

# **Application of Many-Body Techniques to Canonically Quantized Yang–Mills-Theories**

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## Zusammenfassung

In der vorliegenden Arbeit untersuchen wir Yang-Mills-Theorien in der Weyleichung mit Hilfe des Schrödingerbildes. Die Motivation für diese Untersuchung speist sich hauptsächlich aus zwei einander ergänzenden Quellen: einerseits ist die Entwicklung von Techniken jenseits der Störungstheorie in Yang-Mills-Theorien sehr wichtig. Andererseits hat das Schrödingerbild seine Nützlichkeit in kinematischen und topologischen Betrachtungen unter Beweis gestellt, dynamische Rechnungen wurden in diesem Zugang jedoch bisher - zumindest im Fall der Yang-Mills-Theorien - kaum versucht. Daher erscheint die Fragestellung lohnend, ob Methoden aus der Vielteilchenphysik, die sich recht einfach innerhalb des Schrödingerbildes formulieren lassen, auf Yang-Mills-Theorien übertragen werden können. Dabei muss berücksichtigt werden, daß Yang-Mills-Theorien Systeme mit Nebenbedingungen darstellen.

Nach einer kurzen Einführung stellen wir die Yang-Mills-Theorie und ihre kanonische Quantisierung in Weyleichung in knapper Form vor. Wir betrachten dann die verschiedenen Techniken, die im Rest dieser Arbeit Verwendung finden, nämlich das Schrödingerbild, das zeitunabhängige Variationsprinzip von Rayleigh und Ritz und das zeitabhängige Variationsprinzip von Dirac. Im letzten Abschnitt des ersten Kapitels stellen wir einige Methoden vor, die in der Literatur entwickelt wurden, um die in der Weyleichung auftretende Nebenbedingung, das sogenannte Gaußgesetz, zu behandeln.

Das zweite Kapitel ist dem Projektor auf den physikalischen Unterraum der eichinvarianten Zustände gewidmet. Wir beginnen das Kapitel mit der Herleitung eines, für beliebige externe Ladungen gültigen, kompakten Ausdrucks für den Projektor. Da die exakte Auswertung des Projektors in der Feldtheorie unmöglich ist, stellen wir zwei in der Literatur betrachtete Näherungsverfahren vor: entweder behandelt man den Projektor als effektives  $\sigma$ -Modell, was mehr dem Geiste einer Variationsrechnung entspräche, oder man versucht eine systematische störungstheoretische Entwicklung, die auf der Feynmanschen Darstellung der Übergangsamplitude beruht. Wir wenden uns dann einer *mean-field* (Molekularfeld-) Behandlung mit Hilfe Gaußscher Wellenfunktionale zu. In einem ersten Schritt vernachlässigen wir den Einfluss des Projektors völlig. In einem nächsten Schritt betrachten wir, wie dem Gaußgesetz störungstheoretisch durch Modifikationen des Gaußschen Wellenfunktionals Genüge getan werden kann, und zeigen die Grenzen dieses Zugangs auf. Dann wechseln wir den Standpunkt und betrachten, wie man die Zeitabhängigkeit eines Zustandes - zur Verwendung in Diracs zeitabhängigem Variationsprinzip - mittels seiner Deformation, also seiner Eichvarianz, modellieren kann. Das führt zum cranking-Modell, das in der Kernphysik wohlbekannt ist. Es stellt sich allerdings heraus, daß die Ankopplung der externen Ladungen in diesem Zugang, obwohl auf klassischem Niveau noch richtig, auf Ein-Schleifen-Niveau falsch ist.

Das letzte Näherungsschema, das wir in diesem Kapitel betrachten, ist ebenfalls der Kernphysik entlehnt. Es handelt sich um die sog. Kamlah-Entwicklung. Dort betrachtet man die projizierte Energie, wie man sie im Rahmen einer Rayleigh-Ritz-Rechnung benötigt, und entwickelt den Hamiltonoperator in Potenzen derjenigen Symmetriengeneratoren, die den Projektor aufbauen. In Verbindung mit Störungstheorie werden die Erwartungen an ein projiziertes Energiefunktional, die auf den Überlegungen über die störungstheoretische Einhaltung des Gaußgesetzes mittels Modifikationen des Wellenfunktionals gründen, erfüllt. Im letzten Abschnitt dieses Kapitels illustrieren wir den Zugang der mean-field-Behandlung durch eine Berechnung der Energie des Savvidyvakuums, wobei wir auf wohlbekannte Ergebnisse treffen.

Im dritten Kapitel betrachten wir die verallgemeinerte Random Phase Approximation (gRPA). Wir beginnen mit ihrer Formulierung mittels des zeitabhängigen Variationsprinzips, wie sie in

der Feldtheorie wohlbekannt ist, und wenden uns dann dem Operatorzugang, welcher der in der Kernphysik üblichere Zugang ist, zu. Wir übertragen letzteren auf den Fall von Bosesystemen in Gegenwart von Kondensaten, und beweisen, daß unter bestimmten Umständen beide Zugänge dasselbe Spektrum ergeben. Der wesentliche Vorteil des Operatorzugangs besteht darin, daß die Symmetrien der vollen Theorie leichter in die gRPA-Behandlung übersetzt werden können, und daß man Korrekturen zur Energie in mean-field-Näherung, die durch den Erwartungswert des Hamiltonoperators im mean-field-Grundzustand gegeben ist, finden kann, falls der mean-field-Grundzustand deformiert ist. Wir berechnen diese Energiekorrekturen in Störungstheorie in führender Ordnung, und finden, daß sie dieselbe Struktur haben wie die Energiekorrekturen in der Kamlahentwicklung. Der wesentliche Unterschied zur Kamlahentwicklung besteht darin, daß die Korrekturen im Rahmen der gRPA erst berechnet werden, nachdem die Parameter des mean-field-Grundzustandes bestimmt sind, diese also nicht mehr durch die Korrektur beeinflusst werden.

## Abstract

In this thesis we study Yang-Mills theories in the Weyl gauge employing the Schrödinger picture. The main motivation for this study is drawn from two complementing sources: on the one hand, non-perturbative techniques as such are very much sought after in Yang-Mills theories. On the other hand, the Schrödinger picture has proven to be useful in topological and kinematic studies, but dynamical calculations - at least in the case of Yang-Mills theories - have not been carried out very much in this framework. Thus it seems worthwhile to investigate whether techniques from many-body physics that can be formulated quite easily within the Schrödinger picture can be transcribed to Yang-Mills theory with its special difficulties of being a constrained system.

After a short introduction, we give a succinct account of Yang-Mills theory and its canonical quantization in the Weyl gauge. We then consider briefly the techniques that find their application in the remainder of this thesis, namely the Schrödinger picture, the time-independent variational principle of Rayleigh and Ritz and the time-dependent variational principle of Dirac. In the last section of the first chapter we discuss the approaches that have been followed in the literature to overcome the constraint innate in the Weyl gauge treatment of Yang-Mills theory, the so-called Gauss law constraint.

The second chapter is devoted to the projector onto the physical subspace of gauge invariant states. We begin the chapter with the derivation of a compact expression for the projector that is valid for arbitrary external charges. Since in field theory it is impossible to treat the projector exactly, we then present two possibilities of evaluating the projector approximately that have been pursued in the literature: either one can consider the projector as defining an effective  $\sigma$  model, which is more in the spirit of a variational calculation, or one can try a systematic perturbative evaluation based on the Feynman propagation kernel. We then turn to a mean-field treatment based on Gaussian wave functionals. In a first step, we ignore the projector completely. As a next step, we study how the Gauss law constraint can be implemented perturbatively by modifications of the Gaussian wave functional and show the limitations of this approach. Then we change the point of view and consider how one can model the time-dependence of a wave functional (for the usage in Dirac's variational principle) based on its 'deformation', i.e. gauge-noninvariance. This leads to the cranking model well known from nuclear physics. It turns out, however, that in this framework the coupling of external charges, although correct on a classical level, is incorrect on a one-loop level. The last approximation scheme we consider in this chapter, also borrowed from nuclear physics, is the so-called Kamlah expansion. There one considers the projected energy functional as needed for a Rayleigh-Ritz type calculation, and expands the Hamiltonian in powers of the symmetry generators that build up the projector. When combined with perturbation theory, the Kamlah expansion reproduces nicely what is expected of the projected energy functional from the section on perturbative modifications of the wave functional. In the last section of this chapter we illustrate the mean-field approach by a computation of the energy of the Savvidy vacuum where well-known results are reproduced.

In the third chapter we study the generalized Random Phase Approximation (gRPA). We start with the formulation based on the time-dependent variational principle that is known in field theory, but then turn to the operator approach that is more common in nuclear physics. We adapt the latter to the case of bosonic systems in the presence of condensates, and prove that under certain circumstances the two formulations give an identical spectrum. The main advantage of the operator approach lies in the fact that the symmetries of the full theory are more easily translated to the gRPA treatment, and that one can determine the corrections to the mean-field energy, i.e. the expectation value of the Hamiltonian in the mean-field ground state, if the

mean-field ground state is deformed. We evaluate these corrections in leading order perturbation theory and find them to be of identical structure as the corrections of the Kamlah expansion. The main difference to the Kamlah expansion is that these corrections are subtracted *after* the parameters of the mean-field ground state are determined, so the latter are not influenced by the corrections.

# Meinen Eltern





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# Chapter 1

## Introduction

*Detection is, or ought to be, an exact science and should be treated in the same cold and unemotional manner. You have attempted to tinge it with romanticism, which produces much the same effect as if you worked a love-story or an elopement into the fifth proposition of Euclid.*

Sherlock Holmes, The Sign of the Four

### 1.1 Introductory Remarks

Physics is the science that deals with the structure of matter, matter's constituents and the constituents' interactions. During the last centuries, physicists have been very successful at discovering different layers of matter's structure, from molecules over atoms to nuclei, nucleons, and hadrons in general, to the (up to now) last layer of quarks, leptons and gauge bosons.

A very important step leading to the model of this presently last layer was the discovery of the gauge principle<sup>1</sup>. Nowadays, the theories that encompass what is called the Standard Model of particle physics, i.e. the Glashow-Weinberg-Salam theory of the electroweak interaction together with Quantum Chromodynamics (QCD), the theory of the strong interaction, are based on this principle. However, for a scientific endeavour to be meaningful, it is not enough to formulate an aesthetically pleasing theory, one also has to be capable of computing its consequences, and compare these consequences to experimental observations. This has been done for the electroweak theory, and for QCD in a certain kinematical regime where perturbation theory is applicable. In these cases of high energy experiments, satisfactory agreement between theoretical calculations and experimental observations has been reached. For the case of QCD, however, one has to admit that the most successful agreements between theory and experiment are usually obtained when the theoretical predictions *relate* different experiments. *Absolute* predictions from QCD alone have hardly been possible, since usually some information from the low energy domain is needed. Especially in this energy regime of interest for hadronic physics, one has been very much less successful, and well-known experimental quantities like the anomalous magnetic moment of the proton still await their explanation starting from the QCD Lagrangian. At least w.r.t. what Feynman called “*some of the simplest qualitative features of hadronic behaviour, such as the confinement of quarks*” [Fey81], some progress has been made due to numerical lattice studies,

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<sup>1</sup>For a history of the gauge idea, cf. e.g. [OS00].

but certainly an analytical understanding at least of these 'simplest qualitative features' would be desirable. Unfortunately, not many non-perturbative methods are at our disposal. It was the motivation for the studies presented in this thesis to make some methods that have already proved their usefulness in many-body physics available for gauge field theories. In the derivation of the methods, we refrain from including fermions, and restrict ourselves to the gauge field part of QCD, the so-called SU(3) *Yang-Mills theory*<sup>2</sup>.

In the first part of the first chapter, we will introduce the concepts needed in the remainder of the thesis, like basic notions of Yang-Mills theories, the Schrödinger picture in quantum field theory, the Hamiltonian approach and different variational principles. In the second part of this chapter, we introduce some of the approaches that have been followed in the literature up to now in order to deal with the technical problems imposed by gauge invariance. In chapter 2, we formulate a projector that projects an arbitrary state onto a state that is invariant under small gauge transformations, and present several methods of how one can deal with this projector approximately. Whereas in chapter 2 we are mainly interested in methods for determining the ground state of Yang-Mills theory, in chapter 3 we turn to excited states. We introduce an alternative formulation of the Random Phase Approximation, and show how in this formulation one can deal efficiently with a special class of symmetries to which also the gauge symmetry belongs. We conclude this thesis with a critical evaluation of the methods presented.

## 1.2 Yang-Mills Theories

In this section we introduce some basic concepts and notations concerning Yang-Mills theories for later use.

### 1.2.1 Generalities

As an introduction, and in order to fix the notation, we want to give a short overview over some basic concepts of Yang-Mills theories and their canonical quantization. The material is fairly standard and can be found in modern textbooks on quantum field theory, e.g. [IZ80], [Pok87]. A useful reference is also [Jac80].

Yang-Mills theories [YM54] were introduced as a non-Abelian generalization of the (Abelian) gauge theory of electrodynamics. A prominent example of a Yang-Mills theory, namely SU(3) Yang-Mills theory, is given by that part of QCD that is independent of quark degrees of freedom. Yet the very structure of Yang-Mills theories can be simply motivated using the (omitted) matter fields. The basic idea behind a gauge theory is the following: we start with a matter field<sup>3</sup>  $\psi(x)$  that has an internal degree of freedom, in the following to be called *colour*:

$$\psi^a(x). \tag{1.1}$$

The next step consists of introducing a symmetry operation, i.e. a transformation of the  $\psi^a$  that leaves the action invariant. In the case of an ordinary global symmetry<sup>4</sup>,  $\psi^a(x)$  transforms under a representation of the corresponding Lie group<sup>5</sup>:

$$\psi^b(x) = (\exp(i\Theta^i\lambda^i))^{ba}\psi^a(x) = U^{ba}\psi^a(x), \tag{1.2}$$

<sup>2</sup>In fact, for most of the time we will consider SU(N) Yang-Mills theory with N an arbitrary integer.

<sup>3</sup>In the following discussion, we will assume that it is a spinor field, although in general this doesn't have to be the case.

<sup>4</sup>An example is the isospin symmetry.

<sup>5</sup>In the case of isospin: SU(2).

where  $\lambda^i$  denote the *generators* of the Lie group in the appropriate representation and  $\Theta^i$  are the parameters of the transformation which are space-time constants in the case of a global symmetry. In the case of a gauge symmetry, however, the  $\Theta^i$  are functions of space-time

$$\Theta^i = \Theta^i(x). \quad (1.3)$$

The consequences of this space-time dependence of  $\Theta^i$  can be read off a gauge transformation of the kinetic term for the matter field<sup>6</sup>:

$$\mathcal{L}_{\text{kin}} = i\bar{\psi}\not{\partial}\psi \xrightarrow{g.t.} i\bar{\psi}U^\dagger(x)\not{\partial}U(x)\psi = i\bar{\psi}\not{\partial}\psi + i\bar{\psi}U^\dagger(x)(\not{\partial}U(x))\psi = i\bar{\psi}\not{\partial}\psi - i\bar{\psi}(\not{\partial}U^\dagger(x))U(x)\psi. \quad (1.4)$$

In order to render the kinetic part of the matter field Lagrangian gauge invariant, one has to introduce a Lie-algebra valued auxiliary vector field  $A_\mu = A_\mu^a \lambda^a$  which transforms inhomogeneously under gauge transformations such as to compensate the inhomogeneous term generated by the transformation of the derivative:

$$A_\mu \xrightarrow{g.t.} (A_\mu)^U = UA_\mu U^\dagger + iU\partial_\mu U^\dagger. \quad (1.5)$$

If we take  $\Theta$  to be infinitesimal, this transformation can be written as:

$$(A_\mu^a)^U = A_\mu^a + (\delta^{ac}\partial_\mu + f^{abc}A_\mu^b)\Theta^c. \quad (1.6)$$

One combines  $\partial_\mu$  and  $A_\mu$  into an object that transforms homogeneously under gauge transformations, and calls this object *covariant derivative*<sup>7</sup>:

$$D_\mu = \partial_\mu \mathbb{1}_c - iA_\mu \xrightarrow{g.t.} UD_\mu U^\dagger. \quad (1.7)$$

$\mathbb{1}_c$  denotes the unit matrix that has the same dimensions as the generators  $\lambda$ . Usually the matter field is defined in one of the fundamental representations, and thus  $D_\mu$  denotes the covariant derivative where the generators  $\lambda^a$ , multiplying  $A_\mu^a$ , are defined in the corresponding fundamental representation of the algebra. Later on, we will need quite often the covariant derivative in the *adjoint representation*<sup>8</sup>, so we will use a special symbol for it, namely  $\hat{D}$ . In component notation, it reads

$$\hat{D}_\mu^{ab} = \partial_\mu \delta^{ab} + f^{acb}A_\mu^c, \quad (1.8)$$

where  $f^{abc}$  are the *structure constants* of the group that appear in the commutation relations

$$[\lambda^a, \lambda^b] = if^{abc}\lambda^c. \quad (1.9)$$

The first example, where one can use the covariant derivative in the adjoint representation is an infinitesimal gauge transformation of  $A$ , eq. (1.6). This can simply be written as

$$(A_\mu^a)^U = A_\mu^a + \hat{D}_\mu^{ac}\Theta^c. \quad (1.10)$$

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<sup>6</sup>This is the only term of the action of the matter field that contains derivatives and will thus be different for local and global symmetries

<sup>7</sup>The covariant derivative, as well as all of Yang-Mills theory, has a deep geometric interpretation, cf. e.g. [BM94], that will not be needed in the remainder of this thesis. Therefore nothing further will be said about it.

<sup>8</sup>Some group theoretical notions and notations will be given in appendix A.

Now one elevates the auxiliary vector field  $A_\mu$  to a dynamical field by adding a kinetic term to the action. The kinetic term has to be gauge invariant and contain terms quadratic in derivatives. It can be concisely written, if one introduces the Lie-algebra valued *field strength tensor*

$$F_{\mu\nu} = F_{\mu\nu}^a \lambda^a = \partial_\mu A_\nu - \partial_\nu A_\mu - i[A_\mu, A_\nu] = i[D_\mu, D_\nu] \quad (1.11)$$

as

$$\mathcal{L}_{\text{kin},A} = -\frac{1}{4g^2} F_{\mu\nu}^a F^{a\mu\nu} = -\frac{1}{2g^2} \text{tr}(F_{\mu\nu} F^{\mu\nu}). \quad (1.12)$$

The field strength tensor transforms homogeneously under gauge transformations

$$F_{\mu\nu} \rightarrow U F_{\mu\nu} U^\dagger \quad (1.13)$$

and thus  $\mathcal{L}_{\text{kin},A}$  is gauge invariant. In Yang-Mills theories, we only keep this part of the action and dispose of all other parts of the action that contain matter fields. Thus, in the following we will study the system with the action

$$\boxed{S_{\text{YM}} = -\frac{1}{4g^2} \int d^4x F_{\mu\nu}^a F^{a\mu\nu}.} \quad (1.14)$$

### 1.2.2 Classical Yang-Mills Theory

First we can study some classical properties of this action. The classical equations of motion follow as usual from the stationarity of the action:

$$\delta S_{\text{YM}} = 0 \rightarrow [D_\mu, F^{\mu\nu}] = 0. \quad (1.15)$$

In components this can be written as

$$\hat{D}_\mu^{ab} F^{b\mu\nu} = 0. \quad (1.16)$$

The next object to consider is the energy-momentum tensor that can be given in the form

$$\Theta^{\mu\nu} = F^{a\mu\rho} F_\rho^{a\nu} - \frac{1}{4} g^{\mu\nu} F^{a\rho\sigma} F_{\rho\sigma}^a. \quad (1.17)$$

Dilatation invariance of the classical action, i.e. the invariance under rescaling of  $x$  and  $A$  as

$$x \rightarrow \lambda x, \quad A_\mu \rightarrow \frac{1}{\lambda} A_\mu \quad (1.18)$$

implies that its trace vanishes

$$\Theta_\mu^\mu = 0. \quad (1.19)$$

Invariance under space-time translations implies the conservation of  $\Theta^{\mu\nu}$ :

$$\partial_\mu \Theta^{\mu\nu} = 0. \quad (1.20)$$

### 1.2.3 Three Dimensional Notation

For the physical interpretation and the ensuing formalism it will be useful to convert the above equations into a three-dimensional notation. In the remainder of this thesis, three-dimensional vectors will be denoted either by being type-set in boldface<sup>9</sup>, e.g.  $\mathbf{x}$ , or by the use of special symbols, especially

$$\nabla_i = \frac{\partial}{\partial \mathbf{x}_i}. \quad (1.21)$$

Thus

$$\begin{aligned} \partial^\mu &= (\partial_t, -\nabla) & \partial_\mu &= (\partial_t, \nabla) \\ A^\mu &= (A_0, \mathbf{A}) & A_\mu &= (A_0, -\mathbf{A}). \end{aligned}$$

Scalar products between three-dimensional vectors will be denoted by a '.', i.e.

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{a}_i \mathbf{b}_i. \quad (1.22)$$

We also introduce electric and magnetic fields as components of the field strength tensor as

$$\begin{aligned} \mathbf{E}_i^a &= F^{a i 0} = -\partial_t \mathbf{A}_i^a - \hat{\mathbf{D}}_i^{ab} A_0^b \\ \mathbf{B}_i^a &= -\frac{1}{2} \epsilon_{ijk} F^{a j k} = (\nabla \times \mathbf{A})_i^a - \frac{1}{2} f^{abc} (\mathbf{A}^b \times \mathbf{A}^c)_i. \end{aligned}$$

Using these fields, the time-component of eq.(1.20) can be written in the form of a generalized Poynting theorem

$$\partial_t \mathcal{H}(\mathbf{x}, t) + \nabla_i \mathbf{S}_i(\mathbf{x}, t) = 0 \quad (1.23)$$

with

$$\mathcal{H}(\mathbf{x}, t) = \frac{1}{2g^2} \left( \mathbf{E}_i^a(\mathbf{x}, t) \mathbf{E}_i^a(\mathbf{x}, t) + \mathbf{B}_i^a(\mathbf{x}, t) \mathbf{B}_i^a(\mathbf{x}, t) \right) = \Theta^{00}(\mathbf{x}, t) \quad (1.24)$$

$$\mathbf{S}_i(\mathbf{x}, t) = \frac{1}{g^2} \epsilon_{ijk} \left( \mathbf{E}_j^a(\mathbf{x}, t) \mathbf{B}_k^a(\mathbf{x}, t) \right) = \Theta^{0i}(\mathbf{x}, t). \quad (1.25)$$

Eq. (1.24) shows how the energy of the Yang-Mills system can be written in terms of the electric and magnetic fields.

The introduction of the electrical fields is also very useful when exploring the canonical structure of the Yang-Mills system. We compute the canonical momenta corresponding to  $A_0, \mathbf{A}_i$ :

$$\Pi_0^a(\mathbf{x}, t) = \frac{\partial \mathcal{L}}{\partial (\partial_t A_0^a(\mathbf{x}, t))} = 0 \quad (1.26)$$

$$\Pi_i^a(\mathbf{x}, t) = \frac{\partial \mathcal{L}}{\partial (\partial_t \mathbf{A}_i^a(\mathbf{x}, t))} = \frac{1}{g^2} F^{a 0 i}(\mathbf{x}, t) = -\frac{1}{g^2} \mathbf{E}_i^a(\mathbf{x}, t). \quad (1.27)$$

From eq. (1.26) we infer that the system will be subject to a constraint. More about this will be said later on. Using eq. (1.27) we can rewrite the Yang-Mills Lagrangian into a form that is useful for obtaining the Hamiltonian:

$$\mathcal{L} = (\partial_t \mathbf{A}_i^a) \left( -\frac{1}{g^2} \mathbf{E}_i^a \right) + A_0^b (\delta^{ab} \nabla_i - f^{bca} \mathbf{A}_i^c) \left( \frac{1}{g^2} \mathbf{E}_i^a \right) - \frac{1}{2g^2} (\mathbf{E}_i^a \mathbf{E}_i^a + \mathbf{B}_i^a \mathbf{B}_i^a) \quad (1.28)$$

$$= (\partial_t \mathbf{A}_i^a) \Pi_i^a - A_0^b (\delta^{ab} \nabla_i - f^{bca} \mathbf{A}_i^c) \Pi_i^a - \mathcal{H} \quad (1.29)$$

<sup>9</sup>The same notation will also be used, if we want to consider an arbitrary component of a vector, e.g.  $\mathbf{x}_i$  will denote the  $i$ th component of vector  $\mathbf{x}$ . However, if we want to consider a special component, e.g. in the section on the axial gauge the third component of several vectors will play a distinguished role, this component will not be type-set in boldface, e.g.  $x_3$ . This is necessary, since otherwise one could not distinguish between the third component and a labelling of different vectors  $\mathbf{x}_1, \mathbf{x}_2$ , etc.

with  $\mathcal{H}$  as in eq.(1.24). We can see clearly that in a Hamiltonian formalism,  $A_0$  has the special role of a non-dynamical variable, since its conjugate momentum vanishes.  $A_0$  merely serves as a Lagrange multiplier for Gauss' law

$$(\delta^{ab}\nabla_i - f^{bca}\mathbf{A}_i^c)\mathbf{\Pi}_i^a = 0. \quad (1.30)$$

Its time-evolution is not fixed by the equations of motion. It is easy to show that in the absence of boundary conditions in time direction<sup>10</sup> one can always perform a gauge transformation, s.t.

$$A_0 = 0. \quad (1.31)$$

After one has used part of the gauge freedom to achieve  $A_0 = 0$  no further *time-dependent* gauge transformations are allowed, since they would reintroduce a non-vanishing  $A_0$ . One has thus *fixed* part of the gauge freedom by adopting the so-called *Weyl gauge*. This is a gauge well-suited to the Hamiltonian approach, where time has a distinct status anyway<sup>11</sup>. One has left only the canonical coordinates  $\mathbf{A}$  and the conjugate momenta  $\mathbf{\Pi}$ , but one has lost one of the equations of motion, namely the Gauss law equation. Thus, the system described by the action eq.(1.14) can equivalently be described by the Hamilton density  $\mathcal{H}$ , the coordinates  $\mathbf{A}$ , the momenta  $\mathbf{\Pi}$  obeying the Poisson brackets

$$\{\mathbf{A}_i^a(\mathbf{x}, t), \mathbf{\Pi}_j^b(\mathbf{y}, t)\} = \delta_{ij}\delta^{ab}\delta_{\mathbf{xy}} \quad \{\mathbf{A}_i^a(\mathbf{x}, t), \mathbf{A}_j^b(\mathbf{y}, t)\} = 0 \quad \{\mathbf{\Pi}_i^a(\mathbf{x}, t), \mathbf{\Pi}_j^b(\mathbf{y}, t)\} = 0 \quad (1.32)$$

and the constraint  $(\delta^{ab}\nabla_i - f^{bca}\mathbf{A}_i^c)\mathbf{\Pi}_i^a = 0$ .

## 1.3 Canonical Quantization

### 1.3.1 Constraints and Quantization

In this section we discuss very briefly constrained systems and their quantization.

The approach given above can also be phrased in more usual terminology: the fact that

$$\Pi_0 = 0 \quad (1.33)$$

is usually [Dir50], [Dir58], [Wei95] called a *primary constraint*, since it immediately follows from the structure of the Lagrangian. The Gauss law equation is called a *secondary constraint*, since it follows from the requirement of compatibility between the primary constraint and time evolution:

$$0 = \partial_t \Pi_0 = \partial_t \frac{\partial \mathcal{L}}{\partial (\partial_t A_0)} \stackrel{\text{Euler-Lagrange-}}{=} \frac{\partial \mathcal{L}}{\partial A_0} = -(\delta^{ab}\nabla_i - f^{acb}\mathbf{A}_i^c)\mathbf{\Pi}_i^b. \quad (1.34)$$

In the following, we will use the notation

$$\Gamma^a(\mathbf{x}) = (\delta^{ab}\nabla_i - f^{acb}\mathbf{A}_i^c(\mathbf{x}))\mathbf{\Pi}_i^b(\mathbf{x}). \quad (1.35)$$

<sup>10</sup>i.e., this argument does not work if one considers e.g. a system at finite temperature in the so-called imaginary-time formalism, cf. e.g. [Kap89].

<sup>11</sup>A useful reference for properties of non-covariant gauges is [Lei87], cf. also [Lei94].



Alternatively, one can group the constraints into *first class* and *second class* constraints. A constraint is first class, if its Poisson bracket with all other constraints vanishes on the constraint hypersurface. The remaining constraints are called second class constraints. Since  $\Gamma^a$  is independent of  $A_0$ , obviously

$$\{\Gamma^a, \Pi_0\} = 0. \quad (1.36)$$

It is also trivial that

$$\{\Pi_0^a, \Pi_0^b\} = 0. \quad (1.37)$$

The only nontrivial calculation is<sup>12</sup>

$$\{\Gamma^a(\mathbf{x}), \Gamma^b(\mathbf{y})\} = -i\delta_{\mathbf{xy}} f^{abc} \Gamma^c(\mathbf{x}). \quad (1.38)$$

But on the constraint hypersurface this vanishes, too. Thus the constraints are all first class. Whereas a problem that contains second class constraints can be faced by the formalism of *Dirac brackets*, one useful approach to a problem with first class constraints is to choose a gauge which removes the ambiguity in time evolution that is due to the gauge freedom and manifests itself in the presence of the first class constraints [Wei95]. As was indicated above, we choose in this thesis the *Weyl gauge*

$$A_0 = 0. \quad (1.39)$$

We can now proceed straightforwardly with canonical quantization [CL80]. The classical fields  $\mathbf{A}, \mathbf{\Pi}$  become operators  $\hat{\mathbf{A}}, \hat{\mathbf{\Pi}}$  that act on a Hilbert space, and whereas the classical fields  $\mathbf{A}, \mathbf{\Pi}$  satisfied a Poisson algebra, the field operators satisfy certain *equal time* commutation relations

$$[\hat{\mathbf{A}}_i^a(\mathbf{x}, t), \hat{\mathbf{A}}_j^b(\mathbf{y}, t)] = 0, \quad [\hat{\mathbf{\Pi}}_i^a(\mathbf{x}, t), \hat{\mathbf{\Pi}}_j^b(\mathbf{y}, t)] = 0, \quad [\hat{\mathbf{A}}_i^a(\mathbf{x}, t), \hat{\mathbf{\Pi}}_j^b(\mathbf{y}, t)] = i\delta_{ij}\delta^{ab}\delta_{\mathbf{xy}}. \quad (1.40)$$

The constraint  $\Gamma^a = 0$  cannot be imposed as an operator identity since this would be incompatible with the commutation relations<sup>13</sup>. The solution of this problem is well known [Wey50]: one simply uses the constraint to select a part of the Hilbert space as the *physical space*  $\mathcal{H}_{\text{phys}}$ , with the states satisfying

$$\hat{\Gamma}^a|\psi\rangle = 0 \quad \forall |\psi\rangle \in \mathcal{H}_{\text{phys}}. \quad (1.41)$$

This constraint is the main source of difficulties<sup>14</sup> in drawing consequences from Yang-Mills theories. Some of the approaches that have been invented to circumvent the Gauss law constraint will be discussed in sec. 1.7.

<sup>12</sup>The '·' sign on the RHS is noteworthy and will be discussed a bit further in footnote 15.

<sup>13</sup>By using the canonical commutation relations, we can compute the commutator  $\int d^3x \Theta^b(\mathbf{x})[\Gamma^b(\mathbf{x}), \mathbf{A}_i^c(\mathbf{y})] = i\hat{\mathbf{D}}_i^{cb}(\mathbf{y})\Theta^b(\mathbf{y})$ . However, if we set as an operator identity  $\Gamma = 0$ , the commutator would vanish, hence we would have a contradiction between the canonical commutation relations and Gauss' law. This is a phenomenon not restricted to field theory. Let's also consider a simple quantum mechanical example [Tre85]. The Hamiltonian of two particles (moving only in one dimension) of identical mass, that interact via a potential that depends only on the distance between the particles, reads  $H = \frac{1}{2m}(p_1^2 + p_2^2) + V(|x_1 - x_2|)$ . Obviously, the total momentum  $P = p_1 + p_2$  is conserved. Assume that we want to consider the system to be in a state of vanishing total momentum. This cannot be implemented by the operator identity  $P = 0$ , since this would be inconsistent with the canonical commutation relations:  $i = [x_1, p_1] = [x_1, P - p_2] \stackrel{P=0}{=} -[x_1, p_2] = 0$ .

<sup>14</sup>in Weyl gauge, at least

### 1.3.2 Some Properties of $\hat{\Gamma}^a$

Up to now we have assumed that time evolution and the secondary constraint  $\Gamma^a = 0$  are compatible, i.e. no further constraints are generated by requiring  $\partial_t \Gamma^a = 0$ . This is true indeed, since both in the classical theory

$$\partial_t \Gamma^a = \{\Gamma^a, H\} = 0 \quad (1.42)$$

and in the quantum theory

$$\partial_t \hat{\Gamma}^a = [\hat{\Gamma}^a, \hat{H}] = 0. \quad (1.43)$$

Thus  $\hat{\Gamma}^a$  (in the following to be called the *Gauss law operator*) generates a symmetry, and it is easy to see which one:

$$\left[ \int d^3x \Theta^a(\mathbf{x}) \hat{\Gamma}^a(\mathbf{x}), \hat{\mathbf{A}}_j^b(\mathbf{y}) \right] = i \hat{\mathbf{D}}_j^{ba}(\mathbf{y}) \Theta^a(\mathbf{y}). \quad (1.44)$$

Thus the Gauss law operator is the *generator of time-independent gauge transformations*<sup>15</sup>. A first hint at this was already given in eq. (1.38) where one could see that the Gauss law operators satisfy the same commutation relations (up to a sign) as the generators of the Lie algebra eq. (1.9) that was constitutive for the gauge symmetry in the first place. The part of the gauge group that can be continuously deformed to unity can be written with the help of the Gauss law operator as an exponential

$$\mathcal{G} = \exp \left( i \int d^3x \Theta^a(\mathbf{x}) \hat{\Gamma}^a(\mathbf{x}) \right) \quad (1.45)$$

and  $\hat{\mathbf{A}}$  and  $\hat{\mathbf{\Pi}}$  have the transformation properties

$$\mathcal{G} \hat{\mathbf{A}}_i(\mathbf{x}) \mathcal{G}^{-1} = \hat{\mathbf{A}}_i^U(\mathbf{x}) = U(\mathbf{x}) (-i \mathbf{D}_i) U^\dagger(\mathbf{x}) = U(\mathbf{x}) (\mathbf{A}_i - i \nabla_i) U^\dagger(\mathbf{x}) \quad (1.46)$$

$$\mathcal{G} \hat{\mathbf{\Pi}}_i(\mathbf{x}) \mathcal{G}^{-1} = \hat{\mathbf{\Pi}}_i^U(\mathbf{x}) = U(\mathbf{x}) \hat{\mathbf{\Pi}}_i(\mathbf{x}) U^\dagger(\mathbf{x}) \quad (1.47)$$

with  $U(\mathbf{x}) = \exp(i\Theta^a(\mathbf{x})\lambda^a)$ , cf. e.g. [Qua99].

## 1.4 Schrödinger Picture

In this section we introduce the Schrödinger picture, discuss briefly the advantages it offers, and consider three different examples: the appearance of the  $\Theta$  angle in (1+1) dimensional electrodynamics, the free scalar field in (3+1) dimensions, and electrodynamics in (3+1) dimensions.

### 1.4.1 Generalities

The usual approaches to quantum field theory are based on vacuum expectation values of time-ordered products of field operators, often called Green's functions or correlation functions, and their generating functional. From them one tries to extract physical information. The Schrödinger picture is different<sup>16</sup>. Here, one is interested directly in the states and their properties, just as in ordinary quantum mechanics. Instead of abstract state vectors one uses wave

<sup>15</sup>In fact, the generator of (small) time-independent gauge transformations is  $-\hat{\Gamma}^a$ , since only  $-\hat{\Gamma}^a$  fulfils the same Lie algebra eq. (1.9) as the matrix representations  $\lambda^a$ .

<sup>16</sup>Useful references on the Schrödinger picture in general are [Jac87], [Jac88], [Jac89], [Yee92], [Hat92]. For the treatment of fermions in the Schrödinger picture cf. [FJ88], [KW94]. Yang-Mills theories in the Schrödinger picture are dealt with succinctly in [Jac80].

functionals that are either a coordinate or momentum representation of the abstract states:

$$\Psi[\mathbf{A}] = \langle \mathbf{A} | \Psi \rangle \text{ or } \Psi[\mathbf{\Pi}] = \langle \mathbf{\Pi} | \Psi \rangle, \quad (1.48)$$

where  $|\mathbf{A}\rangle, |\mathbf{\Pi}\rangle$  denote eigenstates of the field operators  $\hat{\mathbf{A}}, \hat{\mathbf{\Pi}}$  respectively:

$$\hat{\mathbf{A}}_i^a(\mathbf{x})|\mathbf{A}\rangle = \mathbf{A}_i^a(\mathbf{x})|\mathbf{A}\rangle \quad , \quad \hat{\mathbf{\Pi}}_i^a(\mathbf{x})|\mathbf{\Pi}\rangle = \mathbf{\Pi}_i^a(\mathbf{x})|\mathbf{\Pi}\rangle \quad (1.49)$$

For definiteness we will use in the following the 'A' representation. The operators  $\hat{\mathbf{A}}$  are then realized multiplicatively

$$\hat{\mathbf{A}}_i^a(\mathbf{x})\Psi[\mathbf{A}] = \mathbf{A}_i^a(\mathbf{x})\Psi[\mathbf{A}], \quad (1.50)$$

and the momentum operators are given by functional derivatives

$$\hat{\mathbf{\Pi}}_i^a(\mathbf{x})\Psi[\mathbf{A}] = \frac{1}{i} \frac{\delta}{\delta \mathbf{A}_i^a(\mathbf{x})} \Psi[\mathbf{A}]. \quad (1.51)$$

In this way, the commutation relations are automatically satisfied:

$$[\mathbf{A}_i^a(\mathbf{x}), \frac{1}{i} \frac{\delta}{\delta \mathbf{A}_j^b(\mathbf{y})}] = i\delta^{ab}\delta_{ij}\delta_{\mathbf{x}\mathbf{y}}, \quad (1.52)$$

and from now on, no '^' will be used anymore to indicate the operator nature of an object. Since in the Schrödinger picture the operators are time-independent, the relations eqs. (1.50 - 1.52) are fixed once and for all. The whole time dependence resides in the states which satisfy the Schrödinger equation:

$$\boxed{i\partial_t \Psi[\mathbf{A}, t] = H[\mathbf{A}, \frac{1}{i} \frac{\delta}{\delta \mathbf{A}(\mathbf{x})}] \Psi[\mathbf{A}, t]}. \quad (1.53)$$

The inner product between two states is given via a three-dimensional functional integral

$$\langle \psi_2 | \psi_1 \rangle = \int \mathcal{D}\mathbf{A} \psi_2^*[\mathbf{A}] \psi_1[\mathbf{A}]. \quad (1.54)$$

The Schrödinger picture has a number of attractive features:

1. The most obvious advantage is the proximity of this formulation to ordinary quantum mechanics. Quite a number of features follows directly from this: first, one has a clear *probability interpretation* of the wave functional. Second, one has gained in quantum mechanics a lot of intuition of how wave functions behave. In favourable circumstances one might be able to transfer some of this intuition (cf. e.g. [Fey81]) to quantum field theory. A third aspect is that in quantum mechanics, one has invented a number of approximation schemes, especially variational ones, which can be carried over to field theory.
2. A second main feature is that (at least some of the) topological properties of field theories can be more easily unravelled in the Schrödinger picture, especially the appearance of the  $\Theta$  angle can be interpreted as stemming from the possibility of so-called *large* gauge transformations [Tre85].
3. In the Schrödinger picture one can discuss dynamical questions without having to select a Fock space to work in, i.e. one can discuss dynamics *before* one has to select a vacuum and can let the dynamics decide by itself which vacuum it wants to use. Related to this is the possibility to study quantum field theoretic extensions to Lie algebras without the need of a specific choice of vacuum [FJ88].

4. The last point which we want to mention is the study of the time-evolution of quantum fields that are not in thermal equilibrium. There the Schrödinger equation provides a rather efficient way of solving problems with initial conditions [ERP88].

### 1.4.2 First Application: $\Theta$ Angle in (1+1) Dimensional Electrodynamics

This example is taken from [Jac89]. It illustrates how one can get easily to the  $\Theta$  angle in electrodynamics, and how Gauss' law may help in kinematical and topological investigations. In (1+1) dimensions, one does not have a magnetic term and the Hamiltonian simply reads

$$H = \frac{1}{2} \int dx \Pi_1^2, \quad (1.55)$$

where we have used that in (1+1) dimensions  $\mathbf{\Pi} = \Pi_1$ . In the following it will be important to take a compact manifold as space. Gauss' law reads

$$\frac{d}{dx} \Pi_1(x) \psi[A] = 0. \quad (1.56)$$

This is identical to the requirement

$$\frac{\delta \psi[A]}{\delta A_1(x)} \text{ is independent of } x. \quad (1.57)$$

From this we conclude<sup>17</sup> that  $\psi[A] = f(\int_x A_1)$ , thus  $\psi$  is given by a function of the space integral of  $A$  (since we assume that we are working in a compact space, we could try a Fourier decomposition of the field, and we would see that  $\int_x A_1$  is just the zero frequency part of the Fourier decomposition of  $A_1$ , the so-called zero mode). With this we obtain the stationary Schrödinger equation for  $f(\int_x A_1)$

$$E f(y)|_{y=\int_x A_1} = -\frac{L}{2} \frac{d^2}{dy^2} f(y)|_{y=\int_x A_1}, \quad (1.58)$$

where  $L$  is the length of the interval we are considering. The energy eigenstates are plane waves

$$\psi = e^{(-i\mathcal{E}_1 \int_x A)}, \quad (1.59)$$

with energy  $E = \frac{L}{2} \mathcal{E}_1^2$  and  $\Pi_1 \psi = -\mathcal{E}_1 \psi$ .  $\mathcal{E}_1$  can thus be considered as a background electric field. The  $\Theta$  angle appears when we consider gauge transformations,  $A \rightarrow A - \frac{d}{dx} \Lambda$ . It is important to note that  $\Lambda$  does not have to fulfil periodic boundary conditions, only  $\exp(i[\Lambda(L) - \Lambda(0)]) \stackrel{!}{=} 1$ . Thus  $\Lambda(L) = \Lambda(0) + 2\pi n, n \in \mathbb{N}$  is possible where we would call  $n \neq 0$  a 'large' gauge transformation. Under such a large gauge transformation, the wave functionals do not stay invariant (even though they satisfy Gauss' law) but acquire a phase

$$\psi \rightarrow e^{-in(2\pi\mathcal{E}_1)} \psi, \quad (1.60)$$

where in Yang-Mills theory  $2\pi\mathcal{E}_1$  would be called the 'Theta' angle. A second way the  $\Theta$  angle can appear that we want to illustrate here arises through the possibility of adding total derivatives to the Lagrangian. We start from  $\mathcal{L} = -\frac{1}{4} F^2 = \frac{1}{2} F_{01}^2$  and add a total spatial and a total time derivative, s.t. the total Lagrangian - which is still a gauge invariant Lorentz scalar - reads

$$\mathcal{L} = -\frac{1}{4} F^2 + \Theta F_{01}, \quad (1.61)$$

<sup>17</sup>In the following, we will use the abbreviation  $\int_x A_1 = \int dx A_1$ .

where  $\Theta$  is a constant. The expression for the momentum and the Hamiltonian are changed

$$\Pi_1 = \dot{A}_1 - \Theta + \nabla_1 A_0 \quad (1.62)$$

$$H = \frac{1}{2} \int dx (\Pi_1 + \Theta)^2 \quad (1.63)$$

but Gauss' law not:  $\nabla_1 \Pi_1 | \text{phys} \rangle = 0$ . The operator that implements gauge transformations in the Hilbert space is

$$\mathcal{G} = e^{i \int dx (\nabla_i \Lambda) \Pi_1(\mathbf{x})}, \quad (1.64)$$

e.g.

$$\mathcal{G} A_1(\mathbf{y}) \mathcal{G}^{-1} = A_1(\mathbf{y}) - \nabla_1 \Lambda(\mathbf{y}). \quad (1.65)$$

The  $\Theta$  dependence of the Hamiltonian can be removed by performing a unitary transformation, since

$$U \Pi_1(x) U^\dagger = e^{i\Theta \int dx A_1(x)} \Pi_1(x) e^{-i\Theta \int dx A_1(x)} = \Pi_1(x) - \Theta \quad (1.66)$$

and therefore

$$U H U^\dagger = \frac{1}{2} \int dx \Pi_1^2(\mathbf{x}). \quad (1.67)$$

However, the  $\Theta$  dependence does not disappear altogether. Assume that we had states  $|\psi\rangle$  that were completely gauge invariant, even under large gauge transformations. If we perform the unitary transformation  $U$ , we have to apply it also to the states. Their transformation behaviour under gauge transformations has now changed:

$$\begin{aligned} \mathcal{G} U |\psi\rangle &= \mathcal{G} e^{i\Theta \int dx A_1(x)} \mathcal{G}^{-1} \underbrace{\mathcal{G} |\psi\rangle}_{=|\psi\rangle} = e^{i\Theta \int dx (A_1(x) - \nabla_1 \Lambda)} |\psi\rangle = e^{-i\Theta \int_0^L dx \nabla_1 \Lambda} U |\psi\rangle \\ &= e^{-i\Theta(\Lambda(L) - \Lambda(0))} U |\psi\rangle. \end{aligned} \quad (1.68)$$

If we again require  $\Lambda(L) - \Lambda(0) = 2\pi n$ ,  $n \in \mathbb{N}$ , we obtain the transformation behaviour as before in eq. (1.60)

$$U |\psi\rangle \xrightarrow{g.t.} e^{-i2\pi n \Theta} U |\psi\rangle, \quad (1.69)$$

where in Yang-Mills theory  $2\pi\Theta$  would be called the 'Theta' angle. The last possibility of how the  $\Theta$  angle might appear that we want to illustrate here comes about if we reconsider the canonical quantization. From the commutator

$$[\Pi_1(\mathbf{x}), A_1(\mathbf{y})] = -i\delta_{\mathbf{xy}} \quad (1.70)$$

we have up to now concluded that the momentum operator should be realized as a functional derivative operator

$$\Pi_1(\mathbf{x}) = \frac{1}{i} \frac{\delta}{\delta A_1(\mathbf{x})}. \quad (1.71)$$

However, in (1+1) dimensions, this is not the only possibility [Man85], since the operator

$$\Pi_1^\Theta(\mathbf{x}) = \frac{1}{i} \frac{\delta}{\delta A_1(\mathbf{x})} + \Theta = \Pi_1^{\Theta=0}(\mathbf{x}) + \Theta, \quad (1.72)$$

where  $\Theta$  is a constant, has the same commutation relations as  $\Pi_1(\mathbf{x})$  and may be used as well. In Gauss' law,  $\Theta$  obviously plays no role since it's a constant throughout space-time. With this

generalized momentum operator, we are brought back precisely to the introduction of the  $\Theta$  term via the additional term in the action, cf. eq. 1.61, since in the discussion above it was assumed that  $\Pi_1 = \Pi_1^{\Theta=0}$ .

It should be noted that this ambiguity in the commutation relations plays a role only in (1+1) dimensions, since in this case we have the peculiarity that a constant electric background field is in fact invariant under all permissible Lorentz transformations.

### 1.4.3 Second Application: the Free Scalar Field

As a second application that is instructive for the latter parts of this thesis we consider the free scalar field which is described by the Hamiltonian

$$H = \frac{1}{2} \int d^3x \{ \pi_{\mathbf{x}}^2 + (\nabla \phi_{\mathbf{x}})^2 + m^2 \phi_{\mathbf{x}}^2 \} \quad (1.73)$$

with the commutation relations

$$[\phi_{\mathbf{x}}, \pi_{\mathbf{y}}] = i \delta_{\mathbf{xy}}. \quad (1.74)$$

In the 'position representation' the momentum operator is given by

$$\pi_{\mathbf{x}} = \frac{1}{i} \frac{\delta}{\delta \phi_{\mathbf{x}}}. \quad (1.75)$$

Thus the stationary Schrödinger equation takes the form

$$\frac{1}{2} \int d^3x \left\{ -\frac{\delta^2}{\delta \phi_{\mathbf{x}} \delta \phi_{\mathbf{x}}} + \phi_{\mathbf{x}} (-\Delta + m^2) \phi_{\mathbf{x}} \right\} \psi[\phi] = E \psi[\phi]. \quad (1.76)$$

To determine ground- and excited states it is useful to perform a Fourier transformation

$$\pi_{\mathbf{x}} = \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{x}} \tilde{\pi}_{\mathbf{p}} \quad \phi_{\mathbf{x}} = \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{x}} \tilde{\phi}_{\mathbf{p}}, \quad (1.77)$$

where we now have the commutation relations  $[\tilde{\pi}_{\mathbf{p}}, \tilde{\phi}_{\mathbf{q}}] = i(2\pi)^3 \delta(\mathbf{p} + \mathbf{q})$ , and therefore  $\tilde{\pi}_{\mathbf{p}} = \frac{(2\pi)^3}{i} \frac{\delta}{\delta \tilde{\phi}_{-\mathbf{p}}}$ . We then obtain the Hamiltonian

$$H = \frac{1}{2} \int \frac{d^3p}{(2\pi)^3} \left\{ -\frac{\delta^2}{\delta \tilde{\phi}_{\mathbf{p}} \delta \tilde{\phi}_{-\mathbf{p}}} + (\mathbf{p}^2 + m^2) \tilde{\phi}_{\mathbf{p}} \tilde{\phi}_{-\mathbf{p}} \right\}. \quad (1.78)$$

We can now introduce creation/annihilation operators

$$a^\dagger(\mathbf{p}) = \frac{1}{\sqrt{2}} \frac{1}{(2\pi)^{(3/2)}} \frac{1}{(\mathbf{p}^2 + m^2)^{1/4}} \left( \sqrt{\mathbf{p}^2 + m^2} \tilde{\phi}(\mathbf{p}) - i \tilde{\pi}(\mathbf{p}) \right) \quad (1.79)$$

$$a(\mathbf{p}) = \frac{1}{\sqrt{2}} \frac{1}{(2\pi)^{(3/2)}} \frac{1}{(\mathbf{p}^2 + m^2)^{1/4}} \left( \sqrt{\mathbf{p}^2 + m^2} \tilde{\phi}(\mathbf{p}) + i \tilde{\pi}(\mathbf{p}) \right) \quad (1.80)$$

and write the Hamiltonian in its final form<sup>18</sup>

$$H = \int \frac{d^3p}{(2\pi)^3} \sqrt{\mathbf{p}^2 + m^2} \left( a^\dagger(\mathbf{p}) a(\mathbf{p}) + \frac{1}{2} \delta^{(3)}(\mathbf{0}) \right). \quad (1.81)$$

<sup>18</sup>The  $\delta$  function that appears in eq. (1.81) is the volume of space, since  $\delta^3(\mathbf{0}) = \int d^3x e^{i\mathbf{x}\cdot\mathbf{0}} = \int d^3x = V$ .

We see that the free scalar field is nothing but a collection of infinitely many uncoupled harmonic oscillators. The ground state is therefore given by a Gaussian functional

$$\psi_0[\phi] = \mathcal{N} e^{-\int d^3x \phi(\mathbf{x})(-\Delta+m^2)\phi(\mathbf{x})}, \quad (1.82)$$

where  $\mathcal{N}$  is a normalization constant. Excitations can be built on top of the ground state as usual by acting with a creation operator  $a^\dagger(\mathbf{p})$  upon it. They will have the energy  $E_0 + \sqrt{m^2 + \mathbf{p}^2}$ , as can be easily computed. The interesting lesson we can learn here is that the energy spectrum of the single particle excitations can be read off the *covariance*<sup>19</sup> in the exponent of the Gaussian. This is something we will meet again when discussing the generalized Random Phase Approximation (gRPA) in chapter 3.

#### 1.4.4 Third Application: Electrodynamics in (3+1) Dimensions

We will see that electrodynamics, which in the following is to mean the quantized theory of photons with possibly external, classical charges, is not so very different from the scalar case, but different enough to make it interesting [Gre79]. We start with a pair of canonically conjugate coordinates  $\mathbf{A}$ , and momenta  $\mathbf{\Pi} = -\mathbf{E}$ , and work in the coordinate representation where we have

$$\mathbf{\Pi}_i = -\mathbf{E}_i = \frac{1}{i} \frac{\delta}{\delta \mathbf{A}_i}. \quad (1.83)$$

Apart from the simpler definition of the magnetic field<sup>20</sup> is the Hamiltonian of electrodynamics identical to that of Yang-Mills theory

$$H = \frac{1}{2} \int d^3x \left\{ \mathbf{\Pi}_i(\mathbf{x}) \mathbf{\Pi}_i(\mathbf{x}) + \mathbf{B}_i(\mathbf{x}) \mathbf{B}_i(\mathbf{x}) \right\}. \quad (1.84)$$

A closer look at the potential part<sup>21</sup> shows that it does not depend on the full  $\mathbf{A}$  field, but only on its transversal part:

$$\mathbf{A}_i = \mathbf{A}_i^L + \mathbf{A}_i^T \text{ with } \nabla \cdot \mathbf{A}^T = 0 \text{ and } \nabla \times \mathbf{A}^L = 0. \quad (1.85)$$

Using this we can write the potential part as  $-\mathbf{A}_i^T(\mathbf{x}) \Delta \mathbf{A}_i^T(\mathbf{x})$ . We can also decompose the kinetic part into a part containing only transversal and longitudinal parts, and we end up with a Hamiltonian

$$H = \frac{1}{2} \int \frac{d^3p}{(2\pi)^3} \left\{ -\frac{\delta^2}{\delta \mathbf{A}_i^L(-\mathbf{p}) \mathbf{A}_i^L(\mathbf{p})} - \frac{\delta^2}{\delta \mathbf{A}_i^T(-\mathbf{p}) \mathbf{A}_i^T(\mathbf{p})} + \mathbf{p}^2 \mathbf{A}_i^T(-\mathbf{p}) \mathbf{A}_i^T(\mathbf{p}) \right\}, \quad (1.86)$$

where we use the abbreviation  $\delta/\delta \mathbf{A}_i^{T,L}(\mathbf{p}) = (\mathbf{P}^{T,L}(\mathbf{p}))_{ij} \delta/\delta \mathbf{A}_j(\mathbf{p})$  with the longitudinal(L)/transversal(T) projectors  $\mathbf{P}^{L,T}$ . We have also performed a Fourier transformation just as before in the scalar case. The longitudinal and transversal parts look quite different, since for the former there is no potential term. Up to now, we have not taken into account Gauss' law:  $\nabla_i \frac{\delta}{\delta \mathbf{A}_i} \psi[\mathbf{A}] = 0$ . Using the decomposition of  $\mathbf{A}$  into  $\mathbf{A}^L, \mathbf{A}^T$  we can write Gauss' law in a more practical way

$$\nabla_i \frac{\delta}{\delta \mathbf{A}_i^L} \psi[\mathbf{A}] = 0. \quad (1.87)$$

<sup>19</sup>In a Gaussian functional  $\exp(-(\phi_i G_{ij}^{-1} \phi_j))$  (with i,j super-indices)  $G_{ij}^{-1}$  is often called 'covariance'.

<sup>20</sup> $\mathbf{B} = \nabla \times \mathbf{A}$

<sup>21</sup>The  $\mathbf{B}^2$  term is often referred to as potential, whereas  $\mathbf{\Pi}^2$  is called kinetic energy. The reason for this is quite obvious in the canonical formalism.

In contrast to the discussion of (1+1) dimensional electrodynamics, we don't want to restrict ourselves to a compact manifold, but rather define the theory in  $\mathbb{R}^3$ . Then, discarding the zero mode as usual in this context, we conclude from eq.(1.87) that the wave functional depends on  $\mathbf{A}^T$  only. In this physical subspace of the Hilbert space, the Hamiltonian simplifies,

$$H = \frac{1}{2} \int \frac{d^3p}{(2\pi)^3} \left\{ -\frac{\delta^2}{\delta \mathbf{A}_i^T(-\mathbf{p}) \mathbf{A}_i^T(\mathbf{p})} + \mathbf{p}^2 \mathbf{A}_i^T(-\mathbf{p}) \mathbf{A}_i^T(\mathbf{p}) \right\}. \quad (1.88)$$

Once again we can introduce creation and annihilation operators, where in addition to the scalar case we now have two polarization vectors  $\epsilon_\lambda, \lambda = 1, 2$ , that are perpendicular to  $\mathbf{p}$

$$a^\dagger(\mathbf{p}, \lambda) = \frac{1}{\sqrt{2|\mathbf{p}|}} (\epsilon_\lambda)_i \left( |\mathbf{p}| \tilde{\mathbf{A}}_i^T(\mathbf{p}) - \frac{\delta}{\delta \tilde{\mathbf{A}}_i^T(-\mathbf{p})} \right) \quad (1.89)$$

$$a(\mathbf{p}, \lambda) = \frac{1}{\sqrt{2|\mathbf{p}|}} (\epsilon_\lambda)_i \left( |\mathbf{p}| \tilde{\mathbf{A}}_i^T(\mathbf{p}) + \frac{\delta}{\delta \tilde{\mathbf{A}}_i^T(-\mathbf{p})} \right). \quad (1.90)$$

We end up with the Hamiltonian in a familiar form, cf. eq.(1.81)

$$H = \int \frac{d^3p}{(2\pi)^3} |\mathbf{p}| \left( \sum_{\lambda=1,2} a^\dagger(\mathbf{p}, \lambda) a(\mathbf{p}, \lambda) + \frac{1}{2} \delta^{(3)}(\mathbf{0}) \right). \quad (1.91)$$

In terms of  $\mathbf{A}^T$ , the ground state wave functional looks very similar to eq. (1.82):

$$\psi_0[\mathbf{A}] = \mathcal{N} \exp \left\{ -\frac{1}{2} \int \frac{d^3p}{(2\pi)^3} |\mathbf{p}| \mathbf{A}^T(-\mathbf{p}) \mathbf{A}^T(\mathbf{p}) \right\}. \quad (1.92)$$

An interesting point can be made about the ground state wave functional: it is obviously gauge invariant, since a gauge transformation in electrodynamics affects only the longitudinal degrees of freedom<sup>22</sup>. One can, however, even rewrite the ground state wave functional in terms of *gauge invariant variables*, namely the magnetic field [Gre79]:

$$\psi_0[\mathbf{A}] = \mathcal{N} \exp \left\{ -\frac{1}{2} \int \frac{d^3p}{(2\pi)^3} |\mathbf{p}| \mathbf{A}^T(-\mathbf{p}) \mathbf{A}^T(\mathbf{p}) \right\} \quad (1.93)$$

$$= \mathcal{N} \exp \left\{ -\frac{1}{2} \int \frac{d^3p}{(2\pi)^3} \frac{1}{|\mathbf{p}|} [\mathbf{p} \times \mathbf{A}^T(-\mathbf{p})] \cdot [\mathbf{p} \times \mathbf{A}^T(\mathbf{p})] \right\} \quad (1.94)$$

$$= \mathcal{N} \exp \left\{ -\frac{1}{2} \int d^3x_1 d^3x_2 \frac{\mathbf{B}_i(\mathbf{x}_1) \mathbf{B}_i(\mathbf{x}_2)}{|\mathbf{x}_1 - \mathbf{x}_2|^2} \right\}. \quad (1.95)$$

In contrast to Yang-Mills theory, the magnetic field strength is gauge invariant in electrodynamics.

<sup>22</sup>To make contact with the notation used later on, we write  $\psi_0[\mathbf{A}] = \mathcal{N} \exp(-\mathbf{A}_i G_{ij}^{-1} \mathbf{A}_j)$ ; then a gauge transformation  $\mathbf{A}_i \rightarrow \mathbf{A}_i - \nabla_i \phi$  leads to  $\psi_0[\mathbf{A} - \nabla \phi] = \mathcal{N} \exp(-\mathbf{A}_i G_{ij}^{-1} \mathbf{A}_j) \exp(-\mathbf{A}_i (\nabla_j G_{ij}^{-1}) \phi) \exp(-\phi (\nabla_i G_{ij}^{-1}) \mathbf{A}_j) \exp(-\phi (\nabla_i \nabla_j G_{ij}^{-1}) \phi)$ . Thus for gauge invariance we require a transverse kernel  $\nabla_i G_{ij}^{-1} = 0$ .



## 1.5 The Time-Dependent Variational Principle

We outline first the derivation of the time-dependent variational principle (tdvp) a la Dirac, thereby clearly indicating which quantity is actually minimized. We then will go on to the usual statement of the principle involving an action and thereby study the Hamiltonian structure of the time-dependent variational principle in the spirit of Kerman and Koonin. As a last point we will indicate the connection between the action functional that is introduced in the tdvp and the usual effective action.

### 1.5.1 Dirac's Derivation

The time-dependent variational principle was introduced by Dirac in 1930 [Dir95]. The question he considered was the following: assume that we have a wave function  $|\psi_1\rangle$  of a certain functional form that depends on several parameters. How must these parameters evolve with time such that  $|\psi_1\rangle$  depending on the evolved parameters deviates from the evolved  $|\psi_1\rangle$  using the Schrödinger equation as little as possible? In order to address this question, we consider the exact Schrödinger equation

$$i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle. \quad (1.96)$$

Since  $|\psi_1\rangle$  may vary only through its parameters in time, it will not satisfy the Schrödinger equation, but this can be remedied by introducing a function  $|\psi_2\rangle$  that measures the deviation from the exact time evolution:

$$i\partial_t|\psi_1(t)\rangle = H|\psi_1(t)\rangle + |\psi_2(t)\rangle, \quad (1.97)$$

which in turn can also be read as a defining equation for  $|\psi_2(t)\rangle$ :

$$|\psi_2(t)\rangle = (i\partial_t - H)|\psi_1(t)\rangle. \quad (1.98)$$

As a next step we integrate eq. (1.97) to first order in  $\Delta t$ :

$$i|\psi_1(t + \Delta t)\rangle = i|\psi_1(t)\rangle + \Delta t H|\psi_1(t)\rangle + \Delta t |\psi_2(t)\rangle. \quad (1.99)$$

Now consider a variation of  $|\psi_1(t + \Delta t)\rangle$ :

$$|\psi_1(t + \Delta t)\rangle \rightarrow |\psi_1(t + \Delta t)\rangle + |\delta\psi_1(t + \Delta t)\rangle. \quad (1.100)$$

This has to be absorbed by adding a variation of  $|\psi_2(t)\rangle$  as well

$$|\psi_2(t)\rangle \rightarrow |\psi_2(t)\rangle + |\delta\psi_2(t)\rangle \quad (1.101)$$

and since we do not vary  $|\psi_1(t)\rangle$  in the above context, we get a relation between  $|\delta\psi_1(t + \Delta t)\rangle$  and  $|\delta\psi_2(t)\rangle$ :

$$i|\delta\psi_1(t + \Delta t)\rangle = \Delta t|\delta\psi_2(t)\rangle. \quad (1.102)$$

In the following, we will need only an accuracy up to first order in 'variations'. Having in mind a sort of Taylor expansion, we can replace  $|\delta\psi_1(t + \Delta t)\rangle$  by<sup>23</sup>  $|\delta\psi_1(t)\rangle$  in the formulas needed when  $\Delta t$  is small. This was assumed anyway, since the integration given in eq. (1.99) is only accurate to  $\mathcal{O}((\Delta t)^2)$ :

$$i|\delta\psi_1(t)\rangle \approx \Delta t|\delta\psi_2(t)\rangle. \quad (1.103)$$

<sup>23</sup>Note that  $|\delta\psi_1(t)\rangle$  is not the variation of  $|\psi_1\rangle$  at time  $t$ , since this was assumed to be zero.

Now we come to the quantity that is to be minimized: obviously we want to minimize the deviation from the exact time-evolution. But this deviation is measured by  $|\psi_2\rangle$ . Therefore we want the norm of  $|\psi_2\rangle$  to be minimal (or at least extremal):

$$\delta(\langle\psi_2|\psi_2\rangle) = 0 \leftrightarrow \langle\delta\psi_2|\psi_2\rangle + \langle\psi_2|\delta\psi_2\rangle = 0 \quad (1.104)$$

with arbitrary variations  $|\delta\psi_2\rangle$ . If we take an arbitrary (but fixed) variation  $|\delta\psi_2\rangle$ ,  $i|\delta\psi_2\rangle$  is also a valid variation. From eq. (1.104) we can then conclude

$$\langle\delta\psi_2|\psi_2\rangle + \langle\psi_2|\delta\psi_2\rangle = 0 \quad (1.105)$$

$$-i(\langle\delta\psi_2|\psi_2\rangle - \langle\psi_2|\delta\psi_2\rangle) = 0 \quad (1.106)$$

implying that

$$\langle\delta\psi_2|\psi_2\rangle = 0. \quad (1.107)$$

For the norm of  $|\psi_2\rangle$  to be extremal this must be true for *all*  $|\delta\psi_2\rangle$ . Since we want to express everything in terms of  $|\psi_1\rangle$  (and its variations) we actually have only a restricted range of  $|\delta\psi_2\rangle$  as given by eq. (1.103). If we express in addition  $|\psi_2\rangle$  by its definition eq. (1.98) we obtain as a condition for the minimization of the norm of the deviation from the exact time evolution

$$\boxed{\langle\delta\psi_1(t)|(i\partial_t - H)|\psi_1(t)\rangle = 0.} \quad (1.108)$$

Thus with respect to the possible variations of  $|\psi_1\rangle$ ,  $|\psi_2\rangle$  is as small as possible.

### 1.5.2 Canonical Structure of the Time-Dependent Variational Principle

The formalism is set up a bit differently by Kerman and Koonin [KK76] and they seem to be the standard reference nowadays. They set up an action functional

$$S = \int_{t_1}^{t_2} dt \langle\psi(t)|i\partial_t - H|\psi(t)\rangle \quad (1.109)$$

and determine the equations of motion by requiring that  $S$  be stationary under variations of  $|\psi(t)\rangle$  and  $\langle\psi(t)|$ . The result may be cast into a form identical to eq. (1.108) but also into a form more useful for the following considerations. First we use a coordinate representation of the abstract states (the coordinates are symbolically denoted as  $x$  with integration measure  $[dx]$ ):

$$|\psi(t)\rangle \rightarrow \psi(x, t), \quad \langle\psi(t)| \rightarrow \psi^*(x, t) \quad (1.110)$$

s.t. the action functional reads

$$S = \int_{t_1}^{t_2} dt [dx] \psi^*(x, t)(i\partial_t - H)\psi(x, t). \quad (1.111)$$

We introduce a Hamiltonian function

$$\mathcal{H}[\psi^*, \psi] = \int [dx] \psi^*(x, t) H \psi(x, t). \quad (1.112)$$

Then the equations of motion that result from requiring stationarity of the action can be written as

$$i\dot{\psi} = \frac{\delta\mathcal{H}}{\delta\psi^*} \quad \text{and} \quad i\dot{\psi}^* = -\frac{\delta\mathcal{H}}{\delta\psi}. \quad (1.113)$$

We now decompose  $\psi$  into a real and imaginary part,  $\phi$  and  $\pi$ , in the following way

$$\psi = \frac{1}{\sqrt{2}}(\phi + i\pi) \quad (1.114)$$

and thus eq. (1.113) can be cast into canonical form

$$\boxed{\dot{\phi} = \frac{\delta\mathcal{H}}{\delta\pi} \quad \text{and} \quad \dot{\pi} = -\frac{\delta\mathcal{H}}{\delta\phi}.} \quad (1.115)$$

Thus we have rewritten the Schrödinger equation into a classical Hamiltonian equation for a field and its conjugate momentum. That this is not really surprising can be seen by adding a total time derivative

$$\frac{d}{dt} \int [dx] \left( -\frac{i}{4}(\phi^2 + \pi^2) + \frac{1}{2}\phi\pi \right) \quad (1.116)$$

to the integrand of eq. (1.111). We can then write eq. (1.111) in canonical form

$$S = \int dt [dx] \left( \pi\dot{\phi} - \mathcal{H}[\phi, \pi] \right). \quad (1.117)$$

A last point to mention is that the identification of position and momentum as given in eq. (1.114) is by no means unique. Consider the case that we have found a stationary state

$$\psi(t) = e^{-iEt}\psi(0), \quad (1.118)$$

where  $\psi(0)$  shall be real. We obtain both a time-dependent coordinate and momentum:

$$\phi(t) = \sqrt{2} \cos(Et) \phi(0), \quad \pi(t) = -\sqrt{2} \sin(Et) \phi(0). \quad (1.119)$$

However, if we make a canonical transformation  $\psi \rightarrow e^{-iEt}\tilde{\psi}$ , this results in a more typical behaviour for a stationary state

$$\phi(t) = \sqrt{2}\tilde{\psi}, \quad \pi = 0. \quad (1.120)$$

This last paragraph demonstrates that there is a certain ambiguity in the assignment of coordinates and momentum to a wave function.

### 1.5.3 Connection to the Effective Action

Jackiw and Kerman have shown [JK79] that if one generalizes the action defined in eq. (1.109) in a manner to be defined below it will be equivalent to the ordinary effective action. In order to be able to put the approaches explored in this thesis in relation to more conventional approaches we want to illuminate shortly the connection between the time-dependent variational principle and the effective action. Let  $|\psi_{\pm}, t\rangle$  be states that tend to the true vacuum  $|0\rangle$  of the Hamiltonian  $H$  as the time  $t$  approaches plus or minus infinity

$$|\psi_{\pm}\rangle \xrightarrow{t \rightarrow \pm\infty} |0\rangle \quad (1.121)$$

that are subject to two constraints:

$$\langle \psi_-, t | \psi_+, t \rangle = 1 \quad (1.122)$$

$$\langle \psi_-, t | \Phi(\mathbf{x}) | \psi_+, t \rangle = \phi(\mathbf{x}, t), \quad (1.123)$$

where  $\phi(\mathbf{x}, t)$  is a prescribed value which is kept fixed during the following considerations, and  $\Phi$  denotes the field operators relevant to the system under discussion - one should keep in mind that they are time-independent in the Schrödinger picture. Both  $\Phi$  and  $J$  are taken to be real. We now define the effective action  $\Gamma[\phi]$  to be

$$\Gamma[\phi] = \int_{-\infty}^{+\infty} dt \langle \psi_-, t | i\partial_t - H | \psi_+, t \rangle. \quad (1.124)$$

In order to ensure free variations of  $|\psi_{\pm}, t\rangle$ , we have to couple the constraints with the help of Lagrange multipliers to  $\Gamma$ :

$$\Gamma_{lm}[\phi] = \int_{-\infty}^{+\infty} dt \langle \psi_-, t | i\partial_t - H | \psi_+, t \rangle - \int_{-\infty}^{+\infty} dt w(t) \langle \psi_-, t | \psi_+, t \rangle + \int d^3x dt J(\mathbf{x}, t) \langle \psi_-, t | \Phi(\mathbf{x}) | \psi_+, t \rangle. \quad (1.125)$$

Upon varying this action functional w.r.t  $|\psi_{\pm}, t\rangle$  we obtain

$$\left( i\partial_t - H + \int d^3x J(\mathbf{x}, t) \Phi(\mathbf{x}) \right) |\psi_+, t\rangle = w(t) |\psi_+, t\rangle \quad (1.126)$$

$$\left( i\partial_t - H + \int d^3x J(\mathbf{x}, t) \Phi(\mathbf{x}) \right) |\psi_-, t\rangle = w^*(t) |\psi_-, t\rangle. \quad (1.127)$$

From  $|\psi_{\pm}, t\rangle$  we easily obtain wave functions that satisfy the time-dependent Schrödinger equation  $[i\partial_t - H + \int d^3\mathbf{x} J(\mathbf{x}, t) \Phi(\mathbf{x})] |\pm, t\rangle = 0$ :

$$|+, t\rangle = e^{i \int_{-\infty}^t dt' w(t')} |\psi_+, t\rangle \quad (1.128)$$

$$|-, t\rangle = e^{-i \int_t^{\infty} dt' w^*(t')} |\psi_-, t\rangle. \quad (1.129)$$

They inherit the correct boundary conditions from  $|\psi_{\pm}, t\rangle$  since in the limit  $t \rightarrow \pm\infty$  the exponential prefactor reduces to one. The logarithm of the overlap of  $|\pm, t\rangle$  is known as *vacuum persistence amplitude* and is the generating functional of connected Greens functions:

$$\langle -, t | +, t \rangle = e^{iW} \rightsquigarrow W = \int_{-\infty}^{+\infty} dt w(t). \quad (1.130)$$

We can construct an alternative expression for  $W$  by multiplying eq. (1.126) from the left with  $\langle \psi_-, t |$  and using the fact that  $\langle \psi_-, t | \psi_+, t \rangle = 1$

$$W = \int_{-\infty}^{\infty} dt w(t) = \int_{-\infty}^{\infty} dt \langle \psi_-, t | \left( i\partial_t - H + \int d^3x J\Phi \right) | \psi_+, t \rangle. \quad (1.131)$$

The functional derivative  $\delta W / \delta J$  can be computed by using eqs. (1.122), (1.123), (1.126), (1.127) and keeping in mind that, since at  $t = \pm\infty$  the states  $|\psi_{\pm}, t\rangle$  become independent<sup>24</sup> of  $J$  (they are identical to  $|0\rangle$ ),  $\frac{\delta}{\delta J} |\psi_{\pm}, t\rangle|_{t=\pm\infty} = 0$ . Then

$$\frac{\delta W}{\delta J} = \phi \quad (1.132)$$

<sup>24</sup>This is important since otherwise one obtains  $\frac{\delta W}{\delta J} = \phi + i \langle \psi_-, t | \frac{\delta}{\delta J} | \psi_+, t \rangle|_{t=-\infty}^{+\infty}$ .

and therefore the effective action  $\Gamma_{ea}$  is given by the Legendre transform

$$\Gamma_{ea}[\phi] = W - \int dt d^3x J\phi \quad (1.133)$$

$$\begin{aligned} &= \int dt w(t) - \int dt d^3x J\phi \\ &= \int_{-\infty}^{\infty} dt \langle \psi_-, t | \left( i\partial_t - H + \int d^3x J\Phi \right) | \psi_+, t \rangle - \int dt d^3x J \langle \psi_-, t | \Phi | \psi_+, t \rangle \\ &= \int_{-\infty}^{\infty} dt \langle \psi_-, t | (i\partial_t - H) | \psi_+, t \rangle = \Gamma[\phi] \end{aligned} \quad (1.134)$$

and is thus identical to eq. (1.124) as promised.

## 1.6 The Rayleigh-Ritz Variational Principle

In this section we first state the Rayleigh-Ritz variational principle and show its relation to the effective potential. Then we have a look at a restriction of the space of test wave functionals which leads to the so-called Gaussian effective potentials and consider its advantages and drawbacks.

### 1.6.1 Connection to the Effective Potential

The Rayleigh-Ritz variational principle is well-known from quantum mechanics<sup>25</sup> [RS80]. One starts from two basic observations:

1. the energy functional  $E$ , defined as

$$E[|\psi\rangle] = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \quad (1.135)$$

has as its stationary points, i.e.  $\delta E = 0$ , the solutions of the time-independent Schrödinger equation:

$$(H - E)|\psi\rangle = 0 \quad (1.136)$$

$$\langle \psi | (H - E) = 0. \quad (1.137)$$

2. the energy functional  $E$  is bounded from below by the ground state energy:

$$E[|\psi\rangle] \geq E_{\text{GS}}. \quad (1.138)$$

Note that there is a caveat to this. There might be cases where the state with the lowest energy does not belong to the physical Hilbert space (e.g. in a fermionic problem one might try to ignore the Pauli principle). Then the statement is still true but the ground state refers to an unphysical state and one might underestimate the *physical* ground state energy<sup>26</sup>. If the space of test wave functionals lies completely in the physical Hilbert

<sup>25</sup>For early applications of the Rayleigh-Ritz principle in field theory, cf. [Sch63], [Ros68]. A selection of modern applications can be found in [PP87].

<sup>26</sup>Note that this might also be a problem in gauge theories. In the following chapters we will try in different fashions to extract the energy contributions due to excitations along unphysical directions and, in the cases considered, obtain the result that the sign of these excitation energies are determined by the negative of the eigenvalues of the covariant Laplacian in the background field under consideration (at least for the vacuum, the case that we are mainly considering). Since the spectrum of the covariant Laplacian is negative semi-definite, the excitation energies along unphysical directions determined this way are non-negative.

space these problems may be ignored. Also, if excitations of unphysical degrees of freedom strictly increase the energy, these considerations are irrelevant, since the ground state of the physical Hilbert space has the lowest energy of all states in the complete Hilbert space.

In the following we want to show that the expectation value of the Hamiltonian, which is the basic ingredient of the Rayleigh-Ritz principle, can be found in a more common field theoretical context: it is nothing but the effective potential, i.e. (up to constant factors) that part of the effective action that "survives" if we consider only fields that are constant throughout space-time (i.e. all derivatives vanish), and is accessible by e.g. a loop expansion of the generating functional. For our purposes, a different though equivalent definition is more expedient ([Jon64], [Riv87],[Wei96]): let  $|\psi\rangle$  be the class of states s.t.

$$\langle\psi|\psi\rangle = 1 \quad (1.139)$$

$$\langle\psi|\Phi(\mathbf{x})|\psi\rangle = \phi_0, \quad (1.140)$$

where  $\phi_0$  is a prescribed value. Then the effective potential  $V(\phi)$  is given as

$$V(\phi) = \min_{|\psi\rangle} (\langle\psi|H|\psi\rangle). \quad (1.141)$$

For the proof we follow Coleman and Weinberg [Col85], [Wei96]. We start from the definition of the vacuum persistence amplitude

$$e^{iW[J]} = \langle vac, out | vac, in \rangle_J \quad (1.142)$$

in the presence of the source  $J$ . Then we put the system into a box of dimensions  $V \times T$ . We assume that  $J$  has a constant value  $\mathcal{J}$  inside the box, and is adiabatically turned off outside the box. If  $V$  and  $T$  are large, we can neglect all derivatives of  $J$  in the derivative expansion of  $W[J]$ , and obtain

$$e^{iW} \approx e^{-iVT\mathcal{E}(\mathcal{J})}. \quad (1.143)$$

What happens physically is that the vacuum (in) state changes due to the application of the source into the eigenstate<sup>27</sup> of the Hamiltonian  $H - \mathcal{J} \int d^3x \Phi(\mathbf{x})$  with definite energy  $E[\mathcal{J}] = \mathcal{E}(\mathcal{J})V$ . In this state it stays for the time  $T$ , thereby acquiring the phase given in eq.(1.143).

If we want to minimize on the other hand  $\langle\psi|H|\psi\rangle$  with the constraints eq. (1.139, 1.140) we have to vary

$$\langle\psi|H - \alpha - \int d^3x \beta(\mathbf{x})\Phi(\mathbf{x})|\psi\rangle \quad (1.144)$$

with  $|\psi\rangle$  unrestricted; afterwards we have to choose  $\alpha, \beta$  s.t. eq. (1.139,1.140) are fulfilled. But by our argument above the intermediate state inside the box fulfils all the requirements we have for  $|\psi\rangle$ , thereby determining  $\alpha = V\mathcal{E}(\mathcal{J})$ , and  $\beta = \mathcal{J}$  (since  $\phi_0$  is determined by  $\mathcal{J}$  as  $\phi_0 = dW[J]/dJ$ ). Up to now, we have only determined the lowest eigenvalue of  $H - \mathcal{J} \int d^3x \Phi(\mathbf{x})$ . However, the energy of the corresponding eigenstate is given by the expectation value of the Hamiltonian in this state  $\langle\psi|H|\psi\rangle = -V\mathcal{E}(\mathcal{J}) + \mathcal{J} \int d^3x \Phi(\mathbf{x})$ . This is precisely the Legendre transform of  $-W/T$  for constant sources and fields, which is the negative of the part of the effective action for constant fields divided by  $T$ , and this is effective potential times the spatial volume. This completes the proof.

<sup>27</sup>If there is no level crossing, this is the vacuum state of the theory defined by the Hamiltonian with the source term  $H - \int d^3x \mathcal{J}\Phi(\mathbf{x})$ .

### 1.6.2 The Gaussian Effective Potential

The Gaussian effective potential [Ste84], [Ste85] differs from the effective potential as given above by an additional restriction that is placed upon  $|\psi\rangle$ ; namely, one requires  $|\psi\rangle$  to be a Gaussian state in the coordinate representation,

$$\langle\phi|\psi\rangle = \mathcal{N} \exp \left\{ -\frac{1}{2}(\phi - \phi_0)_i G_{ij}^{-1}(\phi - \phi_0)_j \right\}, \quad (1.145)$$

where  $i, j$  are super-indices, and one performs the minimization indicated in eq.(1.141) only *among the subset of Gaussian states*. In the rest of this section, the set of Gaussian states will be indicated by  $|\psi_G\rangle$ . This defines the so-called *Gaussian effective potential* (GEP):

$$V_G(\phi) = \min_{|\psi_G\rangle} (\langle\psi|H|\psi\rangle). \quad (1.146)$$

At first sight  $V_G$  seems to be a mere approximation to the effective potential  $V$ . However, one may take the point of view that it is physically a much more useful device than the effective potential. This point of view has been particularly advocated by Stevenson (e.g. [Ste84], [Ste85]). The argument runs roughly as follows: the constraint eq.(1.139) does not tell really very much about where the wave function is localized; it might equally well give  $\langle\psi|\Phi(\mathbf{x})|\psi\rangle = \phi_0$  if it consists of several bumps that are distant from  $\phi_0$ , and the probability to actually be in the configuration given by  $\phi_0$  might even be zero. A consequence of this behaviour is that the effective potential is a convex function no matter how many minima the classical potential<sup>28</sup> had. In quantum mechanics, this convexity sometimes leads to absurd results, e.g. in the case when a 'classical' potential is considered that goes to a finite value for  $|\mathbf{x}| \rightarrow \infty$ ; then the effective potential is actually a constant. By restricting oneself to the GEP one has the advantage that the wave function(al) is actually localized at the expectation value of  $\Phi$ . One loses the (sometimes unwanted) convexity property, and obtains a function(al) that mimics a classical potential (i.e. it might have several maxima and minima) but takes into account that quantum mechanical wave functions always have a finite *width* and that curvature of the wave function costs energy. There is also a disadvantage, however; namely, we have shown above that the minimum of the effective potential is indeed the vacuum energy. In the case of the GEP, one only has the statement encoded in the variational principle of Rayleigh and Ritz, i.e. that the calculated energy gives an upper bound to the vacuum energy (with the qualifications made above).

## 1.7 Handling the Gauss Law Constraint

In Yang-Mills theories the physical Hilbert space is only a subset of the complete Hilbert space; the physical Hilbert space is spanned by states that are annihilated by the Gauss law operator. In some theories, like electrodynamics, it is quite simple to construct the physical space explicitly, since it consists of states that in this example depend only on the transversal part of the vector potential. In Yang-Mills theory this is not so simple, and a variety of methods have been developed to deal with the Gauss law constraint. In this section we want to discuss shortly several approaches that have been followed in the literature. They can be roughly categorized as

1. gauge invariant variables, magnetic

<sup>28</sup>By classical potential we mean the potential function(al) that appears in the Hamiltonian.

2. gauge invariant variables, electric
3. resolution of Gauss' law by gauge fixing
4. techniques inspired by nuclear physics
5. introduction of a projector.

We will discuss these different philosophies in turn<sup>29</sup>:

### 1.7.1 Gauge Invariant Variables, Magnetic

One possible way of approaching the problem of the Gauss law constraint is motivated by the observation in electrodynamics, that if one writes down the wave functional in terms of gauge invariant variables (in electrodynamics these are just the transverse components of the vector potential) Gauss' law is satisfied immediately and trivially. Unfortunately, in Yang-Mills theory one cannot identify the gauge invariant degrees of freedom so easily<sup>30</sup>. In the following section, we want to describe a number of approaches which either focus on the coordinate ( $\mathbf{A}$ ) or the momentum ( $\mathbf{\Pi}$ ) representation. Even though historically the first approach along these lines [GJ78] worked in the momentum representation we will first focus on some approaches in the coordinate representation. The approaches we are considering here try to exploit a certain 3-dimensional spatial geometry<sup>31</sup> as a guide. They try to construct quantities from  $\mathbf{A}$  that transform gauge covariantly, and out of these objects they form naturally gauge-invariant quantities. The first approach along these lines [FHJL93] tried to utilize the magnetic field as a gauge covariant object, and proposed to use

$$\phi^{ij} = \mathbf{B}^{ai} \mathbf{B}^{aj} \quad (1.147)$$

as a gauge invariant variable. It became clear soon, however, that due to Wu-Yang ambiguities (gauge-inequivalent  $\mathbf{A}$  configurations may give rise to an identical  $\mathbf{B}$  field configuration) this cannot be a good variable [HJ95]. One then introduces a gauge covariant variable  $\mathbf{u}_i^a$  via

$$\hat{\mathbf{D}}^{ab} \times \mathbf{u}^b = 0 \quad (1.148)$$

so that  $\mathbf{A}$  can be expressed in terms of  $\mathbf{u}$  as

$$\mathbf{A}_i^a = \frac{(\epsilon^{nmk} \partial_m \mathbf{u}_k^b)(\mathbf{u}_n^a \mathbf{u}_i^b - \frac{1}{2} \mathbf{u}_n^b \mathbf{u}_i^a)}{\det(\mathbf{u})}. \quad (1.149)$$

<sup>29</sup>For the discussion of gauge-invariant variables we restrict the gauge group to SU(2).

<sup>30</sup>In the words of P. Haagensen and K. Johnson [HJ97]: "Anyone who has given a certain amount of thought to different treatments of quantum electrodynamics comes inevitably to the conclusion that the reason it is a rather straightforward theory to work out is, in one guise or another, always the same: at some point, one needs to clearly separate what are physical degrees of freedom from what are gauge degrees of freedom, and this separation is absolutely clear in an abelian gauge theory. Unfortunately, no such luck persists with nonabelian gauge theories."

<sup>31</sup>If one assumes that  $\mathbf{A}_i^a$  transforms as a covariant vector density under spatial GL(3) transformations and  $\mathbf{E}^{ai}$  as a contravariant one (and likewise the magnetic field), one sees that all commutation relations that do not involve the Hamiltonian are consistent with this assignment. This is an additional symmetry that is carried by the commutators  $[\mathbf{A}, \mathbf{\Pi}]$ ,  $[\mathbf{A}, \Gamma^a]$ , and  $[\mathbf{E}, \Gamma^a]$ , and is used as a guiding principle for the search of suitable gauge invariant variables. The Hamiltonian does not fit into this scheme since it contracts  $\mathbf{E}^{ai}$  with itself via only a flat metric. Please note that in accordance with [FHJL93], [HJ95], [HJL96] we use  $\mathbf{E}$  instead of  $\mathbf{\Pi}$ , and upper and lower indices for  $\mathbf{E}$ ,  $\mathbf{A}$  respectively to indicate their different transformation behaviour under GL(3) transformations; in contrast to the aforementioned authors, however, we have stuck to usage of boldface vectors.



In this subsection we use  $\partial_i$  instead of  $\nabla_i$  for the gradient, since  $\nabla$  is needed for a different sort of derivative, cf. footnote 33. Eq. (1.148) is motivated by the fact that the thereby defined variables  $u$  are not only  $SU(2)$  covariant but also share the  $GL(3)$  symmetry. From these variables one now constructs the gauge invariant ones, which are suggestively called  $g$ :

$$g_{ij} = \mathbf{u}_i^a \mathbf{u}_j^a. \quad (1.150)$$

If one now considers these new variables to be a metric, one can also define all the other quantities that are connected to metrics, like the Riemann tensor  $R$ , Christoffel symbols  $\Gamma$ , Einstein tensor  $G$  etc. It turns out that eq. (1.148) can be written as

$$\partial_i \mathbf{u}_j^a + \epsilon^{abc} \mathbf{A}_i^b \mathbf{u}_j^c - \Gamma_{ij}^k \mathbf{u}_k^a = 0 \quad (1.151)$$

so we can interpret  $u$  as a dreibein, but more importantly  $\epsilon^{abc} \mathbf{A}^c$  acts as a spin connection. The magnetic field can be written with the help of the Einstein tensor<sup>32</sup>

$$\mathbf{B}^{ai} = \det(\mathbf{u}) \mathbf{u}_j^a G^{ij}. \quad (1.152)$$

In analogy one introduces an electric tensor  $e^{ij}$ , s.t.

$$\frac{\delta}{\delta \mathbf{A}_i^a} = \det(\mathbf{u}) \mathbf{u}_j^a e^{ij} \quad (1.153)$$

and with this the Gauss law operator can be written<sup>33</sup>:

$$iG^a = \hat{\mathbf{D}}_i \frac{\delta}{\delta \mathbf{A}_i^a} = \det(\mathbf{u}) \mathbf{u}_j^a (\nabla_i e^{ij}). \quad (1.154)$$

Since one can show that the wave functions are annihilated by Gauss' law iff they depend only on the metric, one has made quite a step forward towards extracting the important gauge invariant variables. The difficulties start when one considers the electric part of the energy. In order to calculate it, one needs an explicit expression for  $\mathbf{E}^{ai} \mathbf{E}^{ai}$  and in the long run also for  $e^{ij}$ . One can relate the traceless part of  $e^{ij}$ , in the following called  $\tilde{e}$ , to the functional derivative w.r.t.  $g_{ij}$

$$\frac{\delta \psi}{\delta g_{ij}} = \frac{1}{2} \epsilon^{mni} \nabla_m \tilde{e}_n^j \psi. \quad (1.155)$$

Thus one has to invert  $\epsilon^{mni} \nabla_m$  and this already hints at the fact that the Hamiltonian is not a local functional of  $\frac{\delta}{\delta g_{ij}}$ . However, apart from this problem in principle, one has a practical problem as well<sup>34</sup>: one has to determine the inverse of  $\epsilon \nabla$  for every new  $u$  configuration. Since in the approach of Haagensen *et al* [HJL96] the inversion was performed by solving the eigenvalue problem, it cannot be done in general but only for special cases of considerable symmetry<sup>35</sup>, so it seems difficult to make further progress along these lines.

<sup>32</sup>In this way, the geometric Bianchi identity implies the gauge Bianchi identity.

<sup>33</sup>In the following,  $\nabla$  will denote the geometric covariant derivative. One should also note that in [HJ95]  $\mathbf{D}_i$  denotes the covariant derivative in the adjoint representation, whereas we stick here to our notation  $\hat{\mathbf{D}}_i$ .

<sup>34</sup>We have ignored other problems involving unwanted zero modes since it seems that these problems can be solved at the expense of just making the formulas a bit more clumsy [Haa95].

<sup>35</sup>The cases studied mainly consisted of spaces of constant curvature (Einstein spaces) which can be related to instantons.

### 1.7.2 Gauge Invariant Variables, Electric

A similar approach can also be followed in the electric/momentum representation, where one has a similar notion of a metric [Hal77], [BFH94], but we won't give any details here. Rather we will give some details<sup>36</sup> from [GJ78]. Goldstone *et al* also use the momentum representation, but they attained it by a functional Fourier transformation:

$$\phi[\mathbf{E}] = \int \mathcal{D}\mathbf{A} \exp(-i \int d^3x \mathbf{A} \cdot \mathbf{E}) \psi[\mathbf{A}]. \quad (1.156)$$

From this expression one can immediately read off that, whereas  $\psi[\mathbf{A}]$  is gauge invariant,  $\phi[\mathbf{E}]$  is not:

$$\phi[\mathbf{E}] = \exp(-i\Omega[\mathbf{E}, U])\phi[\mathbf{E}^U], \quad (1.157)$$

where  $\mathbf{E}^U$  is the gauge transform of  $\mathbf{E}$ , and

$$\Omega[\mathbf{E}, U] = - \int d^3x \mathbf{E}_a^i ((\partial_i U) U^{-1})^a. \quad (1.158)$$

In the case of electrodynamics, since  $\mathbf{E}^U = \mathbf{E}$ , eq. (1.157) indicates that  $\phi[\mathbf{E}]$  has only support on the transversal part of the electric field, since we have the requirement that  $\Omega[\mathbf{E}, U] = 0$  for  $\phi[\mathbf{E}] \neq 0$ . In a non-Abelian theory one can put eq. (1.157) to a different use. [GJ78] start out by observing that the electric field, having both three spatial and, since we are only dealing with SU(2), three colour indices, might be considered as a  $3 \times 3$  matrix and as such might be decomposed into a product of an orthogonal with a diagonal with an orthogonal matrix:

$$\mathbf{E}_a^i = R_{i\alpha}(\Theta^J) \hat{E}_{\alpha\beta} R_{\beta a}(\Theta^T) \text{ with } \hat{E}_{\alpha\beta} = -\delta_{\alpha\beta} \hat{\pi}_\beta \text{ (no sum over } \beta), \quad (1.159)$$

where  $R(\Theta)$  can be written in terms of angle variables. The point is, that in this decomposition, only  $R_{\beta a}(\Theta^T)$  is affected by a gauge transformation, leaving  $\pi$  and  $\Theta^J$  as gauge invariant variables. We can now use eq. (1.157) to make the dependence of  $\phi$  on  $R(\Theta^T)$  explicit by choosing  $U = R(\Theta^T)^{-1}$ :

$$\phi[\mathbf{E}] = \phi[R(\Theta^J) \hat{\mathbf{E}}] \exp(-i\Omega[\mathbf{E}, R^{-1}(\Theta^T)]).$$

If we now transform every operator  $O$  via

$$\bar{O} = \exp(i\Omega[\mathbf{E}, R^{-1}(\Theta^T)]) O \exp(-i\Omega[\mathbf{E}, R^{-1}(\Theta^T)]) \quad (1.160)$$

we only have to deal with the wave functional depending on the gauge invariant degrees of freedom ( $\pi, \Theta^J$ ). The vector potential, which is given as a functional derivative w.r.t.  $\mathbf{E}$ , can then - via the chain rule - be expressed at each point in space by a body-fixed spin and isospin angular momentum. One ends up realizing that gauge invariant operators don't depend at all on  $R(\Theta^T)$  after the transformation. The computation of the Hamiltonian, however, is plagued by infinities stemming from reordering terms, but since regularization and renormalization have not been incorporated up to now, it is not clear whether they pose any problem. However, apart from that sort of problem, one ends up with a Hamiltonian formulated in terms of gauge invariant variables. One important point should be mentioned, namely that  $\Omega[\mathbf{E}, R^{-1}]$  contains (and even has to contain) singularities, which, in analogy to the quantum mechanical transformation to

<sup>36</sup>In some places we use the simpler notation of [Jac96].

angular -rotation covariant - coordinates may be interpreted as centrifugal barriers.

To put the progress of the last 20 years into perspective, we may quote from [Jac96]: “*It is hoped that analysis of these singularities will provide clues to low energy dynamics - but it is also true that thus far the hope has not been fulfilled.*” To conclude this short section on gauge invariant variables, we have to realize that all approaches presented<sup>37</sup> have serious difficulties. The first class of problems concern the Hamiltonian: either, one cannot even give a general expression for the Hamiltonian, or it is non-local, or it contains fourth-order derivative terms. The second class of problems is related to the question of the integral measure for scalar products, which seems not to have been addressed sufficiently.

### 1.7.3 Gauge Fixing

Another method for dealing with the Gauss law constraint is also well known: *gauge fixing*. This has been the method of choice, to quote Jackiw and Goldstone [GJ78]: “*Gauss’ law is a fixed time constraint and not a hamiltonian equation of motion. The remedy for this problem is well-known: one chooses a gauge by setting selected components of  $A_a^\mu$  to zero and uses Gauss’ law to eliminate from the hamiltonian the corresponding components of  $E_a^i$ .*” However, this is not the end of the story. The procedure indicated is essentially classical - but it is far from clear that resolving Gauss’ law on a classical level and quantizing afterwards is the correct procedure<sup>38</sup>. As is explained in [LNOT94], [LNT94] e.g. it is in this framework not only difficult to prove the equivalence of different versions of gauge fixing of the quantum theory, but also might some parts of the gauge symmetry (on the quantum level) survive the process of gauge fixing, and give rise to global symmetries like the displacement symmetry. This cannot be seen if variables are eliminated on the classical level altogether. However, there is a different path to a gauge fixed theory. Canonical quantization does not require that the classical theory does not contain redundant variables. Rather we consider the theory in the Weyl gauge, perform ordinary canonical quantization and then perform unitary transformations to eliminate the unphysical coordinates from the Hamiltonian<sup>39</sup>. The procedure can be illustrated by an ordinary quantum mechanical example: assume we have a system of two particles interacting via a potential that depends only on the distance vector between them:

$$H = \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} + V(\mathbf{x}_1 - \mathbf{x}_2) \quad (1.161)$$

and assume that the physical states have vanishing total momentum

$$(\mathbf{p}_1 + \mathbf{p}_2)|\psi\rangle = 0. \quad (1.162)$$

This state of affairs can be kept during time evolution since

$$[(\mathbf{p}_1 + \mathbf{p}_2), H] = 0 \quad (1.163)$$

and just like in the case of Yang-Mills theory the Gauss law operator can be brought into connection with gauge transformations,  $(\mathbf{p}_1 + \mathbf{p}_2)$  is the generator of centre-of-mass translations

$$\Omega[\mathbf{b}] = \exp((\mathbf{p}_1 + \mathbf{p}_2) \cdot \mathbf{b}) \text{ and } \langle \mathbf{x}_1, \mathbf{x}_2 | \Omega[\mathbf{b}] | \psi \rangle = \langle \mathbf{x}_1 + \mathbf{b}, \mathbf{x}_2 + \mathbf{b} | \psi \rangle. \quad (1.164)$$

<sup>37</sup>In 2+1 dimensions, more progress seems to have been made, cf. [Sch00] and references therein.

<sup>38</sup>Gauge fixing in this context resembles going from Cartesian to curvilinear coordinates in quantum mechanics. There it is well-known, cf. e.g. [Kle93], that ordinary canonical quantization does not work (i.e. replacing Poisson brackets with commutators) for any other sort of coordinates but Cartesian ones due to *ordering ambiguities*. Cf. in this context [CL80].

<sup>39</sup>One can also consider this problem from the path integral point of view as has been done in [Rei97a].

Similar to the sections above, one could in this example also change variables to relative and centre of mass coordinates and momenta ('choose gauge invariant variables'). Here, we want to follow a different route: we perform a unitary transformation  $U$  on states and operators:

$$U = \exp\left(-\frac{i}{2}\mathbf{x}_1 \cdot \mathbf{p}_2\right) \exp(i\mathbf{x}_2 \cdot \mathbf{p}_1). \quad (1.165)$$

With this unitary transformation the canonical operators become

$$U\mathbf{x}_{1,2}U^\dagger = \mathbf{x}_2 \pm \frac{1}{2}\mathbf{x}_1, \quad U\mathbf{p}_{1,2}U^\dagger = \mathbf{p}_2 \pm \frac{1}{2}\mathbf{p}_1 \quad (1.166)$$

and the generator of translations becomes  $\hat{\Omega}[\mathbf{b}] = \exp(\mathbf{p}_2\mathbf{b})$ ; it thus generates translations only in the variable  $\mathbf{x}_2$ . The constraint eq.(1.162) becomes

$$0 = (\mathbf{p}_1 + \mathbf{p}_2)|\psi\rangle = U^\dagger \underbrace{U(\mathbf{p}_1 + \mathbf{p}_2)U^\dagger}_{=\mathbf{p}_2} U|\psi\rangle = U^\dagger \mathbf{p}_2|\tilde{\psi}\rangle = 0 \rightarrow \mathbf{p}_2|\tilde{\psi}\rangle = 0. \quad (1.167)$$

With this we can see that the Hamiltonian, which in its transformed form looks as follows

$$\hat{H} = UHU^\dagger = \frac{\mathbf{p}_1^2}{m} + V(\mathbf{x}_1) + \frac{\mathbf{p}_2^2}{4m} = H_{\mathbf{p}_1, \mathbf{x}_1} + H_{\mathbf{p}_2}, \quad (1.168)$$

describes in the physical subspace only the relative coordinates, since  $H_{\mathbf{p}_2}|\text{phys}\rangle = 0$ . To put it all in a nutshell: we started with a Hamiltonian that explicitly depended on two positions and two momenta, but which was symmetric under a simultaneous change of both coordinates. In addition we imposed a constraint on the sum of the momenta. Then we performed a unitary transformation s.t. the constraint involves only one momentum, and the Hamiltonian is decomposed into two parts, one depending only on coordinates and momenta that are not affected by the constraint and another part, that depends on the constraint variables in such a way that it is zero when acting on states from the physical subspace.<sup>40</sup>

As an application in field theory we restrict ourselves to QED and the implementation of the axial gauge since this seems to be a gauge that can be implemented profitably in QCD as well [LNT94]. In the following, therefore, we will consider QED including fermions, which in Weyl gauge has the Hamiltonian density

$$\mathcal{H} = -i\psi^\dagger \alpha \cdot (\nabla - ie\mathbf{A})\psi + m\psi^\dagger \beta \psi + \frac{1}{2}(\mathbf{\Pi}^2 + (\nabla \times \mathbf{A})^2). \quad (1.169)$$

In order to avoid infrared problems (which are known to be a nuisance in the axial gauge) we work on a torus with periodic boundary conditions on the gauge fields and quasi-periodic (i.e. periodic up to a phase) ones for the fermions. We will also use frequently the standard definition of the charge density

$$\rho(\mathbf{x}) = \psi^\dagger(\mathbf{x})\psi(\mathbf{x}). \quad (1.170)$$

Classically, the axial gauge amounts to setting  $A_3 = 0$ , and eliminating the conjugate momentum  $\Pi_3$  with the help of Gauss' law

$$\Pi_3 = -\frac{1}{\nabla_3}(\nabla_\perp \cdot \mathbf{\Pi}_\perp + e\rho(\mathbf{x})), \quad (1.171)$$

<sup>40</sup>Here we have an example, where by exciting unphysical modes, one can only increase the energy.

where  $\perp$  refers to the indices 1,2. Note that this is only a formal expression since  $\nabla_3$  has zero modes and cannot be inverted.

The unitary transformation approach to gauge fixing starts by trying to decouple  $A_3$  from the fermions. In order to achieve this, we make the *ansatz*

$$U[\xi] = \exp\left(-i \int d^3x [\nabla_\perp \cdot \mathbf{\Pi}_\perp + e\rho(\mathbf{x})] \xi([A_3], \mathbf{x})\right). \quad (1.172)$$

Then, the  $A_3$ -fermion coupling becomes

$$U[\xi] \psi^\dagger \alpha_3 (\nabla_3 - ieA_3) \psi U^\dagger[\xi] = \psi^\dagger \alpha_3 (\nabla_3 + (\nabla_3 \xi - ieA_3)) \psi, \quad (1.173)$$

and we see that it is eliminated if  $\nabla_3 \xi = A_3$ . Just as in the classical case, one has to invert  $\nabla_3$ . We see that due to the zero mode, we cannot eliminate  $A_3$  completely, but only up to its constant part by choosing

$$\xi([A_3], \mathbf{x}) = \int_0^L dz \vartheta(x_3 - z) A_3(\mathbf{x}_\perp, z), \quad (1.174)$$

where  $\vartheta(z) = \sum_{n \neq 0} \frac{1}{2i\pi n} \exp(2i\pi n(z/L))$  which fulfils  $\frac{d}{dz} \vartheta(z) = \delta(z) - \frac{1}{L}$  and is as close as one can get to an inverse of  $\nabla_3$  with periodic boundary conditions. The most interesting transformation is that of  $\Pi_3$ ,

$$U[\xi] \Pi_3(\mathbf{x}) U^\dagger[\xi] = \Pi_3(\mathbf{x}) - \int_0^L dz \vartheta(x_3 - z) (\nabla_\perp \cdot \mathbf{\Pi}_\perp(\mathbf{x}_\perp, z) + e\rho(\mathbf{x}_\perp, z)), \quad (1.175)$$

which should be compared to eq. (1.171). This also changes the Gauss law operator to

$$U[\xi] G(\mathbf{x}) U^\dagger[\xi] = \nabla_3 \Pi_3(\mathbf{x}) + \frac{1}{L} G^{(2)}(\mathbf{x}_\perp), \quad (1.176)$$

where  $G^{(2)}(\mathbf{x}_\perp)$  is the Gauss law operator of 2-dimensional QED<sup>41</sup> with the two-dimensional charge

$$\rho^{(2)}(\mathbf{x}_\perp) = \int_0^L dx_3 \rho(\mathbf{x}) \quad (1.177)$$

and the zero mode electric field operators

$$\mathbf{p}_l(\mathbf{x}_\perp) = \int_0^L dx_3 \mathbf{\Pi}_l(\mathbf{x}). \quad (1.178)$$

The transformed Gauss law operator as given by eq. (1.176) is a sum of two terms, both of which annihilate the transformed physical states individually<sup>42</sup>, and one can conclude

$$G^{(2)}(\mathbf{x}_\perp) |\tilde{\psi}\rangle = 0, \quad \Pi_3(\mathbf{x}) |\tilde{\psi}\rangle = \frac{1}{L} p_3(\mathbf{x}_\perp) |\tilde{\psi}\rangle. \quad (1.179)$$

We see that the three component of the gauge field is not eliminated completely due to the zero mode of  $\nabla_3$ . Also, we still have a constraint to solve, namely the two-dimensional Gauss'

<sup>41</sup>If it hadn't been for the zero mode of  $\nabla_3$ , this term would not have appeared.

<sup>42</sup>This can be seen very easily: due to the periodicity of  $\Pi_3$  the first term does not contain an  $x_3$  zero mode, whereas the second part is constant w.r.t.  $x_3$ , and thus proportional to the zero mode of  $\nabla_3$ .

law. This can be done by fixing a two-dimensional Coulomb gauge via an additional unitary transformation

$$u^{(2)} = \exp\left(-ie \int d^2x_{\perp} \rho^{(2)}(\mathbf{x}_{\perp}) \int d^2y_{\perp} d(\mathbf{x}_{\perp} - \mathbf{y}_{\perp}) \nabla_{\perp} \cdot \mathbf{a}_{\perp}(\mathbf{y}_{\perp})\right), \quad (1.180)$$

where  $\mathbf{a}_{\perp}$  denotes the zero mode of the gauge fields

$$\mathbf{a}_{\perp}(\mathbf{x}_{\perp}) = \int_0^L dx_3 \mathbf{A}(\mathbf{x}), \quad (1.181)$$

and  $d(\mathbf{x}_{\perp} - \mathbf{y}_{\perp})$  is the periodic Green's function of the two-dimensional Laplace operator. We end up with a theory that contains as cyclic variables the three-component of the vector potential *apart from its zero mode* (which is still a physical variable) and the longitudinal part of the zero mode of  $\mathbf{A}_{\perp}$ , so that in total the same amount of vector potential variables are cyclic as in the Coulomb gauge where the longitudinal part of the vector potential is completely cyclic. The Hamiltonian can - as in the quantum mechanical example above - be decomposed into a part that contains only the unconstrained variables, and one that contains only constrained variables. The unconstrained part of the vector potential and the electric field read respectively

$$\mathbf{A}_{\text{uncon}} = (\mathbf{A}_{\perp}(\mathbf{x}) - \mathbf{a}_{\perp}(\mathbf{x}_{\perp})) + \mathbf{a}_{\perp}^t(\mathbf{x}_{\perp}) + \mathbf{A}_{\perp}^0 + a_3(\mathbf{x}_{\perp})\hat{e}_3, \quad (1.182)$$

$$\mathbf{\Pi}_{\text{uncon}} = (\mathbf{\Pi}_{\perp}(\mathbf{x}) - \frac{1}{L}\mathbf{p}_{\perp}(\mathbf{x}_{\perp})) + \frac{1}{L}\mathbf{p}_{\perp}^t(\mathbf{x}_{\perp}) + \frac{1}{V}\mathbf{\Pi}_{\perp}^0 + \frac{1}{L}p_3(\mathbf{x}_{\perp})\hat{e}_3, \quad (1.183)$$

where  $\mathcal{O}^0$  indicates the volume integral of  $\mathcal{O}$ ,  $\hat{e}_3$  is the unit vector in 3-direction, and  $V$  is the total spatial volume. Introducing the abbreviations

$$\mathcal{E}(\mathbf{x}) = \int_0^L dz \vartheta(x_3 - z) (\nabla_{\perp} \cdot \mathbf{\Pi}_{\perp}(\mathbf{x}_{\perp}, z) + e\rho(\mathbf{x}_{\perp}, z)), \quad (1.184)$$

$$\eta^{(2)}(\mathbf{x}_{\perp}) = e\nabla_{\perp} \int d^2y_{\perp} d(\mathbf{x}_{\perp} - \mathbf{y}_{\perp})\rho^{(2)}(\mathbf{y}_{\perp}) \quad (1.185)$$

we can write the two parts of the Hamiltonian density conveniently as

$$\mathcal{H}_{\text{phys}} = -i\psi^{\dagger}\alpha \cdot (\nabla - ie\mathbf{A}_{\text{uncon}})\psi + m\psi^{\dagger}\beta\psi + \frac{1}{2}(\mathcal{E}^2 + \frac{1}{L^2}\eta^{(2)2}) + \frac{1}{2}(\mathbf{\Pi}_{\text{uncon}}^2 + (\nabla \times \mathbf{A}_{\text{uncon}})^2) \quad (1.186)$$

and

$$\mathcal{H}_{\text{van}} = \frac{1}{2}(\Pi_3 - p_3)(\Pi_3 - p_3 - 2\mathcal{E}) + \frac{1}{2L^2}p_{\perp}^l(p_{\perp}^l - 2\eta^{(2)}). \quad (1.187)$$

The Gauss law constraints on the (now twice) transformed states  $|\psi_{\text{uncon}}\rangle = u^{(2)}U|\psi\rangle$  read

$$(\Pi_3 - p_3)|\psi_{\text{uncon}}\rangle = 0, \quad \mathbf{p}_{\perp}^l|\psi_{\text{uncon}}\rangle = 0, \quad Q|\psi_{\text{uncon}}\rangle = 0, \quad (1.188)$$

where  $Q$  denotes the operator of the total charge. As promised, this ensures  $\mathcal{H}_{\text{van}}|\psi_{\text{uncon}}\rangle = 0$  and can be rather straightforwardly implemented by  $\langle \mathbf{A}|\psi_{\text{uncon}}\rangle$  being independent of  $A_3$  (except its zero mode) and of  $\mathbf{a}_{\perp}^l$ . As is repeatedly emphasized by Lenz *et al* [LNOT94] this is quite in contrast to an interpretation based on the classical constraint equations  $\nabla_3 A_3 = 0$  which rather would indicate a prescribed value for  $A_3$  (apart from its zero mode) but not arbitrary values for it (as one gets now, since the wave functionals are independent of these variables). As a very last point in this section, we shortly want to indicate what complications arise if one

wants to implement this program for QCD. At first sight this seems quite more intricate than the QED case, since one does not have to invert  $\nabla_3$  but the  $A_3$  dependent 3-component of the covariant derivative. However, this problem can be simplified considerably; one has to insert a transformation with the help of the path ordered exponential  $\text{P exp} \left( ig \int_0^{x_3} dz A_3(\mathbf{x}_\perp, z) \right)$ . In order to keep the boundary conditions periodic, one has to perform another transformation which reintroduces the zero modes of  $A_3$ , but only those that are diagonal in the Lie algebra. Thus we end up with having to invert, instead of  $\hat{D}_3 = \nabla_3 - ie\hat{A}_3(\mathbf{x})$ , the operator  $\hat{d}_3 = \nabla_3 - ie\hat{a}_3(\mathbf{x}_\perp)$ , the inverse of which can be given explicitly. One can read off this explicit expression that basically  $a_3$  serves to regularize the limit in which the torus is made large (the infrared problems that are usually associated with the axial gauge are thereby circumvented). The next point that is different from electrodynamics is that the zero mode of the 3-component of the electrical field is not hermitian. This is a phenomenon well-known from curvilinear coordinate systems in quantum mechanics, and results in a kinetic energy term that involves a Jacobian<sup>43</sup>. This Jacobian can be absorbed into a redefined wave function, and by this procedure we obtain (just as in quantum mechanics in cylindrical coordinates, where the redefined wave function has to vanish at the origin) certain boundary conditions. These boundary conditions are the point where the difficulties start, to quote from [LNT94]: “*It appears that even on a symbolic formal level, the construction of a Hamiltonian for QCD with unconstrained degrees of freedom is possible only after some discretization.*” Before leaving this subject of gauge fixing, one should note that all the manipulations that have been carried out above are purely formal, since they contain products of operators at the same space-time point, which are usually divergent quantities.

#### 1.7.4 Inspiration by Nuclear Physics

The approaches we have illustrated up to now aimed at resolving Gauss’ law exactly and separate gauge invariant from gauge variant coordinates. One can take also a different point of view, e.g. to quote from [GS78]: “*From our viewpoint the time-independent gauge transformations should be treated in the same way as any other symmetry of the system.*” This point of view provides the opportunity of transferring techniques from nuclear physics to gauge theories. We will discuss three different approaches: the first one, to be discussed in this section, will consist of considering a colour-rotating (intrinsic) frame, the second one will deal with a *projector* and approximations to this projector; this approach will be presented in chapter 2. The third approach will be concerned with the formulation of the Random Phase Approximation for bosonic theories in the presence of condensates and can be found in chapter 3. To some extent, the latter two approaches are inspired by the Thouless-Valatin approach presented in [HMVI98], [HVM199], [HIMV00].

In this section, we want to follow Levit [Lev95], who has written a very insightful paper on this kind of approach. The main idea is to introduce - as successfully done in nuclear physics - a body-fixed (or intrinsic) frame. Thereby one can distinguish between “gauge rotations” and the intrinsic dynamics just as in nuclear physics where one can (if the coupling is weak) study collective rotations and the vibrational modes in the body-fixed frame. A particular advantage of the approach is that in the body-fixed frame no attention has to be paid to symmetries: whereas in the laboratory frame a nucleus always has good angular momentum<sup>44</sup>, in the intrinsic frame the nucleus may very well be deformed; the symmetry is restored since the intrinsic frame in

<sup>43</sup>This appears to be the first point that one would get wrong by fixing the gauge classically and quantizing afterwards.

<sup>44</sup>Similarly, one can not accept in a gauge theory - due to Elitzur’s theorem - breaking of a gauge symmetry *in the lab frame*.

this example collectively rotates w.r.t. the laboratory frame - this is a point of view that will be particularly emphasized in section 2.5 where the cranking approach is treated. Usually such a decomposition into collective rotations and body-fixed dynamics will be fruitful if a Born-Oppenheimer approximation is allowed, i.e. when inertia connected with the collective rotation is much larger than that of the internal vibration. In the following we want to shortly discuss Levit's "rigid gauge rotor". Most of his considerations are basically classical, since, although he works with a Hamiltonian in Weyl gauge, the electric field does not appear as a canonical momentum, but only in terms of its original definition<sup>45</sup> (Weyl gauge !):

$$-E^i = \partial_0 A^i. \quad (1.189)$$

The decomposition into gauge rotations and internal dynamics is achieved by the ansatz for  $A^i(\mathbf{x}, t)$

$$A^i(\mathbf{x}, t) = U(\mathbf{x}, t) a^i(\mathbf{x}) U^\dagger(\mathbf{x}, t) + \frac{i}{g} U(\mathbf{x}, t) \partial^i U^\dagger(\mathbf{x}, t), \quad (1.190)$$

where  $a^i$  is time-independent. This carries over to the covariant derivative

$$D^i = \partial^i - igA^i = U(\mathbf{x}, t) (\partial^i - iga^i) U^\dagger(\mathbf{x}, t) = U(\mathbf{x}, t) d^i U^\dagger(\mathbf{x}, t), \quad (1.191)$$

where  $d^i$  denotes the covariant derivative in the body-fixed frame. We now consider the Hamiltonian: the magnetic field squared is the same in both lab frame and internal frame since it is invariant under all gauge transformations:

$$\sum_{i,j} [D^i, D^j]^2 = \sum_{i,j} [d^i, d^j]^2, \quad (1.192)$$

whereas the electric field can be written with the help of an angular velocity vector  $\omega = 2iU^\dagger \partial_0 U$  as

$$-E^i = \partial_0 A^i = \frac{1}{2g} U[\omega, d^i] U^\dagger. \quad (1.193)$$

The kinetic energy can then be written suggestively as<sup>46</sup>

$$E_{\text{rot}} = \frac{1}{4} \int d^3x (\omega I \omega) = -\frac{1}{16g^2} \int d^3x \text{Tr}(\omega [d^i, [d^i, \omega]]). \quad (1.194)$$

For the purpose of quantizing the model later on it is useful to formulate this in terms of symmetry generators which are here the Gauss law operators. They can be written as<sup>47</sup>

$$G^A = [\partial^i - igA^i, E^i] = -2gU(I\omega)U^\dagger \stackrel{\dagger}{=} U^\dagger \hat{G} U, \quad (1.195)$$

<sup>45</sup>In this section, we keep Levit's conventions (apart from his different normalization of  $\lambda$ ). They can be easily transcribed into the conventions we follow in the rest of this thesis by noting:  $A^i = \mathbf{A}_i$ ,  $E^i = \mathbf{E}_i$ ,  $\partial^i = -\nabla_i$ ,  $D^i = -\mathbf{D}_i$ .

<sup>46</sup>We have ignored possible surface terms from partial integrations.

<sup>47</sup>One has to note that, since this is a basically classical treatment, the commutator of  $[A_a^i, E_b^j]$  vanishes, and thus  $[A^i, E^j] = A_a^i E_b^j [\lambda^a, \lambda^b] = if_{abc} A_a^i E_b^j \lambda^c$ . If  $[A_a^i, E_b^j] \neq 0$  one obtains an additional term proportional to  $\lambda^a \lambda^a$  that spoils the first relation in eq. (1.195).



where  $\hat{G}$  denotes the symmetry generator in the body fixed frame. With their help, the Hamiltonian of the rigid gauge rotator (in which the magnetic term is ignored) can be written as<sup>48</sup>

$$H_{\text{rot}}^A = \frac{1}{4g^2} \int d^3x d^3y \hat{G}_a(\mathbf{x}) I_{ab}^{-1} \hat{G}_b(\mathbf{y}) \quad (1.196)$$

with  $I_{ab}^{-1} = (1/4)\text{Tr}(\lambda^a I^{-1}(\mathbf{x}, \mathbf{y}) \lambda^b)$  proportional to the Green's function of  $d_{ac}^i d_{cb}^i$  where  $d_{ab}^i$  is the covariant derivative in the intrinsic frame in the adjoint representation. As we will see in the following chapters, this is a result that comes out in one guise or another in (almost) every approach that is based upon nuclear physics techniques, be it the Thouless-Valatin approach, or the (generalized) Random Phase Approximation, or others; at least the Greens function of the covariant d'Alembertian always has to be computed. In the limit  $g \rightarrow 0$  (and vanishing background field) the Green's function reduces to the Coulomb potential, and (in the physical sector)  $\hat{G}$  is related to the electrical charge. Thus, quite naturally, the notion of the Green's function of the covariant d'Alembertian appears as the interaction energy of static charges.

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<sup>48</sup>Note that this Hamiltonian is formulated entirely in terms of body-fixed quantities, and is therefore automatically gauge invariant - gauge transformations only affect the relative position of the body fixed frame w.r.t. to the laboratory frame.

## Chapter 2

# Projector on Physical States

### 2.1 The Projector on Gauge-Invariant States

In this section we want to introduce the projector onto states that satisfy Gauss' law in the presence of external charges. We show that the time-component of the fermionic colour current generates gauge transformations of the fermionic matter. From this we can conclude how Yang-Mills wave functionals transform in the presence of external charges, and also give a concise formulation of the projector. In the last part of this section, we draw the connection to the literature, and show how Kogan and Kovner [KK95] dealt approximately with the projector.

#### 2.1.1 Generalities

The method that we want to discuss in this chapter is the *projection onto gauge invariant states*, and approximations to the exact projection. Projection onto states with good quantum numbers is a technique that has its roots in nuclear physics [RS80]; there one is often faced with the problem that the simple trial states one wants to use (e.g. Slater determinants for Hartree-Fock calculations) do not share the symmetries of the Hamiltonian<sup>1</sup>. In order to restore the symmetry one adds up all symmetry transformed wave functions. Symbolically

$$\psi_{\text{restored}}[A] = \int d\phi \psi_{\text{broken}}[\phi[A]], \quad (2.1)$$

where  $\int d\phi$  abbreviates the summation over the different symmetry transformations and  $\phi[A]$  symbolizes the symmetry transformed variables. Since symmetries form a group, and since we are summing over all symmetry transformations<sup>2</sup>, it follows trivially that  $\psi_{\text{restored}}[A]$  is indeed invariant under symmetry transformations:

$$\psi_{\text{restored}}[\phi_1[A]] = \int d\phi \psi_{\text{broken}}[\phi_1[\phi[A]]] = \int d\phi \psi_{\text{broken}}[(\phi_1 \circ \phi)[A]] = \int d(\phi_1^{-1} \circ \phi) \psi_{\text{broken}}[\phi[A]]$$

---

<sup>1</sup>Of course one can construct trial states in nuclear physics that do share the symmetries of the Hamiltonian; however, the only single-particle wave functions that are compatible with, say, translational invariance are plane waves - and thus the many particle wave function would also be a plane wave; we conclude from this that in some instances one even has to break a symmetry by a variational *ansatz* in order to get sensible physics (like a localized nucleus) with a sufficiently simple wave function.

<sup>2</sup>If one sums over all group elements, a left multiplication (as well as a right multiplication) by a fixed group element only leads to a reshuffling of the terms in the sum, but the sum stays the same. For continuous groups this leads to the requirement that the integration measure (Haar measure) is to be invariant under left multiplication. This is often denoted as 'invariance of the Haar measure'.

$$= \int d\phi \psi_{\text{broken}}[\phi[A]] = \psi_{\text{restored}}[A]. \quad (2.2)$$

In Yang-Mills theory one would sum over all topologically trivial gauge transformations:

$$\psi_{\text{restored}}[A] = \int \mathcal{D}U \psi[A^U], \quad (2.3)$$

where  $A^U$  is given by eq.(1.5). Since one stays in the topologically trivial sector, the gauge transformation can also be written with the help of the operator eq.(1.45) (where  $\phi$  parametrizes  $U$ ):

$$\psi[A^U] = \mathcal{G}[U]\psi[A], \quad (2.4)$$

and thus the averaging over the different gauge copies can be put into a projection operator  $\mathbf{P}$

$$\int \mathcal{D}U \psi[A^U] = \left[ \int \mathcal{D}U \mathcal{G}[U] \right] \psi[A] = \mathbf{P} \psi[A] \quad (2.5)$$

acting upon the wave functional whose symmetry is to be restored<sup>3</sup>. After this introduction into the idea of projecting a state onto the physical subspace, let us briefly outline the rest of this chapter.

First, we introduce external charges into the theory, which allows us to formulate the projector onto arbitrarily charged states in a compact manner. Since the exact treatment of the projector appears to be impossible in field theory, we then consider two approximate treatments of the projector that are known from the literature. The first one is the approach of Kogan and Kovner [KK95]. They interpret the projector as defining an effective  $\sigma$ -model which is then dealt with in a mixture of perturbation theory and mean-field approximation. The second approach we consider is the systematic perturbative evaluation of the influence of the projector in the framework of the Feynman propagation kernel as suggested by Testa and Rossi [TR80a], [TR80b].

We then turn to a mean-field treatment based on Gaussian wave functionals. In a first step, we ignore the projector completely. This will later on allow us to see the influence of the projector clearly. In a next step, we consider how Gauss' law can be implemented order by order in perturbation theory by modifications of the Gaussian wave functional we started with, and demonstrate the problems of this approach.

Then we slightly change the point of view: whereas we hitherto studied how one can implement Gauss' law, we now try to model the time-dependence of states that are not annihilated by the Gauss law operator based on this gauge-noninvariance of the states. This is similar in spirit to nuclear physics, where the time-dependence of a deformed state, i.e. a state that is not invariant under rotations, is usually taken to be a rotation. This sort of time-dependence is not available for a rotationally invariant state. These considerations lead us to the cranking model well known from nuclear physics. Unfortunately, it turns out that this model is insufficient to describe the coupling of charges at the one-loop level, as can be seen from the fact that the known  $\beta$ -function of Yang-Mills theory is not reproduced.

As a last approximate treatment of the projector we then consider the Kamlah expansion, which is also well-known from nuclear physics. In this approach, one expands the Hamiltonian (between projected states) in powers of the generators that build up the projector (between projected states). In combination with perturbation theory this is seen to work nicely - the energy functional does not depend on those parameters of the wave functional that shouldn't have appeared

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<sup>3</sup>The significance of the projector in Yang-Mills theory was emphasized by [JLP91], cf. also [Hua92] and [Qua94].

in the first place according to the studies of perturbative modifications of the Gaussian wave functional mentioned above. However, due to technical difficulties it has not been possible yet to treat charges beyond the classical level.

As a last point in this chapter, we illustrate the treatment based on Gaussian wave functionals by calculating the energy of the Savvidy vacuum, and arrive at a result well-known in the literature.

### 2.1.2 External Charges

In this section we want to introduce external static charges into our system. In the usual formulations (e.g. [Pol97], [HJ97], [Qua99]) one attaches colour indices to the Yang-Mills wave functional and requires new transformation properties under gauge transformations. If we denote the collection of spin indices by  $M$ , then we require<sup>4</sup>, for a gauge transformation  $U$ ,

$$|\psi_M\rangle \xrightarrow{U} \sum_{M'} \mathcal{G}_{MM'} |\psi'_{M'}\rangle \quad \text{with} \quad (2.6)$$

$$\mathcal{G}_{MM'} = \mathcal{G}_{m_1 m'_1 \dots m_n m'_n}[U] = \mathcal{D}_{m_1 m'_1}^{R_1}[U(\mathbf{x}_1)] \cdots \mathcal{D}_{m_n m'_n}^{R_n}[U(\mathbf{x}_n)], \quad (2.7)$$

where  $\mathcal{D}^{R_i}$  denotes the matrix representation  $R_i$  of the gauge group and  $\mathbf{x}_i$  the positions of the charges. It will turn out below that we have to choose the representation matrices  $\mathcal{D}^{R_i}$  to form the conjugate representation of the representation under which the quarks at the points  $\mathbf{x}_i$  in space transform<sup>5</sup>. This formulation has the disadvantage that one does not have a concise formulation of gauge transformations *independent of the fermionic colour charge content* of the wave functional under consideration. As a result, one cannot write down a projector that projects onto the physical sector for all fermionic charges. Since the latter is a very important requirement for the approximations to the projector that we want to carry out later on, we have to look for a different approach that is inspired by [Pol97], [Zar98c], [Zar98d]. We start by adding a fermionic part to the Yang-Mills Hamiltonian appropriate to static quarks:

$$H = H_{\text{YM}} + M \int d^3x \bar{\psi}(\mathbf{x}) \psi(\mathbf{x}), \quad (2.8)$$

where  $M$  denotes the quark mass (we deal only with a single flavour), and we require the usual anti-commutation relations for the quark fields:

$$\{\psi_\alpha^a(\mathbf{x}), \psi_\beta^\dagger{}^b(\mathbf{y})\} = \delta^{ab} \delta_{\alpha\beta} \delta_{\mathbf{x}\mathbf{y}}. \quad (2.9)$$

In eq. (2.9),  $a, b$  denote colour indices,  $\alpha, \beta$  spinor indices, and  $\mathbf{x}, \mathbf{y}$  position indices. We also use the usual notation  $\bar{\psi} = \psi^\dagger \gamma^0$ , and use for  $\gamma^0$  the usual Dirac convention:  $\gamma^0 = \text{diag}(1, 1, -1, -1)$ . Acting upon the bare fermionic vacuum the operators  $\psi, \psi^\dagger$  generate further eigenstates of the Hamiltonian. Their energy can - as usual - be determined via the commutator of  $H$  with  $\psi, \psi^\dagger$ :

$$[H, \psi_\alpha^a(\mathbf{x})] = \begin{cases} -M\psi_\alpha^a(\mathbf{x}) & , \quad \alpha = 1, 2 \\ M\psi_\alpha^a(\mathbf{x}) & , \quad \alpha = 3, 4 \end{cases} \quad (2.10)$$

$$[H, \psi_\alpha^\dagger{}^a(\mathbf{x})] = \begin{cases} M\psi_\alpha^\dagger{}^a(\mathbf{x}) & , \quad \alpha = 1, 2 \\ -M\psi_\alpha^\dagger{}^a(\mathbf{x}) & , \quad \alpha = 3, 4. \end{cases} \quad (2.11)$$

<sup>4</sup>Remember that we set the Yang-Mills  $\Theta$  angle everywhere in this thesis to zero.

<sup>5</sup>The explicit form of eq. (2.7) that one can find in the literature [Pol97], [HJ97], [Qua99] seems to differ superficially from the expression that we use here. However, in none of the references mentioned the authors explicitly state, under which representation their matter fields transform, and therefore it is likely that the superficial difference is no real difference.

In concordance with the common interpretation we associate *creation* operators with operators that create positive energy states, and thus write explicitly

$$\psi_\alpha^a(\mathbf{x}) = \begin{pmatrix} a_1^a(\mathbf{x}) \\ a_2^a(\mathbf{x}) \\ b_1^{\dagger a}(\mathbf{x}) \\ b_2^{\dagger a}(\mathbf{x}) \end{pmatrix}, \quad \psi_\alpha^{\dagger a}(\mathbf{x}) = \begin{pmatrix} a_1^{\dagger a}(\mathbf{x}) \\ a_2^{\dagger a}(\mathbf{x}) \\ b_1^a(\mathbf{x}) \\ b_2^a(\mathbf{x}) \end{pmatrix}. \quad (2.12)$$

We then interpret the operators  $a$  as connected to quarks, and the operators  $b$  as connected to anti-quarks. We now turn to the charge operator. Let  $\lambda^a$  be the (hermitian) generators of the group representation appropriate for the quarks. The charge operator is then given by

$$\rho^a(\mathbf{x}) = J_0^a(\mathbf{x}) = \bar{\psi}(\mathbf{x})\gamma^0\lambda^a\psi(\mathbf{x}), \quad (2.13)$$

where there is no integration over  $\mathbf{x}$  just as in the remainder of this section (unless explicitly stated). In terms of  $a, b$  operators, it can be written as (the fact that the generators of SU(N) are traceless and hermitian has to be used)

$$\rho^a(\mathbf{x}) = a_i^{\dagger b}(\mathbf{x})\lambda_{bc}^a a_i^c(\mathbf{x}) - b_i^{\dagger b}(\mathbf{x})\lambda_{bc}^{a*} b_i^c(\mathbf{x}). \quad (2.14)$$

The matrix  $\lambda^*$  denotes simply the complex conjugate matrix of  $\lambda$ . The charge operators inherit their commutation relations from the  $\lambda$  matrices:

$$[\rho^a(\mathbf{x}), \rho^b(\mathbf{y})] = \delta_{\mathbf{xy}} \left( a_i^{\dagger}(\mathbf{x})[\lambda^a, \lambda^b]a_i(\mathbf{x}) + b_i^{\dagger}(\mathbf{x})[\lambda^{a*}, \lambda^{b*}]b_i(\mathbf{x}) \right) = if^{abc}\rho^c(\mathbf{x})\delta_{\mathbf{xy}}. \quad (2.15)$$

Thus, we can form the Gauss law operator in the presence of external charges<sup>6</sup>

$$\mathcal{G}^a(\mathbf{x}) = -\Gamma^a(\mathbf{x}) + \rho^a(\mathbf{x}), \quad (2.16)$$

where  $\Gamma^a(\mathbf{x})$  is the generator of gauge transformations on the Yang-Mills part of the wave functionals<sup>7</sup>. Note that we have a special situation here: although the Gauss law operators for different colours do not commute, there is one special instance when a state can be a simultaneous eigenstate of all Gauss law operators, namely if it is annihilated by all of the operators. From the relation  $\mathcal{G}^a(\mathbf{x})|\text{phys}\rangle = 0$  we can infer  $\Gamma^a(\mathbf{x})|\text{phys}\rangle = \rho^a(\mathbf{x})|\text{phys}\rangle$  but this does not mean that we have diagonalized all  $\Gamma^a$ , since a state cannot simultaneously be an eigenstate of all charge operators, but only of the charge operators corresponding to the *Cartan subalgebra* (in SU(2), this would usually be  $\rho^3$ , in SU(3),  $\rho^3$  and  $\rho^8$ ).

We want to show that  $\rho^a$  generates the usual gauge transformations of the quark operators, just as the pure Yang-Mills operators  $\mathbf{A}, \mathbf{\Pi}$  are gauge transformed by  $-\Gamma^a(\mathbf{x})$ . We start by considering an infinitesimal transformation:

$$\begin{aligned} e^{-i\int d^3y \varphi^b(\mathbf{y})\rho^b(\mathbf{y})}\psi_\alpha^a(\mathbf{x})e^{i\int d^3y \varphi^b(\mathbf{y})\rho^b(\mathbf{y})} &= \psi_\alpha^a(\mathbf{x}) - i\int d^3y \varphi^b(\mathbf{y})[\rho^b(\mathbf{y}), \psi_\alpha^a(\mathbf{x})] + \mathcal{O}(\varphi^2) \\ &= \psi_\alpha^a(\mathbf{x}) + \delta\psi_\alpha^a(\mathbf{x}) + \mathcal{O}(\varphi^2). \end{aligned} \quad (2.17)$$

<sup>6</sup>This result can also be obtained from the Lagrangian with matter fields. The matter field Lagrangian reads  $\mathcal{L}_m = \bar{\psi}i\not{D}\psi = \bar{\psi}i\gamma^\mu(\partial_\mu - iA_\mu)\psi$  and if we concentrate on the part that is multiplied by  $A_0^a$  this reads  $\bar{\psi}\gamma^0\lambda^a\psi = \rho^a$ . Taking into account the term multiplying  $A_0^a$  in the pure Yang-Mills Lagrangian eq. (1.29), we obtain as generalization of eq. (1.30) the Gauss' law in the presence of external charges:  $-\Gamma^a(\mathbf{x}) + \rho^a = 0$ ; cf. in this context also [CL80].

<sup>7</sup>Depending on the form of the covariant derivative (with or without an explicit factor of  $g$ ) this may either be  $\frac{1}{g}\hat{D}\Pi$  or  $\hat{D}\Pi$ . Please note also that (a) as was discussed above in sec. 1.3.2  $\Gamma^a(\mathbf{x})$  is in fact the *negative* of the generator of gauge transformations, and (b) it is hopefully not confusing that we call both  $\mathcal{G}^a$  and  $\Gamma^a$  Gauss law operator although they differ by a sign in their respective Lie algebra.

We can compute the commutator, and obtain the result

$$\delta\psi_\alpha^a(\mathbf{x}) = i\varphi^b(\mathbf{x})\lambda_{ac}^b\psi_\alpha^c(\mathbf{x}). \quad (2.18)$$

As usual, we can iterate this formula and thereby obtain

$$\boxed{\begin{aligned} e^{-i\int d^3y\varphi^b(\mathbf{y})\rho^b(\mathbf{y})}\psi_\alpha^a(\mathbf{x})e^{i\int d^3y\varphi^b(\mathbf{y})\rho^b(\mathbf{y})} &= (e^{i\varphi^b(\mathbf{x})\lambda^b})_{ac}\psi_\alpha^c(\mathbf{x}) = \mathcal{D}_{ac}^{R_q}[U(\mathbf{x})]\psi_\alpha^c(\mathbf{x}), \\ e^{-i\int d^3y\varphi^b(\mathbf{y})\rho^b(\mathbf{y})}\psi_\alpha^{\dagger a}(\mathbf{x})e^{i\int d^3y\varphi^b(\mathbf{y})\rho^b(\mathbf{y})} &= \psi_\alpha^{\dagger c}(\mathbf{x})(e^{-i\varphi^b(\mathbf{x})\lambda^b})_{ca} = \mathcal{D}_{ac}^{R_p}[U(\mathbf{x})]\psi_\alpha^{\dagger c}(\mathbf{x}), \end{aligned}} \quad (2.19)$$

where we have used the same procedure for  $\psi^\dagger$ , and due to the hermiticity property of  $\lambda$  we have  $(e^{-i\varphi^b(\mathbf{x})\lambda^b})_{ca} = (e^{-i\varphi^b(\mathbf{x})\lambda^{*b}})_{ac}$ .  $\mathcal{D}^{R_p}[U]$  is called the *conjugate representation* of  $\mathcal{D}^{R_q}[U]$ , cf. e.g. [PS95].

### 2.1.3 External Charges and Transformation Properties of Gluonic States

We are now in a position to see how the usual formulation of transformation properties of gluonic states in the presence of external charges comes about. The structure of the states that we are considering is given by a sum of direct products of states from a fermionic Hilbert space (we denote the states as  $|\text{fermion } i\rangle$ , where  $i$  is a collection of indices, cf. eq. 2.21) and states from a Hilbert space that is spanned by  $|\mathbf{A}\rangle$ . The states from the latter Hilbert space are denoted as  $|\text{YM } a\rangle$  with label  $a$ . Thus the complete states we are going to consider (called  $|\text{coupled}\rangle$ ) are

$$|\text{coupled}\rangle = \sum_{a,i} c_i^a |\text{fermion } i\rangle |\text{YM } a\rangle, \quad (2.20)$$

where  $c_i^a$  are probability amplitudes. The fermionic states are generated by acting with quark and antiquark creation operators on the (gauge invariant) fermionic vacuum<sup>8</sup>:

$$|\text{fermion } i\rangle = a_{i_1}^\dagger \cdots a_{i_n}^\dagger b_{j_1}^\dagger \cdots b_{j_m}^\dagger |0\rangle, \quad (2.21)$$

where we have combined colour-, spinor- and spatial indices into a single super-index  $i$  (or  $j$ ), and denoted the fermionic vacuum by  $|0\rangle$ . We can also write suggestively

$$\begin{aligned} \sum_{a,i_1,\dots,j_m} c_{i_1,\dots,j_m}^a a_{i_1}^\dagger \cdots a_{i_n}^\dagger b_{j_1}^\dagger \cdots b_{j_m}^\dagger |0\rangle |\text{YM } a\rangle &= \sum_{i_1,\dots,j_m} a_{i_1}^\dagger \cdots a_{i_n}^\dagger b_{j_1}^\dagger \cdots b_{j_m}^\dagger |0\rangle \underbrace{\sum_a c_{i_1,\dots,j_m}^a}_{a} |\text{YM } a\rangle \\ &= \sum_{i_1,\dots,j_m} a_{i_1}^\dagger \cdots a_{i_n}^\dagger b_{j_1}^\dagger \cdots b_{j_m}^\dagger |0\rangle |\text{YM}\rangle_{i_1,\dots,j_m} \quad \text{with } |\text{YM}\rangle_{i_1,\dots,j_m} = \sum_a c_{i_1,\dots,j_m}^a |\text{YM } a\rangle. \end{aligned} \quad (2.22)$$

We perform a gauge transformation by acting upon the state with<sup>9</sup>  $e^{-i\int\varphi^a\mathcal{G}^a} = \mathbf{U}e^{i\int\varphi^a\Gamma^a}$  (where  $\mathbf{U} = e^{-i\int\varphi^a\rho^a}$ ):

$$e^{-i\int\varphi^a\mathcal{G}^a} \sum_{i_1,\dots,j_m} a_{i_1}^\dagger \cdots a_{i_n}^\dagger b_{j_1}^\dagger \cdots b_{j_m}^\dagger |0\rangle |\text{YM}\rangle_{i_1,\dots,j_m}$$

<sup>8</sup>That the fermionic vacuum is gauge invariant is a trivial consequence of the fact that it is annihilated by the annihilation operators.

<sup>9</sup>We use the abbreviation  $e^{-i\int\varphi^a\mathcal{G}^a} = e^{-i\int d^3x\varphi^a(\mathbf{x})\mathcal{G}^a(\mathbf{x})}$ .

$$\begin{aligned}
&= \sum_{i_1, \dots, j_m} U a_{i_1}^\dagger U^\dagger U \dots U^\dagger U a_{i_n}^\dagger U^\dagger U b_{j_1}^\dagger U^\dagger U \dots U^\dagger U b_{j_m}^\dagger \underbrace{U^\dagger |0\rangle}_{=|0\rangle} e^{i \int \varphi^a \Gamma^a} |\text{YM}\rangle_{i_1 \dots j_m} \\
&= \sum_{i_1, \dots, j_m} \mathcal{D}_{i_1 l_1}^{R_p}[U] a_{l_1}^\dagger \dots \mathcal{D}_{i_n l_n}^{R_p}[U] a_{l_n}^\dagger \mathcal{D}_{j_1 k_1}^{R_q}[U] b_{k_1}^\dagger \dots \mathcal{D}_{j_m k_m}^{R_q}[U] b_{k_m}^\dagger |0\rangle e^{i \int \varphi^a \Gamma^a} |\text{YM}\rangle_{i_1 \dots j_m} \\
&= \sum_{i_1, \dots, j_m} a_{i_1}^\dagger \dots a_{i_n}^\dagger b_{j_1}^\dagger \dots b_{j_m}^\dagger |0\rangle \mathcal{D}_{l_1 i_1}^{R_p}[U] \dots \mathcal{D}_{l_n i_n}^{R_p}[U] \mathcal{D}_{k_1 j_1}^{R_q}[U] \dots \mathcal{D}_{k_m j_m}^{R_q}[U] e^{i \int \varphi^a \Gamma^a} |\text{YM}\rangle_{l_1 \dots k_m},
\end{aligned} \tag{2.23}$$

where we use a super-index notation for  $a_i^\dagger, b_i^\dagger$ . For the representation matrices this has to be understood as follows: if we decompose the super-index  $i_1$  into the colour index  $a_1$ , the spatial index  $m_1$  and the position index  $\mathbf{x}_1$ , and correspondingly  $l_1$  into  $b_1, n_1$  and  $\mathbf{x}_1$  (the position index is in both cases identical since we do not associate an integration over position indices with gauge transformations), then

$$\mathcal{D}_{i_1 l_1}[U] = \delta_{m_1 n_1} \mathcal{D}_{a_1 b_1}[U(\mathbf{x}_1)]. \tag{2.24}$$

This allows us now to determine  $e^{i \int \varphi^a \Gamma^a} |\text{YM}\rangle_{l_1 \dots k_m}$ . From the requirement that the state containing quarks and gluons shall be overall gauge invariant,

$$e^{-i \int \varphi^a \Gamma^a} \left( \sum_{i_1, \dots, j_m} a_{i_1}^\dagger \dots a_{i_n}^\dagger b_{j_1}^\dagger \dots b_{j_m}^\dagger |0\rangle |\text{YM}\rangle_{i_1 \dots j_m} \right) = \sum_{i_1, \dots, j_m} a_{i_1}^\dagger \dots a_{i_n}^\dagger b_{j_1}^\dagger \dots b_{j_m}^\dagger |0\rangle |\text{YM}\rangle_{i_1 \dots j_m}, \tag{2.25}$$

the following relation between a representation  $\mathcal{D}^{R_q}$  and its conjugate representation  $\mathcal{D}^{R_p}$

$$\mathcal{D}_{ji}^{R_q}[U^{-1}] = \mathcal{D}_{ij}^{R_p}[U] \tag{2.26}$$

and eq. (2.23) we can conclude that

$$e^{i \int \varphi^a \Gamma^a} |\text{YM}\rangle_{i_1 \dots j_m} = \mathcal{D}_{i_1 l_1}^{R_q}[U] \dots \mathcal{D}_{i_n l_n}^{R_q}[U] \mathcal{D}_{j_1 k_1}^{R_p}[U] \dots \mathcal{D}_{j_m k_m}^{R_p}[U] |\text{YM}\rangle_{l_1 \dots k_m}. \tag{2.27}$$

Thus, our way of approaching the problem of static charges almost exactly reproduces the usual 'effective' gauge transformation prescription as given in eq. (2.6). However, we obtain a nice interpretation for the spin label attached to a Yang-Mills state, that may be useful in variational calculations: the spin labels are nothing but part of the probability amplitudes  $c_{i_1 \dots i_n j_1 \dots j_m}^a$  and in constructing variational *ansätze* one may choose only certain combinations to be non-zero.

### 2.1.4 The Projector on Physical States

Since we now have an operator that generates gauge transformations on arbitrarily charged state, we can also write down a very simple (formal) expression for the projector onto the physical sector:

$$P^\rho = \int \mathcal{D}\varphi e^{i \int d^3x \varphi^a (\Gamma^a - \rho^a)}. \tag{2.28}$$

$\mathcal{D}\varphi$  denotes the integral over all variables parametrizing the gauge transformation including the Haar measure necessary to make the integral invariant under left multiplication. The integration domain runs over the topologically trivial sector of the gauge transformations. Two points deserve attention: first, we want to consider why  $P^\rho$  is indeed a projector onto the physical

subspace, and second, why it is sufficient to restrict the domain of integration to topologically trivial gauge transformations. In fact these two points are closely related. A state in the physical subspace is characterized by the fact that it is annihilated by the Gauss law operator:  $\mathcal{G}^a|\psi\rangle = 0$ . An identical requirement is  $e^{-i\phi^a\mathcal{G}^a}|\psi\rangle = |\psi\rangle$ , in other words a state has to be invariant under topologically trivial gauge transformations. If we now act with  $e^{-i\phi^a\mathcal{G}^a}$  upon  $\mathcal{P}^\rho$  we can use the fact that topologically trivial gauge transformations form a group, i.e.

$$e^{-i\phi^a\mathcal{G}^a}e^{-i\varphi^a\mathcal{G}^a} = e^{-i\alpha^a(\phi,\varphi)\mathcal{G}^a}, \quad (2.29)$$

the left invariance of the Haar measure

$$\mathcal{D}\varphi = \mathcal{D}\alpha(\phi, \varphi), \quad (2.30)$$

and the fact that a topologically trivial gauge transformation does not change the domain of integration of the projector  $\mathcal{P}^\rho$  to obtain

$$\begin{aligned} e^{-i\phi^a\mathcal{G}^a}\mathcal{P}^\rho &= e^{-i\phi^a\mathcal{G}^a} \int \mathcal{D}\varphi e^{-i\varphi^a\mathcal{G}^a} = \int \mathcal{D}\varphi e^{-i\phi^a\mathcal{G}^a} e^{-i\varphi^a\mathcal{G}^a} = \int \mathcal{D}\varphi e^{-i\alpha^a(\phi,\varphi)\mathcal{G}^a} \\ &= \int \mathcal{D}\alpha e^{-i\alpha^a\mathcal{G}^a} = \mathcal{P}^\rho. \end{aligned} \quad (2.31)$$

Thus we have answered both questions: the projector projects onto the physical subspace since the projector is invariant under small gauge transformations, and since the Gauss law constraint is equivalent to topologically trivial gauge transformation only this domain of integration is required.

### 2.1.5 QED

One main difficulty of the Yang-Mills theory with external charges lies in the fact that the charge operators do not commute and therefore the states cannot be chosen as simultaneous eigenstates of all charge operators. This is - obviously - very different in QED, where there is only one type of charge. Thus we can choose the fermionic part of the states to be eigenstates of the charge operator (this happens quite naturally if we take only states with a fixed number of external charges into account). Then the projector can be simplified very much as well: denote by  $|\rho\rangle$  an eigenstate of the charge operator, and write the charge operator in the rest of this section as  $\hat{\rho}$ , i.e.

$$\hat{\rho}(\mathbf{x})|\rho\rangle = \rho(\mathbf{x})|\rho\rangle. \quad (2.32)$$

Thus, upon a state  $|\rho\rangle \otimes |\text{photons}\rangle$  the projector acts as

$$\begin{aligned} \mathcal{P}^\rho|\rho\rangle \otimes |\text{photons}\rangle &= \int \mathcal{D}\varphi e^{i\int \varphi(\Gamma-\hat{\rho})}|\rho\rangle \otimes |\text{photons}\rangle = \int \mathcal{D}\varphi e^{i\int \varphi(\Gamma-\rho)}|\rho\rangle \otimes |\text{photons}\rangle \\ &= |\rho\rangle \otimes \int \mathcal{D}\varphi e^{i\int \varphi(\Gamma-\rho)}|\text{photons}\rangle. \end{aligned} \quad (2.33)$$

We can get completely rid of the fermionic states by forming scalar products:

$$\langle\rho'|\mathcal{P}^\rho|\rho\rangle \otimes |\text{photons}\rangle = \delta_{\rho\rho'} \int \mathcal{D}\varphi e^{i\int \varphi(\Gamma-\rho)}|\text{photons}\rangle. \quad (2.34)$$

The externally prescribed charge can now be found in the projector as a c-number  $\rho(\mathbf{x})$ . Note that the integration domain (i.e. whether  $\varphi(\mathbf{x})$  runs from e.g.  $0 \dots 2\pi$  or  $-\infty \dots +\infty$ ) determines whether the charges we take into account are quantized or not. In what follows we usually assume that  $\varphi$  runs from  $-\infty \dots +\infty$ , and ignore the fermionic part of the states completely. We implement the prescribed charge content in the projector precisely via the c-number function  $\rho$ .



### 2.1.6 Projection Integral as an Effective Theory

We have indicated that the projector is a very complicated object; until now nobody has been able to deal with it exactly but there have been a number of approximate approaches in the literature. Two of them we want to illustrate in the following: first, we have a look at the calculation by Kogan and Kovner [KK95]. In sec. 2.2 we have a look at a systematic perturbative evaluation, using the static inter-quark potential as an example, of the projector formulation.

In this section we want to consider an approach that has been pioneered by Kogan and Kovner [KK95]. They start out by considering expectation values of local operators<sup>10</sup> using wave functionals ( $\phi$  is used to indicate a generic set of fields):

$$\langle \mathcal{O} \rangle = \int \mathcal{D}\phi \psi^*[\phi] \mathcal{O} \psi[\phi] = \int \mathcal{D}\phi \mathcal{O} e^{-\ln(\psi^*[\phi] \psi[\phi])}. \quad (2.35)$$

Thus, they consider expectation values as Euclidean path integrals with an action that is given by the logarithm of the squared wave function. This point of view will be very useful later on. Since the only path integrals that can be done exactly are polynomials times a Gaussian, they conclude that one should restrict oneself to Gaussian wave functionals in the following. Their arguments that restriction to a Gaussian wave functional is not only done for simplicity reasons are given in sec. 2.3; since in Yang-Mills theories there are no gauge invariant Gaussian functionals (as we will discuss at some length in sec. 2.4) Kogan and Kovner [KK95] propose to enforce gauge invariance as described in eq. (2.1):

$$\psi[\mathbf{A}] = \int \mathcal{D}\phi \exp \left\{ -\frac{1}{2} \int d^3x d^3y \mathbf{A}_i^{U a}(\mathbf{x}) (G^{-1})_{ij}^{ab}(\mathbf{x}, \mathbf{y}) \mathbf{A}_j^{U b}(\mathbf{y}) \right\}, \quad (2.36)$$

where  $\mathbf{A}^U$  denotes the field  $\mathbf{A}$  after a gauge transformation  $U$ , parametrized by  $\phi$ . They use a specific *ansatz* for the parameters in the Gaussian wave functional:

$$(G^{-1})_{ij}^{ab}(\mathbf{x}, \mathbf{y}) = \delta^{ab} \delta_{ij} \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})} G^{-1}(|\mathbf{k}|) \quad \text{with} \quad G^{-1}(|\mathbf{k}|) = \begin{cases} |\mathbf{k}| & \text{for } |\mathbf{k}| > M \\ M & \text{for } |\mathbf{k}| < M. \end{cases} \quad (2.37)$$

This ansatz is inspired by the observation that it has apparently the correct large- $|\mathbf{k}|$  behaviour expected from perturbation theory, and that for small  $|\mathbf{k}|$  one expects the theory to have a (mass) gap. Note, however, that this motivation results from the property of  $G^{-1}$  being the equal-time propagator of the  $\mathbf{E}$ -field in the unprojected theory. If we restrict ourselves to leading order in perturbation theory, the non-Abelian character of the gauge group can be neglected, thus the projection will replace  $G^{-1}$  by its transverse part, and additionally to leading order the correlator  $\langle \mathbf{E}_i(\mathbf{x}) \mathbf{E}_j(\mathbf{y}) \rangle$  is gauge-invariant. Thus at least to leading order in perturbation theory one does not have to distinguish (for motivational purposes) between the projected and the unprojected theory. Where the leading order perturbative approximation is not valid (like in the momentum regions where one would expect a mass gap) the interpretation is also unlikely to be valid. With this *ansatz* one can now start the computation: for the variational calculation, we need two expectation values, the first is the expectation value of  $\mathbb{1}$ , i.e. the norm of the projected states, the second is the expectation value of the Hamiltonian  $H$ . Both  $\mathbb{1}$  and  $H$  share the property of

<sup>10</sup>For simplicity, we assume that  $\mathcal{O}$  will contain only field operators and no momentum operators. This is not a restriction for the following calculation, since in the effective  $\sigma$  model that will be evaluated along these lines, in fact only operators  $\mathcal{O}$  are needed that are constructed from field operators alone.

being gauge invariant under the permissible gauge transformations (i.e. time-independent ones). Thus we have the following simplification

$$\int \mathcal{D}\mathbf{A} \left[ \int \mathcal{D}U_1 \psi^*[\mathbf{A}^{U_1}] \right] \mathcal{O} \left[ \int \mathcal{D}U_2 \psi[\mathbf{A}^{U_2}] \right] = \int \mathcal{D}(U_1 U_2^\dagger) \int \mathcal{D}\mathbf{A} \psi[\mathbf{A}^{(U_1 U_2^\dagger)}] \mathcal{O} \psi[\mathbf{A}], \quad (2.38)$$

where we have used the gauge invariance of  $\mathcal{D}\mathbf{A}$  and the left invariance of  $\mathcal{D}U$ . Furthermore we have assumed that the integration over  $\mathcal{D}U$  is normalized to one<sup>11</sup>. Kogan and Kovner now claim that - having integrated out  $\mathbf{A}$ , which is possible since the path integral over  $\mathbf{A}$  is just Gaussian - the integral over the remaining  $U = U_1 U_2^\dagger$  can be approximated without harming gauge invariance. This statement may be a bit misleading, though. It is true that under a gauge transformation  $\mathbf{A} \rightarrow \mathbf{A}^V$ ,  $U$  does not change:  $U \rightarrow (U_1 V)(U_2 V)^\dagger = U$ . However, gauge invariance means more than that. An analogy from nuclear physics will help here: the Gaussian gauge-non invariant ansatz is similar to a deformed nucleus in nuclear physics. Such a state can be projected onto an s-wave by averaging over all rotated versions of the deformed state. We end up with a state that is itself invariant under rotations; it will be annihilated by the angular momentum operators, very much like a gauge invariant state is annihilated by the Gauss law operators. If we now calculate an expectation value of a rotationally invariant operator, we can hold one of the deformed states fixed, and average only over the directions of the other state. Alas, also a matrix element of a rotationally invariant operator between two deformed states is rotationally invariant. This does not state any more than that the coordinate system that we introduce to perform explicit calculations does not matter. It has nothing to do with the s-wave character of the states. And so, the correct observation that  $U$  does not change under gauge transformations (since it is nothing else but a distance between  $\psi[\mathbf{A}]$  and  $\psi[\mathbf{A}^U]$ ) has nothing to do with the requirement of gauge invariance of the states.

We start now with the computation of the norm  $Z$ :

$$Z = \langle \mathbb{1} \rangle = \int \mathcal{D}U \int \mathcal{D}\mathbf{A} \psi^*[\mathbf{A}^U] \psi[\mathbf{A}] = \int \mathcal{D}U e^{(-\{\frac{1}{2}\text{Tr}(\ln(\mathcal{M})) + \frac{1}{2}\lambda[G + S G S^T]^{-1}\lambda\})} = \int \mathcal{D}U e^{-\Gamma[U]}, \quad (2.39)$$

where we have used an obvious matrix-vector notation, and the abbreviations<sup>12</sup>

$$S^{ab}(\mathbf{x}) = \frac{1}{2} \text{tr}(\tau^a U^\dagger(\mathbf{x}) \tau^b U(\mathbf{x})), \quad \lambda_i^a(\mathbf{x}) = \frac{i}{g} \text{tr}(\tau^a U^\dagger \nabla_i U), \quad (2.40)$$

$$S_{ij}^{ab}(\mathbf{x}, \mathbf{y}) = S^{ab}(\mathbf{x}) \delta_{ij} \delta(\mathbf{x} - \mathbf{y}), \quad \mathcal{M}_{ij}^{ab}(\mathbf{x}, \mathbf{y}) = [\delta^{ab} + S^{T ac}(\mathbf{x}) S^{cb}(\mathbf{y})] G^{-1}(\mathbf{x} - \mathbf{y}) \delta_{ij}. \quad (2.41)$$

In this context,  $\text{tr}$  denotes a colour trace only, and  $\text{Tr}$  a trace over all three types of indices. The matrices  $\tau$  are hermitian generators of (one of) the fundamental representation(s) of  $SU(N)$  normalized as  $\text{tr}(\tau^a \tau^b) = 2\delta^{ab}$ , cf. also footnote 12. Eq. (2.39) implies that one can think about the norm as a partition function of a non-linear  $\sigma$ -model in 3-dimensional Euclidean space with target space  $SU(N)/Z_N$ . One should note that the action is non-local and non-polynomial. The treatment Kogan and Kovner propose is a combination of perturbation theory<sup>13</sup>, mean-field

<sup>11</sup>This is equivalent to the property of a projector  $PP = P$ .

<sup>12</sup>A short comment on notation is in order: whereas in the rest of this thesis, generators of  $SU(N)$  are indicated by  $\lambda$ , and the fundamental representation is normalized as  $\text{tr}(\lambda^a \lambda^b) = \frac{1}{2}\delta^{ab}$ , Kogan and Kovner use a differently normalized fundamental representation  $\tau$ , with  $\tau_{\text{KK95}}^a = 2\lambda_{\text{this thesis}}^a$ .

<sup>13</sup>For the perturbation theory one has to note that they use what we call 'perturbative scaling', i.e. they have put an explicit coupling constant into the covariant derivative, cf. appendix A.5.

approximation and the renormalization group. They start setting up the perturbation theory by writing

$$U(\mathbf{x}) = e^{ig\phi^a\tau^a/2} \quad (2.42)$$

and calculate  $\lambda_i^a$  and  $S^{ab}(\mathbf{x})$  to lowest order<sup>14</sup>, obtaining  $\lambda_i^a(\mathbf{x}) = -\nabla_i\phi^a(\mathbf{x}) + \mathcal{O}(g)$ ,  $S^{ab} = \delta^{ab} + \mathcal{O}(g)$ . The action  $\Gamma[u]$  reduces then to leading order in  $g$  to

$$\frac{1}{16} \int d^3x d^3y (\nabla_i\phi^a(\mathbf{x}))G^{-1}(\mathbf{x}-\mathbf{y})(\nabla_i\phi^a(\mathbf{y})). \quad (2.43)$$

This looks like a free theory with a non-standard propagator. The treatment may be valid for the high-momentum modes<sup>15</sup>. For the low momentum modes, a different expansion may be in order: by ansatz,  $G$  is of short range, and hence for  $U$ s that contain only modes below  $M$ , the action is actually local:

$$\frac{M}{2g^2} \int d^3x \nabla_i U^\dagger(\mathbf{x}) \nabla_i U(\mathbf{x}) + \dots, \quad (2.44)$$

where the spatial dependence of  $S_{ij}^{ab}(\mathbf{x}, \mathbf{y})$  in  $S^TGS$  has been neglected, as have been terms of higher order<sup>16</sup> in  $g$ . Then Kogan and Kovner rewrite the action for the low modes with the help of an additional  $U(1)$  gauge field, s.t. the target space of the model is no longer  $SU(N)/Z_N$ , but rather  $U(N)$ . The gauge symmetry there reduces the physical manifold to  $U(N)/U(1)$  which is isomorphic to  $SU(N)/Z_N$ . The idea is now that one can integrate out the high-momentum modes and thereby produce the running of the parameters of the low-momentum part of the action; the running is assumed to be identical to the QCD running<sup>17</sup>. The coupling constant that enters the low-momentum action would then be  $\alpha_s(M)$  - the strong coupling constant at the scale  $M$ .

The next part of the calculation consists of calculating  $\int \mathcal{D}\mathbf{A} \psi^*[\mathbf{A}^U] H \psi[\mathbf{A}]$ , and reexpressing the result in the high- and low-momentum modes of  $U$ , where the high-momentum modes are treated to lowest order perturbation theory in  $g$ . To the order of  $g$  that is considered, one obtains as energy expectation value a sum of terms that do not contain cross terms between high- and low momentum modes; whereas the high momentum modes give a positive contribution, the low momentum modes give a negative contribution to the energy. In the region of large  $M$ , it is argued that the low momentum theory is weakly coupled, and therefore its contribution to the energy can also be calculated in perturbation theory, resulting in a total (high momentum plus low momentum contribution) energy density

$$\frac{E(M)}{V} = \frac{N^2 - 1}{120\pi^2} M^4, \quad M \gg \Lambda_{QCD}. \quad (2.45)$$

For small  $M$ , it might be useful to look at the phase structure of the  $\sigma$ -model, and therefore use an analogy to classical statistical mechanics: the appearance of the coupling  $g(M)$  is very much like the appearance of the temperature. Thus, one could say that at large  $M$ , the coupling is

<sup>14</sup>A systematic perturbation theory will be set up in sec. 2.2. General expressions for  $\lambda$  and  $S$  that are very well suited to a perturbative expansion beyond lowest order are given in appendix B.

<sup>15</sup>The decomposition of  $U$  into high- and low momentum modes is thought to be permissible due to the gauge-invariant nature of  $U$ .

<sup>16</sup>Apparently, the term  $\text{Tr}(\ln(\mathcal{M}))$  is meant.

<sup>17</sup>This has been investigated in [BK99]. It turned out that the  $\beta$ -function is not quite identical to the QCD  $\beta$ -function (with zero quark flavours) but that (at least to lowest non-trivial order in  $g$ )  $\beta_\sigma = \frac{12}{11}\beta_{QCD}$ . This was interpreted physically in [Brow98].

small, and thus the system is in the low temperature phase, where the  $SU(N)$  symmetry of the  $\sigma$ -model is spontaneously broken. If one decreases  $M$ , thereby increasing  $g$ , one could imagine raising the temperature, and thereby going from the spontaneously broken phase to the disordered, symmetry restored phase. If in this phase transition the internal energy of the  $\sigma$ -model increases, then we might find a minimum of the total energy density at values away from  $M = 0$ , since the contribution of the low-momentum modes, to which this discussion applies, to the total energy is negative. For the rest of the calculation a mean-field approximation is employed, and one obtains indeed a non-zero value for  $M$ . Kogan and Kovner [KK95] then also calculate the value of the gluon condensate, in order to find a physical interpretation for  $M$ , and see that the calculated gluon condensate is of the same order of magnitude as implied by phenomenological studies.

To conclude this section, we want to mention that quite some work has emanated from this study of Kogan and Kovner: there has been some activity to connect the  $\beta$ -function of the  $\sigma$ -model to that of QCD [Brow98], [BK99], and also instanton effects have been studied [BGKK99]. The whole idea of considering the projector integral as a new 'effective' theory has been extended [Dia98], and also been applied to lattice models (topologically massive compact  $U(1)$  theory, compact QED) [KK96],[KS99] and to fermions (Schwinger model) [BGKK00]. However promising the idea in itself may be (as indicated by the number of studies alluded to above), one should also see the shortcomings that are present at least at a technical level: perturbation theory is used throughout (at least for the high momentum modes). As we will see more clearly in the next section, things quickly become quite complicated if one wants to go beyond lowest order. Also the explicit form of the propagator eq. (2.37) was needed in order to ensure a local action for the low-momentum modes<sup>18</sup>. As a last point, the claim that gauge invariance was maintained throughout the calculation is a bit dubious as we have argued in some detail.

*It was indeed our visitor of the afternoon who came bustling in, dangling his glasses more vigorously than ever, and with a very perturbed expression upon his aristocratic features.*

Sherlock Holmes, The Adventure of the Noble Bachelor

## 2.2 Perturbative Evaluation of the Projector

In this section we will present the approach of Testa and Rossi to perturbation theory in the Weyl gauge. We illustrate the general formalism by a calculation of the inter-quark potential up to  $\mathcal{O}(g^4)$ .

In this section we want to illustrate a way of evaluating the projector integral perturbatively that has been pioneered by Testa and Rossi [TR80a], [TR80b] and appreciate the importance of the projector for the static quark potential. In other studies one has seen that the projector basically reinstates the (time-independent) part of the  $A_0$  field<sup>19</sup> [Rei96] and since static charges originally couple only to  $A_0$  it is quite straightforward to see that without the projector there would be no quark potential at all. At tree level, the spatial components of  $A_\mu$  do not contribute

<sup>18</sup>According to [KK95] one obtains practically the same results if one uses a massive scalar propagator with mass  $M$ . However, this propagator is very similar to the one used, so the statement above is not invalidated.

<sup>19</sup>thereby bringing us from the Weyl gauge to the Polyakov gauge

to the interquark potential.

At the heart of the approach is what Testa and Rossi call the *Feynman propagation kernel*:

$$K(\mathbf{A}_2, T/2; \mathbf{A}_1, -T/2) = \langle \mathbf{A}_2 | \exp(-iHT) \mathbf{P} | \mathbf{A}_1 \rangle, \quad (2.46)$$

where  $\mathbf{P}$  denotes the projector as outlined above.  $K$  has the advantage that it can be expressed in several different ways: first, it can be decomposed into gauge invariant eigenstates of the Hamiltonian:

$$H|\psi_n\rangle = E_n|\psi_n\rangle \quad (2.47)$$

with  $|\psi\rangle$  transforming appropriately with respect to the external charge content (cf.eq.(2.6)) under gauge transformations. Using them we can write  $K$  as

$$K(\mathbf{A}_2, T/2; \mathbf{A}_1, -T/2) = \sum_n e^{-iE_n T} \psi_n^*[\mathbf{A}_2] \psi_n[\mathbf{A}_1], \quad (2.48)$$

where the sum  $n$  extends over all physical states. In order to construct the appropriate path integral representation it is more useful, however, to consider first

$$\tilde{K}(\mathbf{A}_2, T/2; \mathbf{A}_1, -T/2) = \sum_{n'} e^{-iE_{n'} T} \psi_{n'}^*[\mathbf{A}_2] \psi_{n'}[\mathbf{A}_1], \quad (2.49)$$

where  $n'$  now extends over the complete Hilbert space. The path integral representation of this can be given straightforwardly as

$$\tilde{K}(\mathbf{A}_2, T/2; \mathbf{A}_1, -T/2) = \int_{\mathbf{A}(t=-T/2)=\mathbf{A}_1}^{\mathbf{A}(t=+T/2)=\mathbf{A}_2} \mathcal{D}\mathbf{A} e^{iS_{YM}}. \quad (2.50)$$

Note that due to gauge invariance (at least w.r.t. time-independent gauge transformations) of the action and the path integral measure, we have

$$\tilde{K}(\mathbf{A}_2, T/2; \mathbf{A}_1, -T/2) = \tilde{K}(\mathbf{A}_2^V, T/2; \mathbf{A}_1^V, -T/2), \quad (2.51)$$

where  $V$  is a time-independent gauge transformation<sup>20</sup>. This will be useful later on. If one uses eq.(2.46) as a starting point, one sees that one can implement the restriction to gauge invariant states by performing the projection procedure at any one time slice; it is particularly convenient to do it at  $t = -T/2$  or  $t = +T/2$ . Note that in the case of presence of external charges, the wave functionals with the appropriate transformation behaviour  $\psi_n$  will carry spin indices, whereas the  $\psi_{n'}$  that span the complete Hilbert space don't<sup>21</sup>; thus  $K$  carries a set of initial spin indices

<sup>20</sup>This property of  $\tilde{K}$  has the same origin as the invariance of  $U$  under gauge transformations in sec.2.1.6 as one can see from the alternative representation of  $\tilde{K}$  as  $\tilde{K} = \langle \mathbf{A}_2 | \exp(-iHT) | \mathbf{A}_1 \rangle$ .

<sup>21</sup>Perhaps it is obvious to the reader, but let us spend a footnote on the topic of spin indices. In sec.2.1.2, we discussed one way of attaching spin indices to Yang-Mills wave functionals. There is, however, a second possibility that is even simpler. Since the Hamiltonian commutes with  $\Gamma^a$ , it commutes also with the Casimir operator(s), like  $\Gamma^a \Gamma^a$ . Thus, we can classify the eigenstates of the Hamiltonian by the eigenvalues of the Casimir operators and of the  $\Gamma^a$ s that span the Cartan subgroup. In other words, at every point in space the eigenstates of the Hamiltonian carry a specific representation of  $SU(N)$ . For simplicity we now restrict ourselves to  $SU(2)$ , where we have only one operator in the Cartan subgroup, but it should work identically for  $SU(N>2)$ . In  $SU(2)$  the states will be, at every point in space, in an eigenstate of  $\Gamma^a \Gamma^a$  (eigenvalue  $j(j+1)$ ) defining the representation, and also in an eigenstate of  $\Gamma^3$  (eigenvalue  $m = -j \dots j$ ); thus if we concentrate on the point  $\mathbf{x}_0$  for a moment, the state looks like  $|\mathbf{x}_0; j, m\rangle$  with  $\Gamma^a \Gamma^a |\mathbf{x}_0; j, m\rangle = j(j+1) |\mathbf{x}_0; j, m\rangle$  and  $\Gamma^3 |\mathbf{x}_0; j, m\rangle = m |\mathbf{x}_0; j, m\rangle$ .  $\Gamma^1, \Gamma^2$  only perform linear combinations of states with the same  $j$  value and different  $m$  values; thus for a state carrying a specific representation of  $SU(2)$  at a point in space, the Gauss law operators act like the matrices of this specific representation. Thus, the spin labels are nothing more (in the case of  $SU(2)$ ) than the eigenvalues  $m$  of  $\Gamma^3$ . Sometimes it is convenient to make them explicit, as in the case of  $K$  if one knows beforehand which representation one wants at which spatial point, and sometimes one leaves them rather implicit as in the case of  $\tilde{K}$ .

$\{s_i\}$  and final spin indices  $\{s_f\}$ . Let  $\lambda^{(j)}$  denote the generators in the appropriate representation  $j$  for the external charges (fundamental, adjoint, etc) that are localized at the points  $\mathbf{x}_j$ ; then the relation between  $K$  and  $\tilde{K}$  can be written as

$$K_{\{s_2\}\{s_1\}}^{\{j\}}(\mathbf{A}_2, T/2; \mathbf{A}_1, -T/2) = \int_{\mathcal{G}_0} \mathcal{D}h \left[ \prod_j e^{ig\lambda_a^{(j)} h^a(\mathbf{x}_j)} \right]_{\{s_2\}\{s_1\}} \tilde{K}(\mathbf{A}_2^{U_h}, T/2; \mathbf{A}_1, -T/2), \quad (2.52)$$

where  $h$  denotes the gauge angles, i.e. the parameters of the gauge transformation.  $\mathcal{D}h$  includes the corresponding Haar measure. It will be further discussed in appendix B.  $\mathcal{G}_0$  denotes the range of integration: only the topologically trivial sector of gauge transformations is integrated over.

### 2.2.1 $\beta$ -Function in this Approach

In the following we have the very modest goal of calculating the  $\beta$ -function to lowest order, since we only want to give an impression of how one can evaluate the projector perturbatively. We follow mainly [TR80b] in our presentation. It appears to be useful to extract the  $\beta$ -function from the perturbative evaluation of the interquark potential to  $\mathcal{O}(g^4)$ . We do this by considering the problem of two static spins evolving from time  $-T/2$  to  $T/2$  and computing the Feynman propagation kernel at imaginary time from zero field to zero field; since at  $g = 0$ , the singlet and  $(N^2 - 1)$ -plet states are degenerate, we have to take them both into account as the lowest energy states<sup>22</sup>. Using the abbreviation  $\chi_{n;sr} = \psi_{n;sr}[\mathbf{A} = 0]$ , where  $r, s$  are spin labels, we write  $K$  as a sum over the  $N^2$  lowest states that are degenerate at  $g = 0$ :

$$K_{s_2 r_2; s_1 r_1}(\mathbf{0}, \mathbf{0}, -iT) \approx \sum_{n=0}^{N^2-1} e^{-E_n T} \chi_{n; s_2 r_2} \chi_{n; s_1 r_1}^*. \quad (2.53)$$

In order to be able to read off  $E_n$  conveniently at the end of the calculation, we perform a Taylor expansion of the exponential<sup>23</sup>, thus

$$K_{s_2 r_2; s_1 r_1}(\mathbf{0}, \mathbf{0}, -iT) \approx \sum_{n=0}^{N^2-1} \chi_{n; s_2 r_2} \chi_{n; s_1 r_1}^* - T \sum_{n=0}^{N^2-1} E_n \chi_{n; s_2 r_2} \chi_{n; s_1 r_1}^* + T^2 \times \dots \quad (2.54)$$

Next, we expand both  $E_n$  and  $\chi$  in powers of  $g$  (assuming  $E_n(g=0) = 0$ ); actually, here we can expand them<sup>24</sup> in powers of  $g^2$ . Using the notation

$$E_n = g^2 \epsilon_n^{(2)} + g^4 \epsilon_n^{(4)} + \dots, \quad \chi_{n; s_2 r_2} = \chi_{n; s_2 r_2}^{(0)} + g^2 \chi_{n; s_2 r_2}^{(2)} + g^4 \chi_{n; s_2 r_2}^{(4)} + \dots \quad (2.55)$$

<sup>22</sup>In the end we want to send  $T \rightarrow \infty$ , so only the states of lowest energy will survive.

<sup>23</sup>This can be done since the radius of convergence of the exponential function is infinity; here, it is not claimed that it is a good approximation, only that one can read off the energy from the term linear in  $T$ .

<sup>24</sup>For  $E_n$  one could argue that for odd powers of  $g$  one would need an odd number of the three gluon vertices, which in the end would result in particle production from the initial to the final state; however, in perturbative expressions for the energy, the initial and final states are always the same (with a fixed number of gluons), and hence operators that comprise particle production don't contribute to perturbative corrections of  $E_n$ . For  $\chi$  the reason lies in the fact that we need  $\psi[\mathbf{0}]$ ; if we start from the perturbative vacuum (that is very much like the QED vacuum), and we want an odd power in  $g$  in the perturbed wave functional, we have to admit a wave functional that is odd in  $\mathbf{A}$  since otherwise the matrix element of the three-gluon vertex will be zero; however, an odd wave functional is zero for  $\mathbf{A} = \mathbf{0}$ , thus  $\chi$  obtains corrections only of even power in  $g$ .

and the relation (to be verified later on in eq. (2.79))

$$\sum_{n=0}^{N^2-1} \chi_{n;s_2 r_2}^{(0)} \chi_{n;s_1 r_1}^{(0)*} = \delta_{s_2 s_1} \delta_{r_2 r_1}, \quad (2.56)$$

we obtain (abbreviating the sets of spins  $(s_2, r_2)$  by  $a_2$ , and  $(s_1, r_1)$  by  $a_1$ )

$$\begin{aligned} & K_{s_2 r_2; s_1 r_1}(\mathbf{0}, \mathbf{0}, -iT) \\ & \approx \delta_{s_2 s_1} \delta_{r_2 r_1} \\ & + g^2 \sum_n \left\{ \chi_{n;a_2}^{(0)} \chi_{n;a_1}^{(2)*} + \chi_{n;a_2}^{(2)*} \chi_{n;a_1}^{(0)} + g^2 \left( \chi_{n;a_2}^{(2)} \chi_{n;a_1}^{(2)*} + \chi_{n;a_2}^{(4)} \chi_{n;a_1}^{(0)*} + \chi_{n;a_2}^{(0)} \chi_{n;a_1}^{(4)*} \right) + \dots \right\} \\ & - T \sum_n g^2 \left\{ \epsilon_n^{(2)} \chi_{n;a_2}^{(0)} \chi_{n;a_1}^{(0)*} + g^2 \left( \epsilon_n^{(4)} \chi_{n;a_2}^{(0)} \chi_{n;a_1}^{(0)*} + \epsilon_n^{(2)} \left( \chi_{n;a_2}^{(2)} \chi_{n;a_1}^{(0)*} + \chi_{n;a_2}^{(0)} \chi_{n;a_1}^{(2)*} \right) \right) + \mathcal{O}(g^4) \right\}. \\ & + \mathcal{O}(T^2) \end{aligned} \quad (2.57)$$

### 2.2.2 Perturbative Evaluation of $K$

The program for the rest of the section is to compute  $K$  from the path integral representation in powers of  $g$ , ignoring all terms that are (at least in the limit of large  $T$ ) not proportional to  $T$  for  $\mathbf{A}_1 = \mathbf{0}, \mathbf{A}_2 = \mathbf{0}$ . We start out by computing  $\tilde{K}$  for arbitrary  $\mathbf{A}_1, \mathbf{A}_2$ , since if we compute  $K$  from  $\tilde{K}$  we have to sum up all  $\tilde{K}$  that have as final configuration a pure gauge potential, cf. eq. (2.52). We consider the action<sup>25</sup> in Weyl gauge and decompose it w.r.t. a free part and the interacting part:

$$\begin{aligned} S & = S_0 + S_I \text{ with} \\ S_0 & = -\frac{1}{2} \int_{-T/2}^{T/2} dt \int d^3x \left( \dot{\mathbf{A}}_i^a \dot{\mathbf{A}}_i^a + (\nabla_i \mathbf{A}_j^a)(\nabla_i \mathbf{A}_j^a) - (\nabla_j \mathbf{A}_i^a)(\nabla_i \mathbf{A}_j^a) \right), \\ S_I & = \frac{g}{2} f^{abc} \int_{-T/2}^{T/2} dt \int d^3x (\nabla_i \mathbf{A}_j^a - \nabla_j \mathbf{A}_i^a) \mathbf{A}_i^b \mathbf{A}_j^c - \frac{g^2}{4} \int_{-T/2}^{T/2} dt \int d^3x f^{abc} f^{ade} \mathbf{A}_i^b \mathbf{A}_j^c \mathbf{A}_i^d \mathbf{A}_j^e. \end{aligned} \quad (2.58)$$

After introducing sources  $\mathbf{J}$ , we can decompose  $\tilde{K}$  into a free part  $\tilde{K}_0$  (which can be explicitly given in terms of the sources  $\mathbf{J}$ , and the initial and final fields  $\mathbf{A}_1, \mathbf{A}_2$ ), and the interaction part that can be written with the help of derivatives w.r.t. the sources:

$$\tilde{K} = e^{S_I[-\frac{\delta}{\delta \mathbf{J}}]} \int_{\mathbf{A}(t=-T/2)=\mathbf{A}_1}^{\mathbf{A}(t=+T/2)=\mathbf{A}_2} \mathcal{D}\mathbf{A} e^{S_0 - \mathbf{J} \cdot \mathbf{A}} = e^{S_I[-\frac{\delta}{\delta \mathbf{J}}]} \tilde{K}_0(\mathbf{A}_1, \mathbf{A}_2; T; \mathbf{J}). \quad (2.60)$$

The free part will be computed as follows: decompose  $\mathbf{A}$  into a classical part that satisfies the classical equations of motion  $\mathbf{A}_{cl}$  with the boundary conditions  $\mathbf{A}_{cl}(t = -T/2) = \mathbf{A}_1, \mathbf{A}_{cl}(t = +T/2) = \mathbf{A}_2$ , and a quantum part  $\mathbf{a}$  with the boundary conditions  $\mathbf{a}(t = -T/2) = \mathbf{a}(t = +T/2) = \mathbf{0}$ . The action  $S_0$ , being quadratic in  $\mathbf{A}$ , is then just a sum of a classical part and the quantum part; the path integral for the quantum part can then be performed in a straightforward manner:

$$\tilde{K}_0(\mathbf{A}_1, \mathbf{A}_2; T; \mathbf{J}) = e^{S_0(\mathbf{A}_2, \mathbf{A}_1, T) - \mathbf{J} \cdot \mathbf{A}_{cl}} \int_{\mathbf{a}(t=-T/2)=\mathbf{0}}^{\mathbf{a}(t=+T/2)=\mathbf{0}} \mathcal{D}\mathbf{a} e^{S_0[\mathbf{a}] - \mathbf{J} \cdot \mathbf{a}}. \quad (2.61)$$

<sup>25</sup>Since we are interested in  $K$  for imaginary times we use already the Wick-rotated action.

We obtain for  $\mathbf{A}_{\text{cl}}$ :

$$\begin{aligned} \mathbf{A}_{\text{cl}}(\mathbf{x}, t) = \int d^3 y \frac{d^3 p}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} & \left\{ \left( -\frac{\sinh(|\mathbf{p}|(t-T/2))}{\sinh(|\mathbf{p}|T)} \mathbf{P}^T(\mathbf{p}) - \frac{t-T/2}{T} \mathbf{P}^L(\mathbf{p}) \right) \mathbf{A}_1(\mathbf{y}) \right. \\ & \left. + \left( \frac{\sinh(|\mathbf{p}|(t+T/2))}{\sinh(|\mathbf{p}|T)} \mathbf{P}^T(\mathbf{p}) + \frac{t+T/2}{T} \mathbf{P}^L(\mathbf{p}) \right) \mathbf{A}_2(\mathbf{y}) \right\}. \end{aligned} \quad (2.62)$$

$\mathbf{P}^T, \mathbf{P}^L$  denote the transversal and longitudinal projectors respectively. Note that even for the non-interacting theory  $\mathbf{A}_{\text{cl}}$  will contain longitudinal contributions if the initial or final configurations contain them. Having obtained  $\mathbf{A}_{\text{cl}}$  we can also compute the classical action:

$$\begin{aligned} S_0^{\text{class}} = -\frac{1}{2} \int \frac{d^3 p}{(2\pi)^3} & \left\{ \frac{1}{T} (\tilde{\mathbf{A}}_2 - \tilde{\mathbf{A}}_1) \mathbf{P}^L (\tilde{\mathbf{A}}_2 - \tilde{\mathbf{A}}_1) \right. \\ & \left. + |\mathbf{p}| \left( \coth(|\mathbf{p}|T) (\tilde{\mathbf{A}}_1 \mathbf{P}^T \tilde{\mathbf{A}}_1 + \tilde{\mathbf{A}}_2 \mathbf{P}^T \tilde{\mathbf{A}}_2) - \frac{2}{\sinh(|\mathbf{p}|T)} \tilde{\mathbf{A}}_1 \mathbf{P}^T \tilde{\mathbf{A}}_2 \right) \right\}, \end{aligned} \quad (2.63)$$

where  $\tilde{\mathbf{A}}$  denotes the Fourier transform of  $\mathbf{A}$  and in eq. (2.63) depends on  $\mathbf{p}$ .

Now we want to deal with the quantum fluctuations. The path integral can be performed by completing the square. One can split  $\mathbf{a}$  into its longitudinal and transversal components and thus has to determine the Green's function for  $(-d^2/dt^2)$  and for  $(-d^2/dt^2 + \mathbf{p}^2)$  (as we integrate over the  $\mathbf{a}$  modes in Fourier space). Here it is important to realize that we need the Green's function for a finite time domain; a possible method of construction can be found in [Kle93] and one obtains for the complete (longitudinal and transversal) Green's function:

$$D_{ij}(\mathbf{x}, t; \mathbf{y}, t') = \int \frac{d^3 p}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} (G_p(t, t') \mathbf{P}_{ij}^T + G_0(t, t') \mathbf{P}_{ij}^L) \quad (2.64)$$

with

$$\begin{aligned} G_p(t, t') = \frac{1}{|\mathbf{p}| \sinh(|\mathbf{p}|T)} & \times \left\{ \Theta(t-t') \sinh\left(|\mathbf{p}|\left(\frac{T}{2}-t\right)\right) \sinh\left(|\mathbf{p}|\left(t'-\frac{T}{2}\right)\right) \right. \\ & \left. + \Theta(t'-t) \sinh\left(|\mathbf{p}|\left(\frac{T}{2}-t'\right)\right) \sinh\left(|\mathbf{p}|\left(t-\frac{T}{2}\right)\right) \right\}, \end{aligned} \quad (2.65)$$

$$G_0(t, t') = \lim_{p \rightarrow 0} G_p(t, t') = \frac{1}{T} \left\{ \Theta(t-t') \left(\frac{T}{2}-t\right) \left(t'-\frac{T}{2}\right) + \Theta(t'-t) \left(\frac{T}{2}-t'\right) \left(t-\frac{T}{2}\right) \right\}. \quad (2.66)$$

With these results we can write the free part of the unprojected Feynman propagation kernel as

$$\begin{aligned} \tilde{K}_0(\mathbf{A}_2, \mathbf{A}_1; T; \mathbf{J}) & = \int_{\mathbf{A}(t=-T/2)=\mathbf{A}_1}^{\mathbf{A}(t=+T/2)=\mathbf{A}_2} \mathcal{D}\mathbf{A} e^{S_0[\mathbf{A}] - \mathbf{A}\cdot\mathbf{J}} \\ & = \mathcal{N} e^{\frac{1}{2} \int d^3 x d^3 y (\mathbf{A}_{2,i}(\mathbf{x}) \chi_1^{ij}(\mathbf{x}, \mathbf{y}) \mathbf{A}_{2,j}(\mathbf{y}) + \mathbf{A}_{1,i}(\mathbf{x}) \chi_1^{ij}(\mathbf{x}, \mathbf{y}) \mathbf{A}_{1,j}(\mathbf{y}) + \mathbf{A}_{1,i}(\mathbf{x}) \chi_2^{ij}(\mathbf{x}, \mathbf{y}) \mathbf{A}_{2,j}(\mathbf{y}))} \\ & \quad \times e^{\int d^3 x d^3 y dt (\mathbf{A}_{1,i}(\mathbf{x}) g_{ij}^-(\mathbf{x}, \mathbf{y}) \mathbf{J}_j(\mathbf{y}, t) - \mathbf{A}_{2,i}(\mathbf{x}) g_{ij}^+(\mathbf{x}, \mathbf{y}) \mathbf{J}_j(\mathbf{y}, t))} \\ & \quad \times e^{\frac{1}{2} \int d^3 x d^3 y dt dt' \mathbf{J}_i^a(\mathbf{x}, t) D_{ij}(\mathbf{x}, t; \mathbf{y}, t') \mathbf{J}_j^a(\mathbf{y}, t')} \end{aligned} \quad (2.67)$$

with

$$\chi_1^{ij}(\mathbf{x}, \mathbf{y}) = - \int \frac{d^3 p}{(2\pi)^3} \left\{ |\mathbf{p}| \coth(|\mathbf{p}|T) \mathbf{P}_{ij}^T + \frac{1}{T} \mathbf{P}_{ij}^L \right\}, \quad (2.68)$$



$$\chi_2^{ij}(\mathbf{x}, \mathbf{y}) = 2 \int \frac{d^3 p}{(2\pi)^3} \left\{ |\mathbf{p}| \frac{1}{\sinh(|\mathbf{p}|T)} \mathbf{P}_{ij}^T + \frac{1}{T} \mathbf{P}_{ij}^L \right\}, \quad (2.69)$$

$$g_{ij}^\pm(\mathbf{x}, \mathbf{y}) = \int \frac{d^3 p}{(2\pi)^3} \left\{ \frac{\sinh|\mathbf{p}|(t \pm \frac{T}{2})}{\sinh|\mathbf{p}|T} \mathbf{P}_{ij}^T + \frac{t \pm T}{T} \mathbf{P}_{ij}^L \right\}. \quad (2.70)$$

From here on, we can use the fact that we want to use a special system, namely one where  $\mathbf{A}_1 = \mathbf{A}_2 = 0$  in the projected propagation kernel; thus in the unprojected kernel, we have to put in initial and final conditions that are pure gauge fields. One could choose  $\mathbf{A}_1 = 0$ ,  $\mathbf{A}_2 = -\frac{i}{g} U_h^\dagger \nabla U_h$  (corresponding to a projector that is applied to the final state); however, in the following we want to be a bit more flexible, and use eq. (2.51) with  $V = e^{i\rho g h_a \lambda^a}$  [LMR84], so that by choosing  $\rho = 0$ , we only integrate, as before, over the final configuration, whereas for  $\rho = -1$  we integrate over the initial configuration. With the results from the appendix B, we can write  $\mathbf{A}_1^V, \mathbf{A}_2^{UV}$  in terms of the matrix<sup>26</sup>  $F$  and  $\nabla h$ :

$$(\mathbf{A}_1^V)^a = \rho(\delta_{ab} + F_{ab}(\rho h)) \nabla h^b, \quad (2.71)$$

$$(\mathbf{A}_2^{UV})^a = (1 + \rho)(\delta_{ab} + F_{ab}((1 + \rho)h)) \nabla h^b. \quad (2.72)$$

We insert these definitions into eq. (2.67) to obtain the exponentiated action for the projector field, cf. eq. (2.52). We see that the free Yang-Mills part with definite boundary conditions has turned into a non-polynomial interacting theory for the projector field albeit in one dimension less, since  $h$  does not depend on time. The integration measure is not flat, however, but one has to use the Haar measure. A rather explicit expression for the Haar measure is given in the appendix, eq. (B.16). In order to get a handle on the  $h$  integration, we again introduce a source term  $-\int d^3 x \{h^a(\mathbf{x}) f^a(\mathbf{x})\}$  and rewrite  $F$  with the help of functional derivatives<sup>27</sup> w.r.t.  $f$ . However, before one can perform the usual completion of squares to perform the path integral<sup>28</sup> over  $h$ , one has to realize that there are other terms besides the newly introduced source term that are linear in  $h$ , resulting from the terms  $\mathbf{A}_{1,2}^{\text{class}} \cdot \mathbf{J}$ . Having done all this, we end up with terms that are

- quadratic in either  $\mathbf{J}$  or  $f$ : they give the  $\mathbf{A}\mathbf{A}$ - or  $hh$  propagators, respectively
- a term that is linear in  $f$  and  $\mathbf{J}$ ; this term gives rise to a mixed propagator
- terms linear in  $\mathbf{J}$  but non-linear in  $f$  - they give rise to new vertices
- terms independent of both  $\mathbf{J}$  and  $f$ : they stem from the three- and four-gluon vertices of the original Yang-Mills action, the Haar measure, and those parts of the classical action that contain  $F$ s.

We use as notation for the propagators:  $\langle \mathbf{A}_i^a(\mathbf{x}) \mathbf{A}_j^b(\mathbf{y}) \rangle$  for the  $\mathbf{A}\mathbf{A}$ -propagator, correspondingly for the others, and thus end up with the perturbative expansion for the projected Feynman propagation kernel (Einstein summation convention even for continuous indices)

$$\begin{aligned} & K(\mathbf{A}_2 = \mathbf{0}, \mathbf{A}_1 = \mathbf{0}, -iT)_{s_2, r_2; s_1, r_1} \\ &= \mathcal{N} \left\{ e^{S_I[-\frac{\delta}{\delta \mathbf{J}}]} e^{S'_I[\mathbf{J}, -\frac{\delta}{\delta \mathbf{f}}]} e^{S_m[-\frac{\delta}{\delta \mathbf{f}}]} \left( e^{-ig\lambda^{as} \frac{\delta}{\delta f_{\mathbf{x}s}^a}} \right)_{s_2 s_1} \left( e^{-ig\bar{\lambda}^{ar} \frac{\delta}{\delta f_{\mathbf{x}r}^a}} \right)_{r_2 r_1} \right. \\ & \quad \left. e^{\frac{1}{2} f_{\mathbf{x}}^a \langle h_{\mathbf{x}}^a h_{\mathbf{y}}^b \rangle f_{\mathbf{y}}^b + f_{\mathbf{x}}^a \langle h_{\mathbf{x}}^a \mathbf{A}_{j,\mathbf{y}}^b \rangle \mathbf{J}_{j,\mathbf{y}}^b + \frac{1}{2} \mathbf{J}_{i,\mathbf{x}}^a \langle \mathbf{A}_{i,\mathbf{x}}^a \mathbf{A}_{j,\mathbf{y}}^b \rangle \mathbf{J}_{j,\mathbf{y}}^b} \right\}, \quad (2.73) \end{aligned}$$

<sup>26</sup>For convenience we give here the definition of  $F$  that is also given in appendix B:  $F = (i\gamma)^{-1}(e^{i\gamma} - i\gamma - 1)$  with  $\gamma_{ab} = i f^{abc} h_c$ .

<sup>27</sup>All the interactions of the projector field come into play because of  $F$ .

<sup>28</sup>In this step one ignores cavalierly that  $h$  is a compact variable.

where the complete expressions for the propagators and the interaction parts are given in appendix B. Here,  $\lambda, \bar{\lambda}$  denote the representations appropriate for the two static sources. In the following we will be concerned with the static inter-quark potential to  $\mathcal{O}(g^4)$ ; this will greatly simplify matters for the following reasons: first, since we are only interested in the potential, we are interested only in that part of  $K$  that depends on both  $\mathbf{x}_s$  and  $\mathbf{x}_r$ ; thus we need only consider the part of eq. (2.73) that contains at least one derivative w.r.t.  $f(\mathbf{x}_s)$  and one w.r.t.  $f(\mathbf{x}_r)$ ; since both terms contain a factor of  $g$ , we only have to consider interaction terms up to  $\mathcal{O}(g^2)$ . Therefore, we expand  $S_m, S'_I$  in powers of  $g$ ; but now comes into play that we are interested also only in contributions that are, in the large- $T$  limit, proportional to  $T$ . This allows to drop a number of terms, especially the complete contribution from the measure, and we don't have to consider terms arising from  $\frac{\delta}{\delta f(\mathbf{x}_s)} \frac{\delta}{\delta f(\mathbf{x}_s)} \frac{\delta}{\delta f(\mathbf{x}_r)} \frac{\delta}{\delta f(\mathbf{x}_r)}$ . These insights can be condensed into using a simplified  $S'_I$ :

$$S'_I = \frac{g}{2} \int d^3x d^3y h_{\mathbf{x}}^c f^{cab} (\nabla_x^i h_{\mathbf{x}}^b) \int dt \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \left\{ \mathbf{P}_{ij}^T \left( \frac{(1+2\rho)}{2} \frac{\sinh(|\mathbf{p}|t)}{\sinh(|\mathbf{p}|T/2)} \right) \right. \\ \left. + \frac{(1+2\rho+2\rho^2)}{2} \frac{\cosh(|\mathbf{p}|t)}{\cosh(|\mathbf{p}|T/2)} \right\} + \mathbf{P}_{ij}^L \left( \frac{1}{2}(1+2\rho+2\rho^2) + \frac{t}{T}(1+2\rho) \right) \left\} \mathbf{J}_j^a(\mathbf{x}, t). \quad (2.74)$$

For the rest of this section, it will be convenient to rewrite the different parts of the action in a form that makes the structures apparent. For this purpose we introduce vertices and a super-index notation:  $a, b, c, \dots$  are supposed to contain all appropriate indices, i.e. position label and colour index and sometimes - when used on a  $\mathbf{J}$  source - also a spatial index. This condensed notation is explain further in app. B.5.3. Then

$$S_I[-\frac{\delta}{\delta \mathbf{J}}] = -g \mathbb{G}_1^{abc} \left( \frac{\delta}{\delta \mathbf{J}^a} \right) \left( \frac{\delta}{\delta \mathbf{J}^b} \right) \left( \frac{\delta}{\delta \mathbf{J}^c} \right) + g^2 \mathbb{G}_2^{abcd} \left( \frac{\delta}{\delta \mathbf{J}^a} \right) \left( \frac{\delta}{\delta \mathbf{J}^b} \right) \left( \frac{\delta}{\delta \mathbf{J}^c} \right) \left( \frac{\delta}{\delta \mathbf{J}^d} \right), \quad (2.75)$$

$$S'_I[\mathbf{J}, -\frac{\delta}{\delta f}] = g \mathbf{J}^a \mathbb{H}_1^{a;bc} \left( \frac{\delta}{\delta f^b} \right) \left( \frac{\delta}{\delta f^c} \right), \quad (2.76)$$

$$S_0 = \frac{1}{2} f^a \langle h^a h^b \rangle f^b + f^a \langle h^a A^b \rangle \mathbf{J}^b + \frac{1}{2} \mathbf{J}^a \langle \mathbf{A}^a \mathbf{A}^b \rangle \mathbf{J}^b. \quad (2.77)$$

With this notation<sup>29</sup> we can write the part of  $K_{s_2s_1; r_2r_1}$  we are interested in as<sup>30</sup>

$$\left[ \begin{aligned} & \delta_{s_2s_1} \delta_{r_2r_1} \\ & - g^2 (\lambda_{s_2s_1}^{a_s} \bar{\lambda}_{r_2r_1}^{a_r}) \frac{\delta}{\delta f_{\mathbf{x}_s}^{a_s}} \frac{\delta}{\delta f_{\mathbf{x}_r}^{a_r}} \\ & - g^4 (\lambda_{s_2s_1}^{a_s} \bar{\lambda}_{r_2r_1}^{a_r}) \frac{\delta}{\delta f_{\mathbf{x}_s}^{a_s}} \frac{\delta}{\delta f_{\mathbf{x}_r}^{a_r}} \left( \mathbb{G}_2^{abcd} \frac{\delta}{\delta \mathbf{J}^a} \frac{\delta}{\delta \mathbf{J}^b} \frac{\delta}{\delta \mathbf{J}^c} \frac{\delta}{\delta \mathbf{J}^d} + \frac{1}{2} \mathbb{G}_1^{abc} \mathbb{G}_1^{def} \frac{\delta}{\delta \mathbf{J}^a} \frac{\delta}{\delta \mathbf{J}^b} \frac{\delta}{\delta \mathbf{J}^c} \frac{\delta}{\delta \mathbf{J}^d} \frac{\delta}{\delta \mathbf{J}^e} \frac{\delta}{\delta \mathbf{J}^f} \right. \\ & \quad \left. - 3 \mathbb{G}_1^{dbc} \mathbb{H}_1^{d;ef} \frac{\delta}{\delta \mathbf{J}^b} \frac{\delta}{\delta \mathbf{J}^c} \frac{\delta}{\delta f^e} \frac{\delta}{\delta f^f} \right] e^{S_0}. \end{aligned} \right. \quad (2.78)$$

This expression still contains terms that are not proportional to  $T$ , but these will be neglected subsequently wherever they appear explicitly. We will now discuss the different orders in  $g^2$  individually.

<sup>29</sup>The complete expressions for the different contributions to the action can be found in appendix B.5.2.

<sup>30</sup>The first term comes from setting  $g = 0$ ; then  $(e^{ig\cdots})_{s_2s_1} = \delta_{s_2s_1}$  etc.; please note also, that we have dropped the normalization constant. We will discuss the normalization after eq. (2.86).

### 2.2.3 $\mathcal{O}(g^0)$ Contribution

To this order, we see that

$$K(\mathbf{A}_2 = \mathbf{0}, \mathbf{A}_1 = \mathbf{0}, -iT)_{s_2 r_2; s_1 r_1}^{\mathcal{O}(g^0)} = \delta_{s_2 s_1} \delta_{r_2 r_1} \quad (2.79)$$

(the restriction to terms proportional to  $T$  obviously does not apply here) thereby proving the claim made in eq. (2.56).

### 2.2.4 $\mathcal{O}(g^2)$ Contribution

The  $\mathcal{O}(g^2)$  contribution to  $K$  that is proportional to  $T$  is given by

$$K_{s_2 r_2; s_1 r_1}^{\mathcal{O}(g^2)} = g^2 (\lambda^{a_s})_{s_2 s_1} (\bar{\lambda}^{a_r})_{r_2 r_1} \langle h^{a_s}(\mathbf{x}_s) h^{a_r}(\mathbf{x}_r) \rangle = -T g^2 (\lambda^a)_{s_2 s_1} (\bar{\lambda}^a)_{r_2 r_1} \frac{1}{4\pi |\mathbf{x}_s - \mathbf{x}_r|}. \quad (2.80)$$

One can represent this also graphically as

$$x_r \leftarrow \text{oooooooooooooooooooo} \rightarrow x_s \quad .$$

By comparing eq. (2.80) with eq. (2.57) we can obtain further information:

$$\sum_n \epsilon_n^{(2)} \chi_{n; s_2 r_2}^{(0)} \chi_{n; s_1 r_1}^{(0)*} = T g^2 \sum_a (\lambda^a)_{s_2 s_1} (\bar{\lambda}^a)_{r_2 r_1} \frac{1}{4\pi |\mathbf{x}_s - \mathbf{x}_r|}. \quad (2.81)$$

In the following we want to assume that the charges are defined in the fundamental representation; then we can reorder the indices on the RHS with the help of the Fierz identity if we note that

$$(\bar{\lambda}^a)_{r_2 r_1} = -(\lambda^{a*})_{r_2 r_1} = -(\lambda^a)_{r_1 r_2} \quad (2.82)$$

since the  $\lambda$ s are hermitian. Then we can use the Fierz identity<sup>31</sup>

$$(\lambda^a)_{s_2 s_1} (\lambda^a)_{r_1 r_2} = \frac{1}{2} \left( 1 - \frac{1}{N^2} \right) \delta_{s_2 r_2} \delta_{s_1 r_1} - \frac{1}{N} (\lambda^a)_{s_2 r_2} (\lambda^a)_{s_1 r_1}. \quad (2.83)$$

This is just the decomposition into singlet and  $(N^2 - 1)$ -plet. Since the latter states are energetically degenerate, this allows an almost direct identification of the energies. One has to give a little thought to the distribution of constant factors between the energies and the wave functions. Of course, one will have distributed correctly if the wave functions are normalized (i.e.  $\text{tr}(\lambda^a \lambda^{b*}) = \delta^{ab}$ , hence  $\chi_{n=0;sr} = \chi_{sr}^{singlet} = \delta_{sr}/\sqrt{N}$ ,  $\chi_{n=1\dots N^2-1;sr} = \chi_{n;sr}^{(N^2-1)\text{-plet}} = \sqrt{2} L_{nb} \lambda_{sr}^b$  where  $L$  is a unitary matrix and  $n$  labels the different  $(N^2 - 1)$ -plet wave functions). Thus the Fierz transform is now written most suggestively as

$$(\lambda^a)_{s_2 s_1} (\lambda^a)_{r_1 r_2} = \frac{1}{2} \left( \frac{N^2 - 1}{N} \right) \frac{\delta_{s_2 r_2}}{\sqrt{N}} \frac{\delta_{s_1 r_1}}{\sqrt{N}} - \frac{1}{2N} \left( \sqrt{2} (\lambda^a)_{s_2 r_2} \right) \left( \sqrt{2} (\lambda^a)_{s_1 r_1} \right). \quad (2.84)$$

<sup>31</sup>e.g. eq. (2.45) in [AR95]; note that the  $\lambda$  matrices are here normalized to 1/2 instead of 2 as in [AR95].

Hence the energies are given by<sup>32</sup>

$$\epsilon_{singlet}^{(2)} = -\frac{N^2 - 1}{2N} \frac{1}{4\pi|\mathbf{x}_r - \mathbf{x}_s|}, \quad (2.85)$$

$$\epsilon_{(N^2-1)\text{-plet}}^{(2)} = \frac{1}{2N} \frac{1}{4\pi|\mathbf{x}_r - \mathbf{x}_s|}. \quad (2.86)$$

Also, one can obtain another piece of information: for the potential, we have considered only the parts of  $K$  that are proportional to  $T$ ; let us now consider the part that is proportional to  $T^0 g^2$ . For this it is important that we have used a rather implicit normalization, namely w.r.t.  $K$  without external static sources<sup>33</sup> [LMR84]. For this reason closed loops that are not connected to the external charges at all can be left out of the considerations. Thus, the only terms we have to consider are source self-energies. However, the only term that involves at least one source and no  $hh$ -propagator (which would make it automatically  $\propto T$ ), is (up to constants)

$$\langle h^{ar}(\mathbf{x}_r) \mathbf{A}_i^b(\mathbf{x}, t) \rangle \langle \mathbf{A}_j^c(\mathbf{y}, t') \mathbf{A}_k^c(\mathbf{z}, t'') \rangle (\mathbb{G}_1)_{ijk}^{bcd}(\mathbf{x}, \mathbf{y}, \mathbf{z}, t, t', t''). \quad (2.87)$$

However,  $\mathbb{G}_1^{bcd} \propto f^{bcd}$  whereas  $\langle \mathbf{A}^c \mathbf{A}^d \rangle \propto \delta^{bc}$ , thus even this term vanishes. Therefore, we conclude that the contribution  $\propto g^2 T^0$  to  $K$  is zero. But then, we can conclude from eq. (2.57) that

$$\sum_{n=0}^{N^2-1} \left( \chi_{n;s_2 r_2}^{(0)} \chi_{n;s_1 r_1}^{(2)*} + \chi_{n;s_2 r_2}^{(2)} \chi_{n;s_1 r_1}^{(0)*} \right) = 0. \quad (2.88)$$

As it stands this equation is not directly useful. However, we can extract with a further argument some information that is very important for the interpretation of the  $\mathcal{O}(g^4)$  contribution (that is also proportional to  $T$ ) to  $K$ : since we are studying a gauge-invariant system, the perturbations should not mix the singlet and the  $(N^2 - 1)$ -plet wave functions. Therefore, (with  $\chi_0^{(0)}$  being the unperturbed singlet wave function)

$$\chi_0^{(2)} = C \chi_0^{(0)}, \quad (2.89)$$

where  $C$  is a constant. Then we can decompose eq. (2.88) into a singlet part, and a sum over the  $(N^2 - 1)$ -plet:

$$(C + C^*) \frac{1}{N} \delta_{s_2 r_2} \delta_{s_1 r_1} + \sum_{n=1}^{N^2-1} \left( \chi_{n;s_2 r_2}^{(0)} \chi_{n;s_1 r_1}^{(2)*} + \chi_{n;s_2 r_2}^{(2)} \chi_{n;s_1 r_1}^{(0)*} \right) = 0. \quad (2.90)$$

The  $(N^2 - 1)$ -plet wave functions are linear combinations of the generators in the fundamental representation; therefore they are traceless. Thus by multiplying eq. (2.90) with  $\delta_{s_2 r_2} \delta_{s_1 r_1}$  and summing over  $s_2, s_1, r_2, r_1$ , the latter part containing the  $(N^2 - 1)$ -plet will vanish, and we obtain  $(C + C^*) = 0$ . Thus, eq. (2.88) simplifies to

$$\sum_{n=1}^{N^2-1} \left( \chi_{n;s_2 r_2}^{(0)} \chi_{n;s_1 r_1}^{(2)*} + \chi_{n;s_2 r_2}^{(2)} \chi_{n;s_1 r_1}^{(0)*} \right) = 0, \quad (2.91)$$

where the sum runs only over the  $(N^2 - 1)$ -plet wave functions. This and the fact that the  $(N^2 - 1)$ -plet states are energetically degenerate allows to simplify drastically the  $Tg^4$  part of

<sup>32</sup>We see that the inter-quark potential is (to lowest order in  $g$ ) proportional to the  $hh$ -propagator.

<sup>33</sup>One should keep in mind that we have set  $E_n(g=0) = 0$ , which is consistent with this normalization.

eq. (2.57), namely

$$\sum_{n=0}^{N^2-1} \left\{ \epsilon_n^{(4)} \chi_{n;s_2r_2}^{(0)} \chi_{n;s_1r_1}^{(0)*} + \epsilon_n^{(2)} \left( \chi_{n;s_2r_2}^{(2)} \chi_{n;s_1r_1}^{(0)*} + \chi_{n;s_2r_2}^{(0)} \chi_{n;s_1r_1}^{(2)*} \right) \right\}. \quad (2.92)$$

We consider the second part of this and decompose it into singlet and  $(N^2 - 1)$ -plet parts

$$\begin{aligned} & \epsilon_{\text{singlet}}^{(2)} \left( \chi_{0;s_2r_2}^{(2)} \chi_{0;s_1r_1}^{(0)*} + \chi_{0;s_2r_2}^{(0)} \chi_{0;s_1r_1}^{(2)*} \right) \\ & + \epsilon_{(N^2-1)\text{-plet}}^{(2)} \sum_{n=1}^{N^2-1} \left( \chi_{n;s_2r_2}^{(2)} \chi_{n;s_1r_1}^{(0)*} + \chi_{n;s_2r_2}^{(0)} \chi_{n;s_1r_1}^{(2)*} \right). \end{aligned} \quad (2.93)$$

But we have shown above that both terms that are multiplied here by energy factors vanish individually, therefore, this part of the  $Tg^4$  part vanishes, and the complete  $Tg^4$  contribution reads now

$$\sum_{n=0}^{N^2-1} \left( \epsilon_n^{(4)} \chi_{n;s_2r_2}^{(0)} \chi_{n;s_1r_1}^{(0)*} \right). \quad (2.94)$$

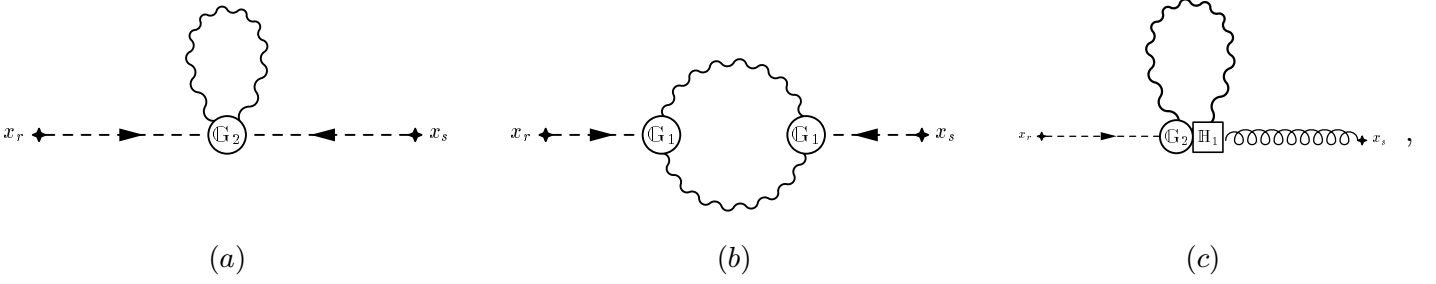
In other words, if the  $T(g^4)$  contribution has the same spin structure as the  $T(g^2)$  contribution, then the singlet and the  $(N^2 - 1)$ -plet energies given in eqs. (2.85, 2.86) are both merely multiplied by a common factor to give the energies up  $\mathcal{O}(g^4)$ .

### 2.2.5 $\mathcal{O}(g^4)$ Contribution

We now turn to the computation of the  $T(g^4)$  part of  $K$ . Its form was already given above in eq. (2.78). When one performs all the derivatives, one realizes that the term containing  $\mathbb{G}_1\mathbb{H}_1$  actually corresponds to two distinct diagrams; fortunately, one of them vanishes, since it contains  $\mathbb{H}_1^{abc} \langle h^b h^c \rangle$  and  $\mathbb{H}_1^{abc}$  is antisymmetric in the colour indices  $b, c$ , but the hh-propagator is symmetric. If one sums up all the identical terms, one ends up with

$$\left[ \begin{aligned} & \delta_{s_2s_1} \delta_{r_2r_1} \\ & - g^2 (\lambda_{s_2s_1}^{a_s} \bar{\lambda}_{r_2r_1}^{a_r}) \langle h_{\mathbf{x}_s}^{a_s} h_{\mathbf{x}_r}^{a_r} \rangle \\ & - g^4 (\lambda_{s_2s_1}^{a_s} \bar{\lambda}_{r_2r_1}^{a_r}) \left\{ \mathbb{G}_2^{abcd} \langle h_{\mathbf{x}_r}^{a_r} \mathbf{A}^a \rangle \langle h_{\mathbf{x}_s}^{a_s} \mathbf{A}^b \rangle \langle \mathbf{A}^c \mathbf{A}^d \rangle \right. \\ & \quad + 18 \mathbb{G}_1^{b_1c_3c_4} \mathbb{G}_1^{b_2b_3b_4} \langle h_{\mathbf{x}_r}^{a_r} \mathbf{A}^{b_1} \rangle \langle h_{\mathbf{x}_s}^{a_s} \mathbf{A}^{b_2} \rangle \langle \mathbf{A}^{b_3} \mathbf{A}^{c_3} \rangle \langle \mathbf{A}^{b_4} \mathbf{A}^{c_4} \rangle \\ & \quad \left. - 12 (\mathbb{G}_1^{dbc} \mathbb{H}_1^{d;ef} \langle h^f \mathbf{A}^b \rangle) (\langle h_{\mathbf{x}_r}^{a_r} h^e \rangle \langle h_{\mathbf{x}_s}^{a_s} \mathbf{A}^c \rangle + \langle h_{\mathbf{x}_s}^{a_s} h^e \rangle \langle h_{\mathbf{x}_r}^{a_r} \mathbf{A}^c \rangle) \right\} \end{aligned} \right]. \quad (2.95)$$

One can also give a diagrammatic representation of the  $\mathcal{O}(g^4)$  contribution to the above expression:



where the propagators are represented by

$\langle h^a h^b \rangle$	$\langle h^a \mathbf{A}^b \rangle$	$\langle \mathbf{A}^a \mathbf{A}^b \rangle$

One can compute now the individual diagrams, which is quite tedious. Also, one is confronted with a subtlety, since the restriction of  $K$  to the lowest  $N^2$  states is valid only in the large- $T$  expansion. One can read off the energies, however, in the construction we've been following so far only if one performs a Taylor expansion in  $T$ . Thus we have to perform, somehow, the large- $T$  limit and at the same time perform a Taylor expansion in  $T$ . This is not so difficult in practice, since in the end, we only want to get rid of terms that are exponentially damped in  $T$ . We do this by replacing  $\sinh(\alpha T)$ ,  $\cosh(\alpha T)$  by  $\frac{1}{2}e^{\alpha T}$  if  $\alpha$  is strictly positive, otherwise we replace them by their definition in terms of exponentials. If one works along these lines, it turns out that all terms that have an exponential dependence on  $T$  are damped, and thus we set them identically to zero. After one has done this, one ends up with integrals that depend on two momenta. If one expands the integrands w.r.t. the ratio of the absolute values of the two momenta involved<sup>34</sup>, one obtains for all three diagrams a result of the structure

$$\frac{-N\delta^{a_s a_r}}{4\pi|\mathbf{x}_s - \mathbf{x}_r|} \times \int \frac{dq}{q}. \quad (2.96)$$

These integrals are obviously UV divergent (which is what we were looking for), but also IR divergent, but this is an artifact of the expansion; one has to introduce an IR cutoff of the same order of magnitude<sup>35</sup> as  $1/|\mathbf{x}_s - \mathbf{x}_r|$ . For definiteness we take the IR cutoff identical to  $1/|\mathbf{x}_s - \mathbf{x}_r|$ . If one adds the three diagrams together (with their respective multiplicities that are given already in eq. (2.95)) one sees that the  $\rho$  dependence (that was introduced artificially in eqs. (2.71), (2.72)) cancels (the diagram involving  $\mathbb{G}_2$  is independent of  $\rho$  whereas the other two have a  $\rho$  dependence of the form  $\rho(1 + \rho)$ ), and one ends up with

$$K_{s_2 r_2; s_1 r_1} = \left[ \delta_{s_2 s_1} \delta_{r_2 r_1} - g^2 T (\lambda_{s_2 s_1}^{a_s} \bar{\lambda}_{r_2 r_1}^{a_r}) \frac{\delta^{a_s a_r}}{4\pi|\mathbf{x}_s - \mathbf{x}_r|} \left\{ 1 + \frac{g^2}{(4\pi)^2} \frac{11N}{3} \ln((\Lambda_{UV}|\mathbf{x}_s - \mathbf{x}_r|)^2) \right\} \right]. \quad (2.97)$$

<sup>34</sup>In fact, one of the diagrams gives such a result after we have dropped the terms exponentially damped in  $T$  without further expansion.

<sup>35</sup>We are only interested in the UV divergence. Thus, we split the integral over the loop momentum into a part where the absolute value of the loop momentum  $q$  is larger than the absolute value of the other momentum (this part will carry the UV divergence) and one where it's smaller. We will drop the latter contribution since it is not UV divergent. We then expand the integrand of the remaining integral in powers of the ratio of the external to the loop momentum, and keep only the leading term. The resulting integral will be IR divergent. However, the expansion is only valid for the loop momentum very much larger than the external momentum. The integral over the external momentum produces the Coulomb potential, since it is of the form  $\int \frac{d^3 p}{(2\pi)^3} e^{i\mathbf{p} \cdot (\mathbf{x}_r - \mathbf{x}_s)} \frac{1}{\mathbf{p}^2}$  and will be dominated by  $|\mathbf{p}| \leq 1/|\mathbf{x}_r - \mathbf{x}_s|$ . Thus, we take as an IR cutoff  $1/|\mathbf{x}_r - \mathbf{x}_s|$  for the loop integral.

Due to the structure of  $K$  when expressed in terms of wave functions and eigenenergies (as indicated above), both the singlet and the  $(N^2 - 1)$ -plet energy are multiplied by the same factor. However, we can also express  $K$  in terms of a renormalized coupling constant, i.e. instead of

$$E_n = g^2 \epsilon^{(2)} + g^4 \epsilon^{(4)} + \dots \quad (2.98)$$

we want to absorb the divergent terms into a renormalized coupling:

$$E_n = g_R^2 \epsilon^{(2)}. \quad (2.99)$$

From this we obtain

$$g_R^2 = g^2 \left( 1 + \frac{g^2}{(4\pi)^2} \frac{11N}{3} \ln \left( (\Lambda_{UV} |\mathbf{x}_s - \mathbf{x}_r|)^2 \right) \right) \quad (2.100)$$

or, if we now express the bare coupling  $g$  in terms of the renormalized one:

$$g^2 = \frac{g_R^2}{1 + \frac{g_R^2}{(4\pi)^2} \frac{11N}{3} \ln \left( (\Lambda_{UV} |\mathbf{x}_s - \mathbf{x}_r|)^2 \right)}, \quad (2.101)$$

which is just what one would expect if  $g_R$  is the renormalized coupling constant at the momentum scale  $\mu = 1/|\mathbf{x}_s - \mathbf{x}_r|$ .

The renormalized coupling is related to the  $\beta$ -function (e.g. [PS95]) as

$$\beta = \mu \frac{\partial g_R}{\partial \mu}, \quad (2.102)$$

where we take the scale  $\mu = 1/|\mathbf{x}_s - \mathbf{x}_r|$ . With this definition the standard one-loop  $\beta$ -function of Yang-Mills theory is reproduced by eq. (2.100):

$$\beta = -\frac{1}{(4\pi)^2} \frac{11N}{3} g_R^3. \quad (2.103)$$

## 2.2.6 Summary

We have seen that one can compute the  $\beta$ -function to lowest order in perturbation theory within the present framework. If one chooses the Weyl gauge, one sees that without a projector, there is no potential between static charges, which however does not come as a surprise since the charges are only coupled via the projector to the Yang-Mills field. Beyond one loop the formalism becomes very tedious, since the number of diagrams explodes due to the non-polynomial action for the projector field. This calculation thus shows how very much more complicated perturbation theory becomes if one includes terms beyond the lowest order. This is interesting since it indicates the order of complexity one is faced with e.g. if one wants to improve the calculation of [KK95].

## 2.3 Mean Field Theory - General Ideas

In this section we will lay the ground for the rest of this chapter. We will start with the most general Gaussian wave functional, interpret the parameters, and demonstrate the important property of factorizability. We will then consider the energy of such a state, and by comparing with the works of Cornwall *et al* [CJT74] will be able to see to which approximation *in field theory* the Gaussian approximation corresponds.

### 2.3.1 Introduction

Whereas the preceding section focused on the Feynman propagation kernel, we now want to return to the main line of thought of this thesis, namely to the usage of *wave functionals*. In the section on the projector as an effective field theory we have already once considered the class of wave functionals that will be the main tool in the rest of this chapter, the class of *Gaussian wave functionals*. For variational calculations it is of course mandatory that we can calculate matrix elements like the expectation value of the Hamiltonian analytically, since these expectation values then depend on the parameters of the wave functional, and may have to be minimized by an appropriate choice of the parameters. If we had to perform e.g. a lattice calculation for evaluation of the matrix elements only (and a new one for every changed parameter set) the situation would be computationally quite hopeless. This fact restricts us in the choice of possible wave functionals to polynomials times Gaussians. As we have seen in the introductory chapter, free field theories have as their ground states Gaussian wave functionals. Thus, the question suggests itself whether the choice of Gaussian wave functionals is physically plausible and not only a mathematical convenience. Kogan and Kovner [KK95] have argued vividly in favour of the physical motivation of a Gaussian ansatz. They argue that in the cases where a Gaussian wave functional was successfully applied (they list self-interacting scalar theories and BCS ground states), the physics is dominated by a single condensate - a situation that apparently is suggested by sum rules also for the case of QCD.

After this motivation for the usage of Gaussian wave functionals we now consider the Gaussians in more detail. The most general Gaussian wave functional is given by (cf. e.g. [KL95])

$$\begin{aligned} \psi[\mathbf{A}] &= \mathcal{N} \exp \left\{ - \left[ \left( \mathbf{A}_i^a(\mathbf{x}) - \bar{\mathbf{A}}_i^a(\mathbf{x}) \right) \left( \frac{1}{4} (G^{-1})_{ij}^{ab}(\mathbf{x}, \mathbf{y}) - i \Sigma_{ij}^{ab}(\mathbf{x}, \mathbf{y}) \right) \left( \mathbf{A}_j^b(\mathbf{y}) - \bar{\mathbf{A}}_j^b(\mathbf{y}) \right) \right] \right\}, \\ &\times \exp \left\{ i \bar{\mathbf{e}}_i^a(\mathbf{x}) \left( \mathbf{A}_i^a(\mathbf{x}) - \bar{\mathbf{A}}_i^a(\mathbf{x}) \right) \right\}, \end{aligned} \quad (2.104)$$

where we have used the Einstein summation convention (cf. app. A.2),  $\mathcal{N}$  is a normalization constant, and all parameters (i.e.  $G^{-1}, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}}$ ) are purely real. We have used a most explicit notation in eq. (2.104), which will often be too clumsy for our purposes. Usually we will combine all the indices (colour-, spatial-, position-) into one super-index, and use the Einstein summation convention also for continuous indices like  $\mathbf{x}$ . In this compact notation, eq. (2.104) reads  $\psi[\mathbf{A}] = \mathcal{N} \exp \left\{ - \left[ (\mathbf{A}_i - \bar{\mathbf{A}}_i) \left( \frac{1}{4} (G^{-1})_{ij} - i \Sigma_{ij} \right) (\mathbf{A}_j - \bar{\mathbf{A}}_j) \right] + i \bar{\mathbf{e}}_i (\mathbf{A}_i - \bar{\mathbf{A}}_i) \right\}$ . The physical interpretation of the parameters becomes clearer if we compute the following expectation values:

$$\langle \mathbf{A}_i^a(\mathbf{x}) \rangle = \bar{\mathbf{A}}_i^a(\mathbf{x}) \quad (2.105)$$

$$\langle \mathbf{\Pi}_i^a(\mathbf{x}) \rangle = \bar{\mathbf{e}}_i^a(\mathbf{x}) \quad (2.106)$$

$$\langle \mathbf{A}_i^a(\mathbf{x}) \mathbf{A}_j^b(\mathbf{y}) \rangle = G_{ij}^{ab}(\mathbf{x}, \mathbf{y}) + \bar{\mathbf{A}}_i^a(\mathbf{x}) \bar{\mathbf{A}}_j^b(\mathbf{y}), \quad (2.107)$$

$$\begin{aligned} \langle \mathbf{\Pi}_i^a(\mathbf{x}) \mathbf{\Pi}_j^b(\mathbf{y}) \rangle &= \frac{1}{4} (G^{-1})_{ij}^{ab}(\mathbf{x}, \mathbf{y}) + 4 \Sigma_{i_1 i_1}^{a c_1}(\mathbf{x}, \mathbf{x}_1) G_{i_1 j_1}^{a_1 b_1}(\mathbf{x}_1, \mathbf{y}_1) \Sigma_{j_1 j}^{b_1 b}(\mathbf{y}_1, \mathbf{y}) \\ &+ \bar{\mathbf{e}}_i^a(\mathbf{x}) \bar{\mathbf{e}}_j^b(\mathbf{y}). \end{aligned} \quad (2.108)$$

Later on, we are frequently going to use the notation  $\langle AB \rangle_c = \langle AB \rangle - \langle A \rangle \langle B \rangle$  to denote the 'connected' part of a matrix element. With this notation, we see that  $G_{ij}^{ab}(\mathbf{x}, \mathbf{y}) = \langle \mathbf{A}_i^a(\mathbf{x}) \mathbf{A}_j^b(\mathbf{y}) \rangle_c$ . We therefore can interpret  $\bar{\mathbf{A}}, \bar{\mathbf{e}}$  as condensates, and  $G$  as equal-time  $\mathbf{A}\mathbf{A}$  correlation function.



The interpretation of  $\Sigma$  is unfortunately not so transparent, but in the formalism of the time-dependent variational principle (where all the parameters of the Gaussian carry an additional time-dependence) we will be able to interpret it as the conjugate momentum to  $G$ , cf. sec.3.2 and e.g. [KL95]. The appearance of apparently finite, non-vanishing expectation values of obviously gauge-dependent operators demonstrates quite clearly<sup>36</sup> the gauge dependence of the wave functionals. One last comment should be made w.r.t. normalizability of the wave functional. We will always assume in the following that the wave functional can be properly normalized, although there are situations where this might not be the case. This occurs when  $G^{-1}$  contains zero modes, i.e. there exist functions  $f_i^a(\mathbf{x})$ , s.t.  $G_{ij}^{-1}f_j = 0$ . Then the integral along the direction spanned by  $f_i^a(\mathbf{x})$  will give a divergent contribution to the path integral and the norm of the state will diverge. Usually, the existence of such zero modes is even required by Gauss' law as we will see in the next section. This will however not be a problem if we consider operators that are not sensitive to these modes, since then the divergences contained in their expectation values will be the same as the divergence of the norm; then we can drop both divergencies, and pretend that we deal with a properly normalized state, but usually a case-by-case analysis is required (see also footnote 36). One could argue that the avoidance of such zero modes is a virtue of the procedure that we will use later on, utilizing so-called deformed states, i.e. states which are not gauge invariant, and thereby regularizing the divergences due to the flat directions associated with gauge invariance; subsequent projection then makes matrix elements independent of the gauge variant parts. This procedure need not be in contradiction to the discussion of footnote 36 due to the following reasons: (a) the projection methods that we are going to use work only if we consider matrix elements of gauge invariant operators. This is different from the cases considered in footnote 36 where the difficulties arose when we considered matrix elements of gauge variant operators. (b) The difficulty with undefined matrix elements arises only (in the  $\mathbf{A}$  representation) for gauge variant field operators, not the conjugate momenta. The latter's matrix elements between gauge invariant states are well-defined, namely zero. If one considers these operators between deformed states, one may obtain non-zero expectation values which then have to be subtracted by a projection procedure.

### 2.3.2 Factorizability

After these general considerations, we now want to come to the statement on factorizability. It seems quite obvious that such a property must exist, since a Gaussian wave functional does not

<sup>36</sup> The comparison with electrodynamics reveals some subtleties in this point: there also one can calculate  $\langle \mathbf{A}_i \mathbf{A}_j \rangle_c = G_{ij}$ . However, the matrix element on the LHS has some *gauge invariant content*, namely  $\langle (\mathbf{P}^T \mathbf{A})_i (\mathbf{P}^T \mathbf{A})_j \rangle_c$  which gives the (non-vanishing) transversal part  $G_{ij}^T$ , whereas the other parts of  $\langle \mathbf{A}_i \mathbf{A}_j \rangle_c$  are indefinite, thus it does not make much sense to consider their gauge transforms: they stay indefinite. Even more subtle is the question of a background field: if one considers the state  $\psi[A] = \mathcal{N} \exp -(A - \bar{A})_i G_{ij}^{-1} (A - \bar{A})_j$  with  $G^{-1}$  transversal, a longitudinal background field is not possible, since  $G_{ij}^{-1} A_j^L = G_{ij}^{-1} \nabla_j \phi = -\nabla_j G_{ij}^{-1} \phi = 0$ . Thus, if the kernel  $G^{-1}$  has zero modes, along these zero modes no background field can exist. This is something one cannot see if one thinks in terms of 'let's add an infinitesimal longitudinal part to the real kernel to avoid divergences and send it to zero later, so that - if we consider normalized states - all infinities can cancel out', since taking the limit 'longitudinal part  $\rightarrow 0$ ' and the integration are not interchangeable, as one can see in the following seemingly trivial example: take the function  $f_\epsilon(x) = \exp(-\epsilon(x - x_0)^2)$ ; one can compute the norm  $N = \int_{-\infty}^{+\infty} f_\epsilon(x) = \sqrt{\pi/\epsilon}$ ; if one now considers the normalized first moment  $\int_{-\infty}^{+\infty} dx x f_\epsilon(x)/N$  for all non-zero  $\epsilon$  this is obviously  $x_0$ , ostensibly independent of  $\epsilon$ . However, for  $\epsilon = 0$ , the integral  $\int_{-\infty}^{+\infty} dx x$  does not exist (since  $\int_{-\infty}^{+\infty} dx |x|$  is ill-defined) as one can see quite simply either by noting that  $0 = \int_{-\infty}^{+\infty} dx x = \int_{-\infty}^{+\infty} dx (x + x_0) = x_0 \times \infty$ , or, if one uses a cut-off procedure to make the integral finite, by noting that the value that the integral gives depends on the way the integral is cut off:  $\lim_{\Lambda \rightarrow \infty} \int_{-\Lambda+a}^{\Lambda} dx x / \int_{-\Lambda+a}^{\Lambda} dx = a/2$ .

contain information about higher correlations than those of two  $\mathbf{A}$  operators. Thus every higher correlation function must factorize into expectation values of one or two  $\mathbf{A}$  operators. Formally this can be seen as follows: first compute<sup>37</sup>

$$\langle e^{ij_i \mathbf{A}_i} \rangle = e^{ij_i \bar{\mathbf{A}}_i} e^{-\frac{1}{2} j_i G_{ij} j_j}. \quad (2.109)$$

Now consider

$$\begin{aligned} \langle (\mathbf{A}_{i_1} - \bar{\mathbf{A}}_{i_1}) \cdots (\mathbf{A}_{i_n} - \bar{\mathbf{A}}_{i_n}) \rangle &= \left( \frac{1}{i} \frac{\delta}{\delta j_{i_1}} \right) \cdots \left( \frac{1}{i} \frac{\delta}{\delta j_{i_n}} \right) \langle e^{ij_i (\mathbf{A}_i - \bar{\mathbf{A}}_i)} \rangle \Big|_{j=0} \\ &= \left( \frac{1}{i} \frac{\delta}{\delta j_{i_1}} \right) \cdots \left( \frac{1}{i} \frac{\delta}{\delta j_{i_n}} \right) e^{-\frac{1}{2} j_i G_{ij} j_j} \Big|_{j=0} \\ &= \left( \frac{1}{i} \frac{\delta}{\delta j_{i_1}} \right) \cdots \left( \frac{1}{i} \frac{\delta}{\delta j_{i_{n-2}}} \right) (G_{i_{n-1} i_n} - G_{i_{n-1} k} j_k G_{i_n l} j_l) e^{-\frac{1}{2} j_i G_{ij} j_j} \Big|_{j=0} \\ &= \langle (\mathbf{A}_{i_1} - \bar{\mathbf{A}}_{i_1}) \cdots (\mathbf{A}_{i_{n-2}} - \bar{\mathbf{A}}_{i_{n-2}}) \rangle \langle (\mathbf{A}_{i_{n-1}} - \bar{\mathbf{A}}_{i_{n-1}}) (\mathbf{A}_{i_n} - \bar{\mathbf{A}}_{i_n}) \rangle \\ &\quad - G_{i_{n-1} k} G_{i_n l} \left( \frac{1}{i} \frac{\delta}{\delta j_{i_1}} \right) \cdots \left( \frac{1}{i} \frac{\delta}{\delta j_{i_{n-2}}} \right) j_k j_l e^{-\frac{1}{2} j_i G_{ij} j_j} \Big|_{j=0}. \end{aligned}$$

The last line can be quite easily evaluated, by noting that the only non-vanishing contributions will stem from terms, where two derivatives annihilate both  $j_k$  and  $j_l$ , thus leaving only  $n - 4$  derivatives to act upon the exponential function. The minus sign will be cancelled by the fact that  $\left( \frac{1}{i} \frac{\delta}{\delta j_i} \right) \left( \frac{1}{i} \frac{\delta}{\delta j_j} \right) j_k j_l = -\delta_{ik} \delta_{jl}$ . The derivatives that are used to cancel  $j_k j_l$  can obviously act no more onto the exponential, thus we obtain

$$\begin{aligned} &-G_{i_{n-1} k} G_{i_n l} \left( \frac{1}{i} \frac{\delta}{\delta j_{i_1}} \right) \cdots \left( \frac{1}{i} \frac{\delta}{\delta j_{i_{n-2}}} \right) j_k j_l e^{-\frac{1}{2} j_i G_{ij} j_j} \Big|_{j=0} \\ &= \sum_{\substack{k, l = i_1 \\ k \neq l}}^{i_{n-2}} G_{i_{n-1} k} G_{i_n l} \langle (\mathbf{A}_{i_1} - \bar{\mathbf{A}}_{i_1}) \cdots (\mathbf{A}_k - \bar{\mathbf{A}}_k) \cdots (\mathbf{A}_l - \bar{\mathbf{A}}_l) \cdots (\mathbf{A}_{i_{n-2}} - \bar{\mathbf{A}}_{i_{n-2}}) \rangle, \end{aligned}$$

where we have used the notation  $\mathbf{A}$  to indicate that this particular  $\mathbf{A}$  should not be contained in the correlation function. We have thus constructed a recursion relation whereby an expectation value of  $n$   $\mathbf{A}$  operators is expressed as a product of a two- $\mathbf{A}$  expectation value times an  $(n-2)$ - $\mathbf{A}$  expectation value plus a sum of products of two two- $\mathbf{A}$  expectation values times an  $(n-4)$ - $\mathbf{A}$  expectation value. Thus, in the end, everything will be reduced to two- $\mathbf{A}$  expectation values just as claimed above. Note that, since  $\langle \mathbf{A} - \bar{\mathbf{A}} \rangle = 0$ , every expectation value of an odd number of factors  $(\mathbf{A} - \bar{\mathbf{A}})$  will be zero.

### 2.3.3 Comparison with Other Approximations

The interpretation of the usage of Gaussian trial wave functionals as an approximation equivalent to the Hartree (or Hartree-Fock) approximation can be justified on several grounds: the first is the property illustrated above, namely that expectation values of products of field operators factorize into expectation values of one or two field operators. The second reason lies in the fact that one can construct in a simple manner creation and annihilation operators, and formulate

<sup>37</sup>The fact that one can give a closed expression for the expectation value of  $e^{ij_i \mathbf{A}_i}$  already very strongly points to the factorizability property.

the (generalized) Random Phase Approximation very similarly to the construction in nuclear physics. This we will do in Chapter 3. The most direct connection, however, is found in the works of [CJT74]. The authors considered a generalization of the effective action which was constructed as a double Legendre transform of the vacuum persistence amplitude  $W$  in the presence of a one-particle- and a two-particle source:

$$e^{iW[J,K]} = \int \mathcal{D}\phi e^{iI[\phi] + \int d^4x J(x)\phi(x) + \frac{1}{2} \int d^4x d^4y \phi(x)K(x,y)\phi(y)}. \quad (2.110)$$

In the following  $\phi$  denotes a generic field. The theory is then specified via the classical action  $I[\phi]$ . Defining

$$\frac{\delta W}{\delta J(x)} = \bar{\phi}(x) \quad \text{and} \quad \frac{\delta W}{\delta K(x,y)} = \bar{\phi}(x)\bar{\phi}(y) + G(x,y) \quad (2.111)$$

one obtains the generalized effective action as

$$\Gamma[\bar{\phi}, G] = W[J, K] - \int d^4x J(x)\bar{\phi}(x) - \frac{1}{2} \int d^4x d^4y \bar{\phi}(x)K(x,y)\bar{\phi}(y) - \frac{1}{2} \int d^4x d^4y G(x,y)K(y,x). \quad (2.112)$$

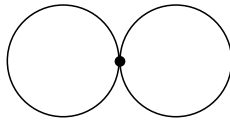
By the nature of the Legendre transforms, eqs. (2.111) imply corresponding equations for derivatives of  $\Gamma$ :

$$\frac{\delta \Gamma}{\delta \bar{\phi}(x)} = -J(x) - \int d^4y K(x,y)J(y) \quad \text{and} \quad \frac{\delta \Gamma}{\delta G(x,y)} = -\frac{1}{2}K(x,y). \quad (2.113)$$

Thus, for vanishing external sources, the effective action is stationary under variations of  $\bar{\phi}$  and  $G$ . Since for  $K = 0$ , this generalized effective action is the same as the ordinary effective action, we can also say that  $\Gamma[\bar{\phi}, G_0]$  (where  $G_0$  is a solution of  $\delta\Gamma/\delta G = 0$ ) is identical to the ordinary effective action, and  $G_0$  is the full  $\phi$  propagator. Since  $\Gamma[\bar{\phi}, G]$  is the generating functional for all two-particle irreducible graphs, one can construct a series representation for the generalized effective action that is given as

$$\Gamma[\bar{\phi}, G] = I(\bar{\phi}) + \frac{i}{2} \text{Tr}(\ln(DG^{-1})) + \frac{i}{2} \text{Tr}(\ln(\mathcal{D}^{-1}G)) + \Gamma_2[\bar{\phi}, G] + \text{const}, \quad (2.114)$$

where  $i\mathcal{D}^{-1}(\bar{\phi}; x, y) = \frac{\delta^2 I(\bar{\phi})}{\delta \bar{\phi}(x)\delta \bar{\phi}(y)} = iD^{-1}(x-y) + \frac{\delta^2 I_{int}(\bar{\phi})}{\delta \bar{\phi}(x)\delta \bar{\phi}(y)}$ .  $D(x-y)$  is the free propagator of  $\phi$  that results from the part of  $I[\phi]$  that is quadratic in  $\phi$ .  $I_{int}[\phi]$  is that part of  $I[\phi]$  that is at least cubic in  $\phi$ .  $\Gamma_2$  has a diagrammatic representation: one starts from the classical action  $I(\phi)$ , and replaces  $\phi$  by  $\phi + \bar{\phi}$ . This action has terms that are cubic or of higher order in  $\phi$ ; they define the new ( $\bar{\phi}$  dependent) vertices. The graphs that constitute  $\Gamma_2$  are the two-particle irreducible vacuum graphs constructed from these vertices and  $G$  as the propagator that connects these vertices. The Hartree-Fock<sup>38</sup> approximation consists of taking the contribution to  $\Gamma_2$  that is of lowest order in the coupling constant; in  $\phi^4$  theory, this would be the 'double-bubble':



<sup>38</sup>This name is used in [CJT74] also for bosonic theories like scalar  $\phi^4$  theories.

We can now draw the connection to the Rayleigh-Ritz calculation with Gaussian wave functionals. If we consider the static generalized effective action<sup>39</sup>, we can show with an argument quite similar to the one we used when drawing the connection between the time-dependent variational principle and the (ordinary) effective action in sec. 1.5.3, that

$$\Gamma[\phi, G]|_{static} = -E[\phi, G] \int dt \quad (2.115)$$

where  $\int dt$  denotes the time during which action is accumulated, and  $E[\phi, G]$  is the minimum of the expectation value of the Hamiltonian corresponding to  $I[\phi]$ , where the (normalized) states are constrained to

$$\langle \phi(\mathbf{x}) \rangle = \bar{\phi}(\mathbf{x}), \quad (2.116)$$

$$\langle \phi(\mathbf{x})\phi(\mathbf{y}) \rangle = \bar{\phi}(\mathbf{x})\bar{\phi}(\mathbf{y}) + \tilde{G}(\mathbf{x}, \mathbf{y}), \quad (2.117)$$

where  $\tilde{G}(\mathbf{x}, \mathbf{y}) = G(x_0 - y_0 = 0; \mathbf{x}, \mathbf{y})$ , and where the operators  $\phi(\mathbf{x})$  are taken at some fixed time. After this identification is made, one can compare the result of an approximation to  $\Gamma|_{static}$  with the result of a restriction of the space of test wave functionals. The comparison will be made using the expressions for the energy that one obtains in both cases. The authors of [CJT74] computed the static effective action in the Hartree-Fock approximation by retaining from the two-particle irreducible graphs only the double-bubble, and via the identification given in eq. (2.115) they then computed the energy for the example of a one-component scalar field with a  $\phi^4$  interaction. On the other hand, they computed the expectation value of the Hamiltonian between Gaussian states that were constructed to reproduce eqs. (2.116, 2.117). The expressions obtained for the energy are precisely the same. Here the fact that  $\Gamma|_{static}$  gives already the lowest possible energy under the constraints eqs. (2.116, 2.117) is no restriction since those parameters are the only variational parameters in the Gaussian, and they have not been varied up to now, but are simply prescribed. We thus see that at least for this theory the Hartree-Fock approximation and the restriction to Gaussian states are identical in their content, since the parameters available have identical interpretations and the equations that determine the parameters are identical as well.

### 2.3.4 Energy Expectation Value

Later on it will be useful in several instances to have the expectation value of the Hamiltonian at hand. For the case of Yang-Mills theory, it is most easily computed between Gaussian states if we (instead of evaluating  $H$  between states with  $\langle \mathbf{A} \rangle = \bar{\mathbf{A}}$ ) shift  $\mathbf{A} \rightarrow \bar{\mathbf{A}} + \mathbf{a}$  (with  $\langle \mathbf{a} \rangle = 0$  and  $\langle \mathbf{a}_i \mathbf{a}_j \rangle = G_{ij}$ ). This technique we will use quite often in the following. In contrast to the introduction, we will now use 'perturbative scaling' as defined in appendix A.5; however, we will use a slight modification since we don't want the background field to be decoupled in the perturbative limit. Therefore, we rescale  $\bar{\mathbf{A}}$  by a factor of  $\frac{1}{g}$ ; thus, in the end, the replacement reads<sup>40</sup>

$$\mathbf{A} \rightarrow \frac{1}{g} \bar{\mathbf{A}} + \mathbf{a}. \quad (2.118)$$

<sup>39</sup>Static means the following here:  $\bar{\phi}$  is taken to be time-independent, and  $G$  is taken to be translationally invariant. In order to obtain the static generalized effective action, one has to express  $G(x_0 - y_0; \mathbf{x}, \mathbf{y})$  in terms of  $\tilde{G}(\mathbf{x}, \mathbf{y}) = G(x_0 - y_0 = 0; \mathbf{x}, \mathbf{y})$ ;  $\Gamma$  expressed in terms of these time-independent quantities  $\bar{\phi}, \tilde{G}$  is then dubbed the static generalized effective action.

<sup>40</sup>This procedure is obviously identical to using the non-perturbative scaling from the outset, and then replacing  $\mathbf{A} \rightarrow \bar{\mathbf{A}} + g\mathbf{a}$ .

The kinetic energy is given in this case by

$$T = \frac{1}{2} \int d^3x \Pi_i^a(\mathbf{x}) \Pi_i^a(\mathbf{x}) = -\frac{1}{2} \int d^3x \left\{ \frac{\delta^2}{\delta \mathbf{a}_i^a(\mathbf{x}) \delta \mathbf{a}_i^a(\mathbf{x})} \right\}, \quad (2.119)$$

whereas the potential is given by

$$V = \int d^3x \mathbf{B}_i^a \left[ \frac{1}{g} \bar{\mathbf{A}} + \mathbf{a} \right](\mathbf{x}) \mathbf{B}_i^a \left[ \frac{1}{g} \bar{\mathbf{A}} + \mathbf{a} \right](\mathbf{x}). \quad (2.120)$$

The expectation value of the kinetic energy follows straightforwardly from eq. (2.108),

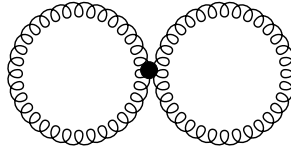
$$\langle T \rangle = \frac{1}{2} \int d^3x \{ \bar{\mathbf{e}}_i^a(\mathbf{x}) \bar{\mathbf{e}}_i^a(\mathbf{x}) \} + \frac{1}{8} \text{Tr}(G^{-1}) + 2 \text{Tr}(\Sigma G \Sigma), \quad (2.121)$$

where the trace  $\text{Tr}$  is to be taken over spatial, colour and position indices. The potential is a bit harder to evaluate, but eventually we end up with<sup>41</sup>

$$\begin{aligned} \langle V \rangle = \frac{1}{2} \int d^3x \left\{ \frac{1}{g^2} \bar{\mathbf{B}}_i^a(\mathbf{x}) \bar{\mathbf{B}}_i^a(\mathbf{x}) + \text{tr} \left( (\hat{\mathbf{D}} \hat{\mathbf{D}} - \hat{\mathbf{B}}) G_{\mathbf{xy}} \right) \Big|_{\mathbf{y} \rightarrow \mathbf{x}} \right. \\ \left. + \frac{g^2}{2} \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}} S_i \hat{T}^a G_{\mathbf{xx}}) + \frac{g^2}{4} \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}}) \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}}) \right\}, \quad (2.122) \end{aligned}$$

where we have used the notation  $(S_i)_{jk} = \epsilon_{jik}$ ,  $(\hat{T}^a)^{bc} = f^{bac}$ ,  $\hat{\mathbf{D}}_{jk}^{ab} = (S_i)_{jk} \hat{\mathbf{D}}_i^{ab}$ ,  $\hat{\mathbf{B}}_{jk}^{bc} = (S_i)_{jk} (\hat{T}^a)^{bc} \bar{\mathbf{B}}_i^a$ , and  $\bar{\mathbf{B}} = \mathbf{B}[\bar{\mathbf{A}}]$ . The symbol 'tr' denotes here a trace both over colour and spatial indices, but not over position indices.

We see explicitly the two double bubble terms in the second line of eq. (2.122),



which are of different origin: the first one stems from the four-gluon vertex, whereas the second one results from two three-gluon-vertices. This is reflected in the different distribution of traces for colour and spatial indices.

In the remainder of this section and in the next section we will ignore the fact that our wave functionals should satisfy Gauss' law. This will allow us later on to compare the effects of the projector and its approximations to this naïve treatment. We see from eq. (2.121) that the expectation value of the Yang-Mills Hamiltonian is quadratic both in  $\bar{\mathbf{e}}$  and in  $\Sigma$ . Thus, minimizing the energy will result in  $\bar{\mathbf{e}}$  and  $\Sigma$  vanishing. Physically this is understandable, since if one considers static situations (as we do when we consider the Rayleigh-Ritz principle, and look for energy minima) one would classically expect zero kinetic energy, and the tribute that has to be paid to the uncertainty principle has to be raised via  $G$  alone, since this is the only parameter that also appears in the potential; thus we end up with  $\bar{\mathbf{e}} = \Sigma = 0$  at the stationary

<sup>41</sup>This result can also be found in [KV89].

point<sup>42</sup>. Now this has an interesting consequence. If we consider  $\langle \Gamma^a(\mathbf{x}) \rangle$ , we can compute this expectation value easily:

$$\langle \Gamma^a(\mathbf{x}) \rangle = \hat{\mathbf{D}}_i^{ab}(\mathbf{x}) \bar{\mathbf{e}}_i^b(\mathbf{x}) + 2g \int d^3y \operatorname{tr}(\hat{T}^a \Sigma_{\mathbf{xy}} G_{\mathbf{yx}}). \quad (2.123)$$

We see therefore that at the stationary point w.r.t.  $\bar{\mathbf{e}}$  and  $\Sigma$  the expectation value of  $\Gamma^a(\mathbf{x})$  is *automatically zero* even though the wave functional itself is by no means gauge invariant.

### 2.3.5 Equations of Motion

In this section, we want to discuss shortly the solution of the equation of motion for  $G^{-1}$  in the perturbative limit. This will be useful for the considerations to be taken later on; we will for the time being not solve the equations for  $\bar{\mathbf{A}}$ . The special case of a quasi-Abelian  $\bar{\mathbf{A}}$  that leads to a constant magnetic field will be discussed in section 2.7. In the perturbative limit, we neglect the  $\mathcal{O}(g^2)$  terms in the potential energy, so that we end up with<sup>43,44</sup>

$$E[G, \bar{\mathbf{A}}] = \frac{1}{8} \operatorname{Tr}(G^{-1}) + \frac{1}{2} \int d^3x \left\{ \operatorname{tr} \left( (\hat{\mathbf{D}}\hat{\mathbf{D}} - \hat{\mathbf{B}}) G_{\mathbf{xy}} \right) \Big|_{\mathbf{y} \rightarrow \mathbf{x}} \right\} + \frac{1}{2g^2} \int d^3x \bar{\mathbf{B}}_i^a(\mathbf{x}) \bar{\mathbf{B}}_i^a(\mathbf{x}). \quad (2.124)$$

One should once again emphasize that in writing down this expression, we have assumed that both  $G^{-1}$  and  $G$  exist. When performing the variation of  $E$  w.r.t.  $G$ , we need for the kinetic term the relation

$$\frac{\delta}{\delta G_{i_1 i_2}^{a_1 a_2}(\mathbf{z}_1, \mathbf{z}_2)} \operatorname{Tr}(G^{-1}) = -(G^{-1} G^{-1})_{i_1 i_2}^{a_1 a_2}(\mathbf{z}_1, \mathbf{z}_2) \quad (2.125)$$

and the contribution from the potential energy can be written as (since  $(\hat{\mathbf{D}}\hat{\mathbf{D}} - \hat{\mathbf{B}})$  is symmetric)

$$\frac{\delta \langle V \rangle}{\delta G_{i_1 i_2}^{a_1 a_2}(\mathbf{z}_1, \mathbf{z}_2)} = \frac{1}{2} \int d^3x \delta_{\mathbf{xz}_1} (\hat{\mathbf{D}}\hat{\mathbf{D}} - \hat{\mathbf{B}})_{i_1 i_2}^{a_1 a_2} \delta_{\mathbf{xz}_2}. \quad (2.126)$$

If we consider  $(G^{-1})_{i_1 i_2}^{a_1 a_2}(\mathbf{z}_1, \mathbf{z}_2)$  as the matrix elements of an operator<sup>45</sup>  $\mathbb{G}^{-1}$ , s.t.

$$\langle \mathbf{z}_1; i_1, a_1 | \mathbb{G}^{-1} | \mathbf{z}_2; i_2, a_2 \rangle = (G^{-1})_{i_1 i_2}^{a_1 a_2}(\mathbf{z}_1, \mathbf{z}_2), \quad (2.127)$$

and similarly the RHS of eq. (2.126) as

$$\int d^3x \delta_{\mathbf{xz}_1} (\hat{\mathbf{D}}\hat{\mathbf{D}} - \hat{\mathbf{B}}) \delta_{\mathbf{xz}_2} = \langle \mathbf{z}_1; i_1, a_1 | \hat{\mathbb{D}}\hat{\mathbb{D}} - \hat{\mathbb{B}} \int d^3x | \mathbf{x} \rangle \langle \mathbf{x} | \mathbf{z}_2; i_2, a_2 \rangle, \quad (2.128)$$

then one can write the variational equation that results from eqs. (2.125, 2.126) as a simple operator equation

$$\mathbb{G}^{-1} \mathbb{G}^{-1} = 4(\hat{\mathbb{D}}\hat{\mathbb{D}} - \hat{\mathbb{B}}). \quad (2.129)$$

<sup>42</sup>If one inserts  $\Sigma = 0$  and  $\bar{\mathbf{e}} = 0$  into  $\langle H \rangle = \langle T + V \rangle$ , one ends up with the expectation value of the energy considered by [KV89].

<sup>43</sup>We have also set  $\bar{\mathbf{e}} = \Sigma = 0$  as discussed above.

<sup>44</sup>Taking into account the  $\mathcal{O}(g^2)$  terms in the potential energy will complicate matters, e.g. since in the equations of motion for  $G$ , i.e.  $\delta E / \delta G = 0$ ,  $G_{\mathbf{xx}}$  will appear which is usually a divergent quantity and thus necessitates considerations of regularization and renormalization already at this point.

<sup>45</sup>This useful notion can be found e.g. in [KV89].

This in turn can be inserted into the equation for the energy

$$E[\bar{\mathbf{A}}] = \frac{1}{8}\text{Tr}(G^{-1}) + \frac{1}{2}\text{Tr}\left(\underbrace{(\hat{\mathbf{D}}\hat{\mathbf{D}} - \hat{\mathbf{B}})}_{\frac{1}{4}G^{-1}G^{-1}}\right)G + \frac{1}{2g^2} \int d^3x \bar{\mathbf{B}}_i^a(\mathbf{x})\bar{\mathbf{B}}_i^a(\mathbf{x}) \quad (2.130)$$

resulting in<sup>46</sup>

$$E[\bar{\mathbf{A}}] = \frac{1}{4}\text{Tr}(G^{-1}) + \frac{1}{2g^2} \int d^3x \bar{\mathbf{B}}_i^a(\mathbf{x})\bar{\mathbf{B}}_i^a(\mathbf{x}) = \frac{1}{2}\text{Tr}\left((\hat{\mathbf{D}}\hat{\mathbf{D}} - \hat{\mathbf{B}})^{\frac{1}{2}}\right) + \frac{1}{2g^2} \int d^3x \bar{\mathbf{B}}_i^a(\mathbf{x})\bar{\mathbf{B}}_i^a(\mathbf{x}), \quad (2.131)$$

which is now a functional of  $\bar{\mathbf{A}}$  alone. One word of caution has to be said at this point: whereas the last expression for the energy is perfectly well-defined, regardless of whether  $M = \hat{\mathbf{D}}\hat{\mathbf{D}} - \hat{\mathbf{B}}$  contains zero modes or not, this is not so straightforward for the intermediate steps. Assume that  $M$  does contain zero modes<sup>47</sup>, then  $G^{-1}$  also contains zero modes, and along those directions,  $G$  is infinite. For the energy this does not matter, since this infinity is cancelled by the zero mode of  $M$ ; however, for other operators that do not contain a zero mode in this direction, the infinity will become important, as we will see below. The problem can, to some extent, be cured if we use a projector, cf. sec. 2.6.

## 2.4 Requirements for Perturbative Satisfaction of Gauss' Law

In this section we try to modify a pure Gaussian wave functional by multiplying it with a polynomial, s.t. it is annihilated by the Gauss law operator  $\Gamma^a$  to a given order in  $g$ . It turns out that one can indeed construct a recursion relation, s.t. the coefficients needed for a given order in  $g$  depend only on the Gaussian and the coefficients needed for lower orders. Unfortunately, the construction works only in a part of the space of gauge field configurations, so that we have to use a background gauge condition, and even then some problems remain.

In this section we want to address the following problem: assume that we start with a wave functional that has Gaussian form. Since this wave functional is not annihilated by the Gauss law operator  $\Gamma^a(\mathbf{x})$  we multiply it by a polynomial. How do we have to fix the coefficients of the polynomial s.t. Gauss' law is satisfied to a given order in the coupling constant  $g$  [Cea88]? In order to proceed, we have to use the same procedure as in sec. 2.3.4: start out from 'perturbative scaling', and then rescale  $\bar{\mathbf{A}}$  by  $1/g$  so that the background field does not decouple in the perturbative limit. The covariant derivative can then be split into a part containing the background field (which is completely of  $\mathcal{O}(g^0)$ ) and a part that contains the fluctuation part and an explicit factor of  $g$ :

$$\hat{\mathbf{D}}_i^{ab}(\mathbf{x}) = \hat{\mathbf{D}}_i^{ab}(\mathbf{x}) - gf^{acb}\mathbf{a}_i^c(\mathbf{x}) \quad \text{with} \quad \hat{\mathbf{D}}_i^{ab}(\mathbf{x}) = \nabla_i\delta^{ab} - f^{acb}\bar{\mathbf{A}}_i^c(\mathbf{x}) \quad (2.132)$$

Thus the Gauss law operator reads

$$\Gamma^a(\mathbf{x}) = \hat{\mathbf{D}}_i^{ab}(\mathbf{x})\frac{1}{i}\frac{\delta}{\delta\mathbf{a}_i^b(\mathbf{x})} = \frac{1}{i}\hat{\mathbf{D}}_i^{ab}(\mathbf{x})\frac{\delta}{\delta\mathbf{a}_i^b(\mathbf{x})} - gf^{acb}\mathbf{a}_i^c(\mathbf{x})\frac{1}{i}\frac{\delta}{\delta\mathbf{a}_i^b(\mathbf{x})}. \quad (2.133)$$

The wave functional is of the form

$$\Psi = P(\mathbf{a})e^{-\frac{1}{2}\mathbf{a}K\mathbf{a}+i\bar{\mathbf{e}}\cdot\mathbf{a}}, \quad (2.134)$$

<sup>46</sup>A similar result was obtained in [KV89].

<sup>47</sup>It will if  $\bar{\mathbf{A}}$  fulfils the classical equations of motion, but more on that in sec. 2.6.

where we have used a (hopefully) obvious shorthand notation together with the abbreviation<sup>48</sup>  $K = \frac{1}{2}G^{-1} - 2i\Sigma$ , and  $P(\mathbf{a})$  indicates a power series in  $g$ :

$$P(\mathbf{a}) = \sum_{n=0}^{\infty} g^n P^{(n)}(\mathbf{a}). \quad (2.135)$$

If we now require

$$\Gamma^a(\mathbf{x})\Psi = 0 + \mathcal{O}(g^{N+1}) \quad (2.136)$$

we obtain a recursion relation between the different  $P^{(n)}$ s:

$$\begin{aligned} 0 = & \sum_{n=0}^N g^n (\hat{\mathbf{D}}_i^{ab} ((-K\mathbf{a})_i^b + i\bar{\mathbf{e}}_i^b) P^{(n)}) - \sum_{n=1}^N g^n \mathbf{a}_i^c (\hat{T}^c)^{ab} ((-K\mathbf{a})_i^b + i\bar{\mathbf{e}}_i^b) P^{(n-1)} \\ & + \sum_{n=1}^N g^n \hat{\mathbf{D}}_i^{ab} \frac{\delta P^{(n)}}{\delta \mathbf{a}_i^b} - \sum_{n=2}^N g^n \mathbf{a}_i^c (\hat{T}^c)^{ab} \frac{\delta P^{(n-1)}}{\delta \mathbf{a}_i^b} = 0, \end{aligned} \quad (2.137)$$

where it is sufficient to terminate the sums at  $n = N$  since we require Gauss' law only up to  $\mathcal{O}(g^N)$ . Note that the summation indices start at different lower values. Thus we study the  $\mathcal{O}(g^0)$  and  $\mathcal{O}(g^1)$  cases separately<sup>49</sup>:

$$\mathcal{O}(g^0): \quad \hat{\mathbf{D}}_i^{ab} ((-K\mathbf{a})_i^b + i\bar{\mathbf{e}}_i^b) = 0. \quad (2.138)$$

Since this equation has to be valid for all  $\mathbf{a}$ , one actually obtains two conditions<sup>50</sup>:

$$\boxed{\begin{aligned} \hat{\mathbf{D}}K &= 0 \\ \hat{\mathbf{D}}\bar{\mathbf{e}} &= 0. \end{aligned}} \quad (2.139)$$

We will meet these conditions later on again in section 2.6 on the Kamlah expansion. If these conditions are satisfied, eq.(2.137) will simplify, since the first term vanishes exactly:

$$- \sum_{n=1}^N g^n \mathbf{a}_i^c (\hat{T}^c)^{ab} ((-K\mathbf{a})_i^b + i\bar{\mathbf{e}}_i^b) P^{(n-1)} + \sum_{n=1}^N g^n \hat{\mathbf{D}}_i^{ab} \frac{\delta P^{(n)}}{\delta \mathbf{a}_i^b} - \sum_{n=2}^N g^n \mathbf{a}_i^c (\hat{T}^c)^{ab} \frac{\delta P^{(n-1)}}{\delta \mathbf{a}_i^b} = 0. \quad (2.140)$$

The  $\mathcal{O}(g^1)$  case is still special, since only the first two terms contribute:

$$\hat{\mathbf{D}}_i^{ab} \frac{\delta P^{(1)}}{\delta \mathbf{a}_i^b} = \mathbf{a}_i^c (\hat{T}^c)^{ab} ((-K\mathbf{a})_i^b + i\bar{\mathbf{e}}_i^b). \quad (2.141)$$

The solution to this is given by<sup>51</sup>

$$\begin{aligned} P^{(1)}[\mathbf{a}] &= \frac{1}{2!} \int d^3x_1 d^3x_2 \chi_{i_1 i_2}^{a_1 a_2}(\mathbf{x}_1, \mathbf{x}_2) \mathbf{a}_{i_1}^{a_1}(\mathbf{x}_1) \mathbf{a}_{i_2}^{a_2}(\mathbf{x}_2) \\ &\quad - \frac{1}{3!} \int d^3x_1 d^3x_2 d^3x_3 \chi_{i_1 i_2 i_3}^{a_1 a_2 a_3}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \mathbf{a}_{i_1}^{a_1}(\mathbf{x}_1) \mathbf{a}_{i_2}^{a_2}(\mathbf{x}_2) \mathbf{a}_{i_3}^{a_3}(\mathbf{x}_3) \end{aligned} \quad (2.142)$$

<sup>48</sup>The usage of this abbreviation will be restricted to this section.

<sup>49</sup>We set  $P^{(0)} = 1$ , since in the end it will be fixed by the overall normalization anyway; it has to be nonzero, s.t. the state can be normalized as  $g \rightarrow 0$ .

<sup>50</sup>Note the similarity with the QED condition of having a purely transversal kernel. Note also that  $\hat{\mathbf{D}}$  does not mix real and imaginary parts, and thus  $\hat{\mathbf{D}}K = 0$  implies both  $\hat{\mathbf{D}}G^{-1} = 0$  and  $\hat{\mathbf{D}}\Sigma = 0$ .

<sup>51</sup>The solution with  $\bar{\mathbf{e}} = 0$  was provided by [Lae01].



with

$$\begin{aligned}\chi_{i_1 i_2}^{a_1 a_2}(\mathbf{x}_1, \mathbf{x}_2) &= i \left( \frac{a_1}{i_1} [\hat{\mathbf{D}}_{\mathbf{x}_1} G_{\mathbf{x}_1 \mathbf{x}_2} \hat{T}^{a_2} \bar{\mathbf{e}}_{\mathbf{x}_2}]_{i_2} + \frac{a_2}{i_2} [\hat{\mathbf{D}}_{\mathbf{x}_2} G_{\mathbf{x}_2 \mathbf{x}_1} \hat{T}^{a_1} \bar{\mathbf{e}}_{\mathbf{x}_1}]_{i_1} \right), \\ \chi_{i_1 i_2 i_3}^{a_1 a_2 a_3}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) &= \frac{a_1}{i_1} [\hat{\mathbf{D}}_{\mathbf{x}_1} G_{\mathbf{x}_1 \mathbf{x}_2} \hat{T}^{a_2} K_{\mathbf{x}_2 \mathbf{x}_3}^{i_2}]_{i_3}^{a_3} + \frac{a_1}{i_1} [\hat{\mathbf{D}}_{\mathbf{x}_1} G_{\mathbf{x}_1 \mathbf{x}_3} \hat{T}^{a_3} K_{\mathbf{x}_3 \mathbf{x}_2}^{i_3}]_{i_2}^{a_2} \\ &+ \frac{a_2}{i_2} [\hat{\mathbf{D}}_{\mathbf{x}_2} G_{\mathbf{x}_2 \mathbf{x}_1} \hat{T}^{a_1} K_{\mathbf{x}_1 \mathbf{x}_3}^{i_1}]_{i_3}^{a_3} + \frac{a_2}{i_2} [\hat{\mathbf{D}}_{\mathbf{x}_2} G_{\mathbf{x}_2 \mathbf{x}_3} \hat{T}^{a_3} K_{\mathbf{x}_3 \mathbf{x}_1}^{i_3}]_{i_1}^{a_1} \\ &+ \frac{a_3}{i_3} [\hat{\mathbf{D}}_{\mathbf{x}_3} G_{\mathbf{x}_3 \mathbf{x}_1} \hat{T}^{a_1} K_{\mathbf{x}_1 \mathbf{x}_2}^{i_1}]_{i_2}^{a_2} + \frac{a_1}{i_1} [\hat{\mathbf{D}}_{\mathbf{x}_1} G_{\mathbf{x}_1 \mathbf{x}_2} \hat{T}^{a_2} K_{\mathbf{x}_2 \mathbf{x}_3}^{i_2}]_{i_3}^{a_3},\end{aligned}\tag{2.143}$$

$$(2.144)$$

where the following abbreviations have been used

$$\frac{a_1}{i_1} [\hat{\mathbf{D}}_{\mathbf{x}_1} G_{\mathbf{x}_1 \mathbf{x}_2} \hat{T}^{a_2} \bar{\mathbf{e}}_{\mathbf{x}_2}]_{i_2} = \hat{\mathbf{D}}_{i_1}^{a_1 d}(\mathbf{x}_1) G_{\Delta}^{da}(\mathbf{x}_1, \mathbf{x}_2) f^{aa_2 d_3} \bar{\mathbf{e}}_{i_2}^{d_3}(\mathbf{x}_2)\tag{2.145}$$

$$\frac{a_1}{i_1} [\hat{\mathbf{D}}_{\mathbf{x}_1} G_{\mathbf{x}_1 \mathbf{x}_3} \hat{T}^{a_3} K_{\mathbf{x}_3 \mathbf{x}_2}^{i_3}]_{i_2}^{a_2} = \hat{\mathbf{D}}_{i_1}^{a_1 d}(\mathbf{x}_1) G_{\Delta}^{da}(\mathbf{x}_1, \mathbf{x}_3) f^{aa_3 c} K_{i_3 i_2}^{ca_2}(\mathbf{x}_2, \mathbf{x}_3)\tag{2.146}$$

and  $G_{\Delta}^{da}(\mathbf{x}_1, \mathbf{x}_3)$  denotes the Green's function of the covariant Laplacian in the background field  $\hat{\mathbf{A}}$ :

$$\left( \hat{\mathbf{D}}_{i, \mathbf{x}_1}^{bc} \hat{\mathbf{D}}_{i, \mathbf{x}_1}^{cd} \right) G_{\Delta}^{da}(\mathbf{x}_1, \mathbf{x}_3) = \delta^{ab} \delta_{\mathbf{x}_1 \mathbf{x}_3}.\tag{2.147}$$

Having determined  $P^{(1)}$ , we see that we are not completely done yet. Putting  $P^{(1)}$  back into eq.(2.141), we see that the equation is only satisfied if we restrict  $\mathbf{a}$  (*after* having performed the derivative) to the space of functions that satisfy<sup>52</sup>

$$\hat{\mathbf{D}}_i^{ab} \mathbf{a}_i^b = 0,\tag{2.148}$$

i.e.  $P(\mathbf{a})e^{-\frac{1}{2}\mathbf{a}K\mathbf{a}+i\bar{\mathbf{e}}\mathbf{a}}$  satisfies Gauss' law to  $\mathcal{O}(g^1)$  only on the gauge fixing surface defined by the background field condition eq.(2.148). In other words:  $P(\mathbf{a})e^{-\frac{1}{2}\mathbf{a}K\mathbf{a}+i\bar{\mathbf{e}}\mathbf{a}}$  does not satisfy Gauss' law; if we compute however

$$\int \mathcal{D}\mathbf{a} \Delta_{FP} \delta(\hat{\mathbf{D}}\mathbf{a}) \psi^*[\mathbf{a}] \mathcal{O} \Gamma^a(\mathbf{x}) \psi[\mathbf{a}],\tag{2.149}$$

where  $\Delta_{FP}$  is the Faddeev-Popov determinant appropriate for this background field gauge, this will be zero (up to  $\mathcal{O}(g^2)$ ) for every operator  $\mathcal{O}$ , that does not contain functional derivatives w.r.t. modes of  $\mathbf{a}$  that are longitudinal in a generalized sense, i.e.  $\hat{\mathbf{D}}\mathbf{a} \neq 0$ . A prominent example of an operator that does not belong to this class is the  $\mathcal{O}(g^0)$  contribution of the Gauss law operator. We therefore considered

$$\int \mathcal{D}\mathbf{a} \Delta_{FP} \delta(\hat{\mathbf{D}}\mathbf{a}) \psi^*[\mathbf{a}] \Gamma^b(\mathbf{y}) \Gamma^a(\mathbf{x}) \psi[\mathbf{a}]\tag{2.150}$$

and found that this vanishes only (up to terms of  $\mathcal{O}(g^2)$ ), if  $\bar{\mathbf{e}} = 0$ . If  $\mathcal{O}$  consists of more than one Gauss law operator, all the matrix elements are zero (up to terms of  $\mathcal{O}(g^2)$ ), even in the presence of  $\bar{\mathbf{e}}$ . This demonstrates that even if the wave functional is annihilated by the Gauss law operator on the gauge fixing surface this is not sufficient for expectation values of arbitrary

<sup>52</sup>The additional factors that make this condition necessary are due to the symmetry requirements on  $\chi_{i_1 i_2}^{a_1 a_2}, \chi_{i_1 i_2 i_3}^{a_1 a_2 a_3}$ .

operators times a Gauss law operator to be zero, but that a case by case analysis is required. For higher orders in  $g$  we obtain from the recursion relation eq. (2.137) the equations

$$\hat{\mathbf{D}}_i^{ab} \frac{\delta P^{(n)}}{\delta \mathbf{a}_i^b} = \mathbf{a}_i^c (\hat{T}^c)^{ab} ((-K\mathbf{a})_i^b + i\bar{\mathbf{e}}_i^b) P^{(n-1)} + \mathbf{a}_i^c (\hat{T}^c)^{ab} \frac{\delta P^{(n-1)}}{\delta \mathbf{a}_i^b} = 0. \quad (2.151)$$

We thus see that (at least in principle)  $P(\mathbf{a})$  can be calculated recursively, since  $\frac{\delta}{\delta \mathbf{a}} P^{(n)}$  can be expressed in terms of polynomials that have been computed before. For which operators problems occur to higher order in  $g$  (taking into account that the Faddeev-Popov determinant becomes non-trivial at  $\mathcal{O}(g^2)$  [Lae01]) we have not investigated in detail. The main lesson from this section is that a pure Gaussian state can satisfy Gauss' law only to order  $g^0$ . This is the reason why we can formulate an exactly gauge invariant Gaussian ground state for electrodynamics.

“Who is she?” - “She is Frankland’s daughter.” -  
“What? Old Frankland the crank?”

Sherlock Holmes, The Hound of the Baskervilles

## 2.5 The Time-Dependent Variational Principle and Cranking

In this section we want to discuss a technique that stems from nuclear physics and is based on the time-dependent variational principle, the so-called cranking model. We start by giving a physical motivation for the approach, and study some general properties. Then we restrict ourselves to Gaussian states and discuss the inter-quark potential to lowest order in  $g$ . We also apply the model to electrodynamics, and see that the Coulomb interaction between static charges is reproduced. The study of the static inter-quark potential to one-loop order, however, demonstrates the short-comings of the cranking approach, since it does not reproduce the one-loop  $\beta$ -function.

### 2.5.1 Generalities

In sec. 2.3 we discussed the variational approach, and ignored the problem that Gaussian states in general violate the gauge invariance required. In this section, we don't want to ignore the problem, but want to use the violation of gauge invariance by the state to approximate its time-dependence. The idea we follow is inspired by [HIMV00] and related to the approach presented in sec. 1.7.4, cf. also [RS80]. We start from Dirac's time-dependent variational principle

$$\delta S = \delta \int_{t_1}^{t_2} dt \langle \psi(t) | i\partial_t - H | \psi(t) \rangle \stackrel{!}{=} 0. \quad (2.152)$$

Whereas for the Rayleigh-Ritz principle only a static *ansatz* for the wave functional is needed, here we also have to make an *ansatz* for the time dependence. We could use a Gaussian wave functional where all parameters  $G^{-1}, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}}$  are now time-dependent, but we rather choose as an *ansatz*

$$|\psi(t)\rangle = e^{-iEt} e^{-i \int d^3x \varphi^a(\mathbf{x}, t) \Gamma^a(\mathbf{x})} |\psi\rangle, \quad (2.153)$$

where  $|\psi\rangle$  is a time-independent state, the coordinate representation of which later on will be restricted to a Gaussian functional. Note that, if  $|\psi\rangle$  is normalized, so is  $|\psi(t)\rangle$ . This *ansatz* for the time dependence is motivated as follows: the general time dependence of a state (unless it is

an energy eigenstate) will consist of vibrations. However, if there are directions in configuration space without restoring forces, we will end up not with a (small-amplitude) vibration, but with a large amplitude motion. If there are states that are degenerate in energy and are connected by an infinitesimal symmetry transformation, the motion from one state to the other does not experience a restoring force. Usually, there are then not only two states which are energetically degenerate and connected by an infinitesimal symmetry transformation, but rather a whole continuous infinity of such states, that are then connected by finite symmetry transformations characterized by (at least) one continuous parameter. In the following, we will call motion within this collection of states 'motion along the zero mode'. We see that if we have a state that is not an eigenstate<sup>53</sup> of the complete set of commuting operators that commute with the Hamiltonian, in other words, if the state is deformed, we necessarily have such a zero mode along which the state could move during the time evolution. To be concrete, if we start from a state that is not gauge invariant, we have a continuous infinity of states that have the same energy. These are the gauge transforms of the original state. Our ansatz for the time dependence draws its form from this consideration: we have approximated the whole time dependence of the state (apart from the energy phase) by its rotation along the zero modes. If one considers a time-averaged picture, the restoration of gauge invariance seems also plausible, since in due time the state will have rotated over all its gauge transformations, thereby mimicking effectively the projector. The second approximation that we are going to make seems also plausible from our considerations; namely, while moving along a zero mode there should be no considerable accelerations. Thus, an ansatz where  $\varphi^a(\mathbf{x}, t)$  and  $\dot{\varphi}^a(\mathbf{x}, t)$  are parallel in colour space<sup>54</sup> appears to be justified. If we insert this time dependence, we obtain an integrand in the action that is time-independent, and we are left with a time-independent variational principle with an effective Hamiltonian

$$\delta\langle\psi|E - \left(H - \int d^3x \omega^a(\mathbf{x})\Gamma^a(\mathbf{x})\right)|\psi\rangle \stackrel{!}{=} 0. \quad (2.154)$$

We can interpret - just as is done in nuclear physics<sup>55</sup> [Bar63], [RS80], [BR86] - the *cranking Hamiltonian*  $H_{cr}$

$$H_{cr} = H - \int d^3x \omega^a(\mathbf{x})\Gamma^a(\mathbf{x}) \quad (2.155)$$

as the Hamiltonian in the internal colour-rotating frame, whereas  $H$  is the Hamiltonian in the 'lab frame'. On the other hand, we may consider the variational problem given in eq. (2.154) as a constrained variational problem with  $\omega$  as a set of Lagrange multipliers that are used s.t.  $\langle\Gamma^a(\mathbf{x})\rangle$  acquires prescribed values. The interpretation of these prescribed values is not as straightforward as one would wish; we have studied before in sec. 2.1 the implementation of external colour charges. One lesson one could draw from that discussion is that, due to the non-Abelian nature of the charge operators, static charges are necessarily quantized in a theory that is based on a compact group like  $SU(N)$  (this is not the case in electrodynamics, where we have a non-compact group that allows for arbitrary charges). Thus, even though it appears that we can prescribe arbitrary values for  $\langle\Gamma^a(\mathbf{x})\rangle$ , this is not the case if we want to interpret them as

<sup>53</sup>The following is obviously only true if the operators of which the state is not an eigenstate are generators of a continuous symmetry, e.g. to take a quantum mechanical example,  $J_3$  could be considered as a valid operator, whereas the parity operator does not serve our purpose.

<sup>54</sup>A specific ansatz that is very popular in nuclear physics [RS80] which fulfils this condition is  $\varphi^a(\mathbf{x}, t) = t\omega^a(\mathbf{x})$ .

<sup>55</sup>Phenomenological applications of the cranking model in nuclear physics can be found in e.g. [VDS83]. Further theoretical considerations can be found in [KO81] where also a connection to the Random Phase Approximation is drawn, cf. also [TV62]. For an application of the cranking approach in hadronic physics, cf. e.g. [ARW96].

static external charges<sup>56</sup>. To put everything in a nutshell: in order to have a clean interpretation in terms of external charges, one should use an extra space on which operators creating static charges can act; here, however, we will interpret  $\langle \Gamma^a \rangle$  as the colour content of the wave functional, and call that 'charge' as well<sup>57</sup>. In the following, we will denote by  $|\psi_\omega\rangle$  a state that minimizes the expectation value of  $H_{cr}$  for a prescribed value of  $\omega$ . Its colour content is then given by

$$\rho_\omega^a(\mathbf{x}) = \langle \psi_\omega | \Gamma^a(\mathbf{x}) | \psi_\omega \rangle. \quad (2.156)$$

If we furthermore assume that the colour content is not discontinuous at  $\omega = 0$ , then we can perform a Taylor expansion for small  $\omega$ :

$$\rho_\omega^a(\mathbf{x}) = \rho_{\omega=0}^a(\mathbf{x}) + \left. \frac{\delta \rho_\omega^a(\mathbf{x})}{\delta \omega^b(\mathbf{y})} \right|_{\omega=0} \omega^b(\mathbf{y}) + \dots \quad (2.157)$$

We call  $\delta \rho_\omega^a(\mathbf{x}) / \omega^b(\mathbf{y}) \big|_{\omega=0} = I^{ab}(\mathbf{x}, \mathbf{y})$  the colour moment of inertia, cf. [HMVI98], [HIMV00], since if we have no colour charge<sup>58</sup> at  $\omega = 0$ , then we have the relation  $\langle \Gamma \rangle = I\omega + \dots$ , and thus precisely the same relationship as in ordinary mechanics of rotating bodies. Of course, we are also interested in the *energy* of the state in the *laboratory* system:

$$E[\omega] = \langle \psi_\omega | H | \psi_\omega \rangle \quad (2.158)$$

$$= \langle \psi_\omega | H_{cr} | \psi_\omega \rangle + \langle \psi_\omega | \int d^3x \omega^a(\mathbf{x}) \Gamma^a(\mathbf{x}) | \psi_\omega \rangle. \quad (2.159)$$

Since the energy will not depend on the sign of  $\omega$ , upon expanding  $E[\omega]$  in powers of  $\omega$  the linear term will vanish, and we end up with

$$E[\omega] = E[0] + \frac{1}{2} \int d^3x d^3y \omega^a(\mathbf{x}) T^{ab}(\mathbf{x}, \mathbf{y}) \omega^b(\mathbf{y}) + \dots \quad (2.160)$$

or, expressed in terms of the charges  $\rho^a$ :

$$E[\omega] = E[0] + \frac{1}{2} \int d^3x d^3y d^3x_1 d^3y_1 \left\{ (\rho_\omega - \rho_{\omega=0})^a(\mathbf{x}) (I^{-1})^{a_1a}(\mathbf{x}_1, \mathbf{x}) T^{a_1b_1}(\mathbf{x}_1, \mathbf{y}_1) \right. \quad (2.161) \\ \left. \times (I^{-1})^{b_1b}(\mathbf{y}_1, \mathbf{y}) (\rho_\omega - \rho_{\omega=0})^b(\mathbf{y}) \right\}.$$

In nuclear physics (where the Gauss law operators are replaced by angular momentum operators  $\mathbf{J}_a$ ), one usually has the situation [RS80] that  $|\psi_\omega\rangle$  is an eigenstate of  $H - \omega_a \mathbf{J}_a$ , and thus one can use the Feynman-Hellman theorem

$$\frac{\partial E_{cr}[\omega]}{\partial \omega_a} = \frac{\partial}{\partial \omega_a} \langle \psi_\omega | H - \omega_b \mathbf{J}_b | \psi_\omega \rangle = \langle \psi_\omega | \left( \frac{\partial}{\partial \omega_a} (H - \omega_b \mathbf{J}_b) \right) | \psi_\omega \rangle = -\langle \psi_\omega | \mathbf{J}_a | \psi_\omega \rangle = -I^{ab} \omega_b + \dots \quad (2.162)$$

to conclude that  $T^{ab} = I^{ab}$ . Then the energy in the laboratory system  $E[\omega] = \langle \psi_\omega | H | \psi_\omega \rangle$  can be simplified, and one ends up with

$$E[\omega] = E[0] + \frac{1}{2} \int d^3x d^3y (\rho_\omega - \rho_{\omega=0})^a(\mathbf{x}) (I^{-1})^{ab}(\mathbf{x}, \mathbf{y}) (\rho_\omega - \rho_{\omega=0})^b(\mathbf{y}). \quad (2.163)$$

<sup>56</sup>In low orders of perturbation theory the group  $SU(N)$  becomes a direct product of  $U(1)$  groups; then we may again have arbitrary charge values. This will also be utilized in sec. 2.6.

<sup>57</sup>It would be more appropriate to call it a charge density distribution.

<sup>58</sup>We have seen in section 2.3 that if we consider the minimum of the Hamiltonian  $H$  alone (i.e.  $\omega = 0$ ), we indeed have  $\rho_{\omega=0} = 0$ .

If the state  $|\psi_\omega\rangle$  is not an eigenstate of the cranking Hamiltonian (as it might be if it is determined by a variational procedure), it has to be checked explicitly whether  $T^{ab}(\mathbf{x}, \mathbf{y}) = I^{ab}(\mathbf{x}, \mathbf{y})$ , and if not one has to use eq. (2.161) as an expression for the energy. In the perturbative calculation that follows in secs. 2.5.3 and 2.5.5 it turns out that  $T = I$  at least to order  $\mathcal{O}(g^4)$ .

### 2.5.2 Gaussian Wave Functionals

After these general considerations, let us come back to our special case, namely states that have a Gaussian structure. The functional to be minimized reads

$$E_{cr} = \langle \psi | H - \int d^3x \omega^a(\mathbf{x}) \Gamma^a(\mathbf{x}) | \psi \rangle, \quad (2.164)$$

where we choose  $\langle \mathbf{A} | \psi \rangle$  to be the Gaussian wave functional defined by eq. (2.104). Then  $E_{cr}$  is given as

$$\begin{aligned} E_{cr} = & \frac{1}{2} \int d^3x \left\{ \bar{\mathbf{e}}_i^a(\mathbf{x}) \bar{\mathbf{e}}_i^a(\mathbf{x}) + \frac{1}{4} \text{tr}(G_{\mathbf{xx}}^{-1}) + 4 \text{tr}(\Sigma G \Sigma)_{\mathbf{xx}} + \frac{1}{g^2} \bar{\mathbf{B}}_i^a(\mathbf{x}) \bar{\mathbf{B}}_i^a(\mathbf{x}) \right. \\ & \left. + \text{tr} \left( (\hat{\mathbf{D}} \hat{\mathbf{D}} - \hat{\mathbf{B}}) G_{\mathbf{xy}} \right) \Big|_{\mathbf{y} \rightarrow \mathbf{x}} + \frac{g^2}{2} \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}} S_i \hat{T}^a G_{\mathbf{xx}}) + \frac{g^2}{4} \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}}) \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}}) \right\} \\ & - \int d^3x \omega^a(\mathbf{x}) \left( \hat{\mathbf{D}}_i^{ab}(\mathbf{x}) \bar{\mathbf{e}}_i^b(\mathbf{x}) + 2g \int d^3y \text{tr}(\hat{T}^a \Sigma_{\mathbf{xy}} G_{\mathbf{yx}}) \right). \end{aligned} \quad (2.165)$$

The last term can also be brought into a form that will be more useful later on. By using the anti-symmetry of  $\hat{T}$ , we can write

$$\int d^3y \text{tr}(\hat{T}^a \Sigma_{\mathbf{xy}} G_{\mathbf{yx}}) = \frac{1}{2} \text{tr}(\hat{T}^a [\Sigma, G]_{\mathbf{xx}}), \quad (2.166)$$

where the commutator is to be taken w.r.t. all indices. In contrast to the case without the extra cranking term, we will obtain non-vanishing values for both  $\bar{\mathbf{e}}$  and  $\Sigma$  upon variation. With a partial integration,  $\int d^3x \omega^a(\mathbf{x}) \hat{\mathbf{D}}_i^{ab}(\mathbf{x}) \bar{\mathbf{e}}_i^b(\mathbf{x}) = - \int d^3x (\hat{\mathbf{D}}_i^{ba}(\mathbf{x}) \omega^a(\mathbf{x})) \bar{\mathbf{e}}_i^b(\mathbf{x})$ , and the variational equation for  $\bar{\mathbf{e}}$  can be solved easily:

$$\frac{\delta E_{cr}}{\delta \bar{\mathbf{e}}_i^a(\mathbf{x})} \stackrel{!}{=} 0 \rightarrow \bar{\mathbf{e}}_i^a(\mathbf{x}) = -\hat{\mathbf{D}}_i^{ab}(\mathbf{x}) \omega^b(\mathbf{x}). \quad (2.167)$$

Next, we consider the equation of motion for  $\Sigma$ :

$$\frac{\delta}{\delta \Sigma_{ij}^{bc}(\mathbf{y}, \mathbf{z})} \left( 2 \text{Tr}(\Sigma G \Sigma) - g \int d^3x \omega^a(\mathbf{x}) \text{tr}(\hat{T}^a [\Sigma, G]_{\mathbf{xx}}) \right) \stackrel{!}{=} 0, \quad (2.168)$$

which results in

$$2(\Sigma G + G \Sigma)_{ij}^{bc}(\mathbf{y}, \mathbf{z}) + g(\omega^a \hat{T}^a G - G \hat{T}^a \omega^a)_{ij}^{bc}(\mathbf{y}, \mathbf{z}) = 0, \quad (2.169)$$

and last the equation for  $G^{-1}$ :

$$\frac{\delta E_{cr}}{\delta G_{ij}^{bc}(\mathbf{y}, \mathbf{z})} = -\frac{1}{8} (G^{-2})_{ij}^{bc}(\mathbf{y}, \mathbf{z}) + \frac{1}{2} (K^2)_{ij}^{bc}(\mathbf{y}, \mathbf{z}) + 2(\Sigma \Sigma)_{ij}^{bc}(\mathbf{y}, \mathbf{z}) - g(\omega^a \hat{T}^a \Sigma - \Sigma \hat{T}^a \omega^a)_{ij}^{bc}(\mathbf{y}, \mathbf{z}) \stackrel{!}{=} 0, \quad (2.170)$$

where in view of the results of sec. 2.3.5 we write the operator  $\hat{\hat{\mathbf{D}}}\hat{\hat{\mathbf{D}}} - \hat{\hat{\mathbf{B}}}$  as  $K^2$ . If we solve this equation w.r.t.  $K^2$  and insert the resulting expression, as well as eq. (2.167), into eq. (2.165), we obtain as an expression for the energy

$$E_{cr}|_{\text{stat.point}} = \frac{1}{2g^2} \int d^3x \bar{\mathbf{B}}_i^a(\mathbf{x})\bar{\mathbf{B}}_i^a(\mathbf{x}) + \frac{1}{4}\text{Tr}(G^{-1}) - \frac{1}{2} \int d^3x (\hat{\hat{\mathbf{D}}}_i^{ab}(\mathbf{x})\omega^b(\mathbf{x}))(\hat{\hat{\mathbf{D}}}_i^{ac}(\mathbf{x})\omega^c(\mathbf{x})). \quad (2.171)$$

In order to give a definite value, however, we first have to solve the equation of motion for  $\Sigma$ , eq. (2.169), since by eq. (2.170)  $G^{-1}$  is given in terms of both the known  $K$  and - until now unknown -  $\Sigma$ .

### 2.5.3 Potential between Static Charges - Lowest Order in $g$

Before we solve the equation<sup>59</sup> for  $\Sigma$ , a short comment about powers of  $g$  is in order. From eq. (2.169) we see that  $\Sigma$  is always of one power higher in  $g$  than  $\omega$  or  $\bar{\mathbf{e}}$ . Thus, the leading power of  $\langle \Gamma^a(\mathbf{x}) \rangle$  is determined by the power of  $\bar{\mathbf{e}}$ , or rather the other way around. In the general discussion in sec. 2.1, we saw that (using perturbative scaling) Gauss' law implies<sup>60</sup>

$$\langle \Gamma^a(\mathbf{x}) \rangle = \left\langle \left( -\frac{1}{g} \hat{\hat{\mathbf{D}}}_i^{ab}(\mathbf{x})\Pi_i^b(\mathbf{x}) + \rho^a(\mathbf{x}) \right) \right\rangle = 0 \rightarrow \langle \hat{\hat{\mathbf{D}}}_i^{ab}(\mathbf{x})\Pi_i^b(\mathbf{x}) \rangle = g\langle \rho^a(\mathbf{x}) \rangle, \quad (2.172)$$

i.e. the expectation value of  $\hat{\hat{\mathbf{D}}}\Pi$  is of order  $g$ , since the charges  $\rho^a$  are of  $\mathcal{O}(1)$ . Thus, we conclude that  $\bar{\mathbf{e}}$  and  $\omega$  are of  $\mathcal{O}(g)$ , and therefore  $\Sigma$  is of  $\mathcal{O}(g^2)$ . Inserting this into eq. (2.170), we see that the corrections to  $G^{-1} = 2K$  (due to the  $\Sigma\Sigma$  and the  $g\omega\Sigma$  terms) are of  $\mathcal{O}(g^4)$ . Before we solve the equation for  $\Sigma$ , let us first consider the energy attributed to the charges to lowest order in  $g$ . The leading term is of  $\mathcal{O}(g^2)$ :

$$-\frac{1}{2} \int d^3x (\hat{\hat{\mathbf{D}}}_i^{ab}(\mathbf{x})\omega^b(\mathbf{x}))(\hat{\hat{\mathbf{D}}}_i^{ac}(\mathbf{x})\omega^c(\mathbf{x})). \quad (2.173)$$

To obtain from this expression which is given in the colour-rotating frame the leading term in  $g$  in the lab frame, we have to add the leading ( $\mathcal{O}(g^2)$ ) contribution of  $\int d^3x \omega^a(\mathbf{x})\Gamma^a(\mathbf{x})$  to it. Using eq. (2.167) this results in

$$\begin{aligned} & -\frac{1}{2} \int d^3x (\hat{\hat{\mathbf{D}}}_i^{ab}(\mathbf{x})\omega^b(\mathbf{x}))(\hat{\hat{\mathbf{D}}}_i^{ac}(\mathbf{x})\omega^c(\mathbf{x})) + \int d^3x \omega^a(\mathbf{x})\hat{\hat{\mathbf{D}}}_i^{ac}(\mathbf{x})\bar{\mathbf{e}}_i^c(\mathbf{x}) \\ & = +\frac{1}{2} \int d^3x (\hat{\hat{\mathbf{D}}}_i^{ab}(\mathbf{x})\omega^b(\mathbf{x}))(\hat{\hat{\mathbf{D}}}_i^{ac}(\mathbf{x})\omega^c(\mathbf{x})). \end{aligned} \quad (2.174)$$

Re-expressing  $\omega$  in terms of charges gives to lowest order in  $g$ :

$$g\rho^a = \hat{\hat{\mathbf{D}}}_i^{ac}(\mathbf{x})\bar{\mathbf{e}}_i^c(\mathbf{x}) = -\hat{\hat{\mathbf{D}}}_i^{ac}(\mathbf{x})\hat{\hat{\mathbf{D}}}_i^{cb}(\mathbf{x})\omega^b(\mathbf{x}) \quad (2.175)$$

and, using the Green's function of the covariant Laplacian:  $\hat{\hat{\mathbf{D}}}_i^{ac}(\mathbf{x})\hat{\hat{\mathbf{D}}}_i^{cb}(\mathbf{x})G_{\Delta}^{bd}(\mathbf{x}, \mathbf{y}) = \delta^{ad}\delta_{\mathbf{x}\mathbf{y}}$ , we have

$$\omega^b(\mathbf{x}) = -g \int d^3y G_{\Delta}^{ba}(\mathbf{x}, \mathbf{y})\rho^a(\mathbf{y}). \quad (2.176)$$

<sup>59</sup>The final result for  $\Sigma$  will be given in eq. (2.189).

<sup>60</sup>This can also be seen in an alternative way, if we consider the eigenstates of the Gauss law operator. Using perturbative scaling, the operators fulfilling the  $SU(N)$  algebra are  $-\frac{1}{g}\hat{\hat{\mathbf{D}}}\Pi$ . Thus, they will have the eigenvalues  $0, \pm(1/2), \dots$  (at each point in space), s.t. the eigenvalues of  $\Gamma$  will be  $0, \pm(g/2), \pm g, \dots$ .

Then the energy in the laboratory system can be written as

$$E = \frac{1}{2g^2} \int d^3x \bar{\mathbf{B}}_i^a(\mathbf{x}) \bar{\mathbf{B}}_i^a(\mathbf{x}) + \frac{1}{2} \text{Tr} K + g^2 \int d^3x d^3y \rho^a(\mathbf{x}) \left( -G_{\Delta}^{ab}(\mathbf{x}, \mathbf{y}) \right) \rho^b(\mathbf{y}). \quad (2.177)$$

From this, one can read off the result that we repeatedly arrive at from different directions in this thesis, namely that the potential between charges to lowest order in perturbation theory is  $-G_{\Delta}^{ab}(\mathbf{x}, \mathbf{y})$ .

One should note that the expression for  $E$  as given here is not complete to  $\mathcal{O}(g^2)$ , since we have obviously neglected the  $\mathcal{O}(g^2)$  that comes from the  $\mathbf{B}^2$ -term, both in the energy and in its effect on the solution for  $G^{-1}$ . However, these contributions should not depend on  $\rho$  and thus do not contribute to the potential.

### 2.5.4 Electrodynamics with External Charges

Before we try to evaluate the  $\mathcal{O}(g^4)$  correction to the inter-quark potential, let us shortly digress to the simpler case of electrodynamics in the presence of external charges. The necessary calculations have already been performed in the previous section; we only have to simplify them slightly. In order to go from the lowest order in  $g$  in Yang-Mills theory to electrodynamics we simply have to make the formal substitution  $(\hat{T}^a)^{bc} = f^{bac} \rightarrow 0$ , and dispose of all the colour indices. Then  $E_{cr}$  is given as

$$E_{cr} = \frac{1}{2} \int d^3x \left\{ \bar{\mathbf{e}}_i(\mathbf{x}) \bar{\mathbf{e}}_i(\mathbf{x}) + \frac{1}{4} \text{tr}(G_{\mathbf{xx}}^{-1}) + 4 \text{tr}(\Sigma G \Sigma)_{\mathbf{xx}} + \frac{1}{g^2} \bar{\mathbf{B}}_i(\mathbf{x}) \bar{\mathbf{B}}_i(\mathbf{x}) \right. \\ \left. + \text{tr}((\nabla \nabla - \mathbb{1} \Delta) G_{\mathbf{xy}}) |_{\mathbf{y} \rightarrow \mathbf{x}} \right\} - \int d^3x \omega^a(\mathbf{x}) \nabla_i \bar{\mathbf{e}}_i(\mathbf{x}), \quad (2.178)$$

where the expression  $\nabla \nabla - \mathbb{1} \Delta$  is a matrix in the spatial indices, s.t.  $(\nabla \nabla - \mathbb{1} \Delta)_{ij} = \nabla_i \nabla_j - \delta_{ij} \Delta$ . The equation for  $\bar{\mathbf{e}}$  simplifies correspondingly,

$$\frac{\delta E_{cr}}{\delta \bar{\mathbf{e}}_i^a(\mathbf{x})} \stackrel{!}{=} 0 \rightarrow \bar{\mathbf{e}}_i(\mathbf{x}) = -\nabla_i \omega(\mathbf{x}), \quad (2.179)$$

and also the equations of motion for  $\Sigma$  are simplified:

$$\frac{\delta}{\delta \Sigma_{ij}^{bc}(\mathbf{y}, \mathbf{z})} (2 \text{Tr}(\Sigma G \Sigma)) \stackrel{!}{=} 0, \quad (2.180)$$

which leads automatically to  $\Sigma = 0$ . The equation for  $G^{-1}$  reads

$$\frac{\delta E_{cr}}{\delta G_{ij}^{bc}(\mathbf{y}, \mathbf{z})} = -\frac{1}{8} (G^{-2})_{ij}^{bc}(\mathbf{y}, \mathbf{z}) + \frac{1}{2} (K_0^2)_{ij}^{bc}(\mathbf{y}, \mathbf{z}) + 2(\Sigma \Sigma)_{ij}^{bc}(\mathbf{y}, \mathbf{z}) \stackrel{!}{=} 0. \quad (2.181)$$

In view of the results of sec. 2.3.5 we write the operator  $(\nabla \nabla - \mathbb{1} \Delta)$  as  $K_0^2$ . Here,  $(K_0)_{ij}(\mathbf{x}, \mathbf{y})$  can be given explicitly as  $(K_0)_{ij}(\mathbf{x}, \mathbf{y}) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})} |\mathbf{k}| P_{ij}^T(\mathbf{k})$ . From eq. (2.179) we see that  $\bar{\mathbf{e}}$  has only a longitudinal component, and that we can relate it to the external charge via Gauss' law<sup>61</sup>. Analogously to eq. (2.175) we obtain:

$$g\rho^a = \nabla_i \bar{\mathbf{e}}_i(\mathbf{x}) = -\nabla_i \nabla_i \omega(\mathbf{x}). \quad (2.182)$$

<sup>61</sup>In contrast to the Yang-Mills case, there are no commutation relations in the Abelian case that would fix the overall normalization; we use here the same normalization as in the Yang-Mills case.

Thus, at the stationary point w.r.t.  $\Sigma, \bar{\mathbf{e}}$  and  $G^{-1}$  (but not  $\bar{\mathbf{A}}$ ), we have the expression for the energy

$$E_{cr}|_{\text{stat.point}} = \frac{1}{2g^2} \int d^3x \bar{\mathbf{B}}_i(\mathbf{x}) \bar{\mathbf{B}}_i(\mathbf{x}) + \frac{1}{2} \text{Tr}(K_0) - \frac{1}{2} \int d^3x (\nabla_i \omega(\mathbf{x})) (\nabla_i \omega(\mathbf{x})) \quad (2.183)$$

and in the laboratory frame

$$E|_{\text{stat.point}} = \frac{1}{2g^2} \int d^3x \bar{\mathbf{B}}_i(\mathbf{x}) \bar{\mathbf{B}}_i(\mathbf{x}) + \frac{1}{2} \text{Tr}(K_0) + \frac{g^2}{2} \int d^3x d^3y \rho(\mathbf{x}) \left( -G_\Delta(\mathbf{x}, \mathbf{y}) \right) \rho(\mathbf{y}), \quad (2.184)$$

where  $G_\Delta(\mathbf{x}, \mathbf{y})$  is the Green's function of the ordinary Laplacian:  $\Delta G_\Delta(\mathbf{x}, \mathbf{y}) = \delta_{\mathbf{x}\mathbf{y}}$ . The three terms in eq. (2.184) are easily interpretable: the first is obviously the classical energy of the external magnetic field (which has not vanished, since we haven't varied  $\bar{\mathbf{A}}$  yet), the second is the zero point energy of the transversal photons, and the last is the Coulomb energy of the static charges; we see that, at the stationary point, electrodynamics is treated exactly.

### 2.5.5 Potential between Static Charges - Next Order in $g$

After this short digression let us return to Yang-Mills theory. Before we solve the equations of motion for  $\Sigma$ , we have to take one fact into account: if  $\bar{\mathbf{A}}$  satisfies the classical equations of motion (or is zero), then  $\hat{\mathbf{D}}K = 0$ , i.e.  $K$ , and with it  $G^{-1}$ , will be transversal in the generalized sense<sup>62</sup>. In other words, the longitudinal components will be zero, and therefore the corresponding components of  $G$  do not exist, as we have already discussed in sec. 2.3.5. There it was no problem, but here we have a term  $\text{tr}(\Sigma G \Sigma)$ . From the longitudinal components of  $G$  being infinite, we can conclude that the corresponding longitudinal components of  $\Sigma$  have to be zero, thus restricting  $\Sigma$  to being purely transversal<sup>63</sup> (in the generalized sense).

After these introductory comments we turn now to solving the equation of motion for the transversal components of  $\Sigma$ . For simplicity, we will solve the equations only for  $\bar{\mathbf{A}} = 0$ . Then the expression for  $K^2$  simplifies, and we will call it in the following  $K_0^2$ :

$$(K_0^2)_{ij}^{ab}(\mathbf{x}, \mathbf{y}) = \delta^{ab} \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \mathbf{k}^2 \left( \delta_{ij} - \frac{\mathbf{k}_i \mathbf{k}_j}{\mathbf{k}^2} \right). \quad (2.185)$$

The square root of this operator can in fact be given explicitly:

$$(K_0)_{ij}^{ab}(\mathbf{x}, \mathbf{y}) = \delta^{ab} \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \sqrt{\mathbf{k}^2} \left( \delta_{ij} - \frac{\mathbf{k}_i \mathbf{k}_j}{\mathbf{k}^2} \right) = \frac{1}{2} (G^{-1})_{ij}^{ab}(\mathbf{x}, \mathbf{y}) + \mathcal{O}(g^2). \quad (2.186)$$

If one now introduces the Fourier transform  $\tilde{\Sigma}$  via

$$\Sigma_{ij}^{ab}(\mathbf{x}, \mathbf{y}) = \int \frac{d^3k_1}{(2\pi)^3} \frac{d^3k_2}{(2\pi)^3} e^{i(\mathbf{k}_1 \cdot \mathbf{x} - \mathbf{k}_2 \cdot \mathbf{y})} \tilde{\Sigma}_{ij}^{ab}(\mathbf{k}_1, \mathbf{k}_2) \quad (2.187)$$

and notes that, by requirement,  $\mathbf{P}_{i_1}^T(\mathbf{k}_1) \tilde{\Sigma}_{i_1 j}^{ab}(\mathbf{k}_1, \mathbf{k}_2) = \tilde{\Sigma}_{i_1 j}^{ab}(\mathbf{k}_1, \mathbf{k}_2) \mathbf{P}_{j_1}^T(\mathbf{k}_2) = \tilde{\Sigma}_{ij}^{ab}(\mathbf{k}_1, \mathbf{k}_2)$ , then eq. (2.169) can be written as

$$2\tilde{\Sigma}_{ij}^{bc}(\mathbf{k}_1, \mathbf{k}_2) \left( \frac{1}{|\mathbf{k}_2|} + \frac{1}{|\mathbf{k}_1|} \right) = g\tilde{\omega}^a(\mathbf{k}_1 - \mathbf{k}_2) (\hat{T}^a)^{bc} \left( \frac{1}{|\mathbf{k}_2|} \mathbf{P}_{ij}^T(\mathbf{k}_2) - \frac{1}{|\mathbf{k}_1|} \mathbf{P}_{ij}^T(\mathbf{k}_1) \right), \quad (2.188)$$

<sup>62</sup>This point will be discussed in a bit more detail in sec. 2.6.3.

<sup>63</sup>This is consistent with our findings of sec. 2.4 where it turned out that, for the Gaussian wave functional to be annihilated by the Gauss law operator to  $\mathcal{O}(g^0)$ , both  $G^{-1}$  and  $\Sigma$  had to be transversal.



where  $\tilde{\omega}$  denotes the Fourier transform of  $\omega$ . It has to be observed that, contrary to our assumptions, the RHS is not purely transversal. This is due to the fact that eq. (2.169) was obtained from varying the energy functional *without the constraint* that  $\Sigma$  should be purely transversal. However, this is easily remedied. If one wants to perform a variation w.r.t the transversal components of  $\Sigma$ , one only has to act with a transversal projector from the left and with a transversal projector from the right onto  $\frac{\delta E}{\delta \Sigma_{ij}}$ , i.e. one has to compute  $\mathbf{P}_{i_1 i}^T \frac{\delta E}{\delta \Sigma_{ij}} \mathbf{P}_{j j_1}^T$ . This is especially easy for the equation containing the Fourier transform of  $\Sigma$ , since in this case we simply have to multiply it from the left with  $\mathbf{P}_{i_1 i}^T(\mathbf{k}_1)$  and from the right with  $\mathbf{P}_{j j_1}^T(\mathbf{k}_2)$ . Then we end up with<sup>64</sup>

$$\tilde{\Sigma}_{ij}^{bc}(\mathbf{k}_1, \mathbf{k}_2) = \frac{g}{2} \tilde{\omega}^a(\mathbf{k}_1 - \mathbf{k}_2) (\hat{T}^a)^{bc} \left( \frac{|\mathbf{k}_1| - |\mathbf{k}_2|}{|\mathbf{k}_1| + |\mathbf{k}_2|} \right) (\mathbf{P}^T(\mathbf{k}_1) \mathbf{P}^T(\mathbf{k}_2))_{ij}. \quad (2.189)$$

Using this expression for  $\Sigma$ , we see that the connection between  $\rho$  and  $\omega$  is altered; in fact the contribution of the second term of  $\langle \Gamma^a \rangle$  in eq. (2.123) has a logarithmic divergence (if we assume that  $\rho$  is a smooth charge distribution - in view of the point-like nature of real static charges, this might be a non-valid assumption):

$$\text{tr}(\hat{T}^a[\Sigma, G]_{\mathbf{xx}}) = -\frac{g^2 N}{48\pi^2} \int \frac{d^3 p}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{x}} \mathbf{p}^2 \tilde{\omega}^a(\mathbf{p}) \ln \left( \frac{\Lambda^2}{\Lambda_{IR}^2} \right), \quad (2.190)$$

where  $\Lambda$  is a sharp cutoff that had to be used in an intermediate momentum integration, and  $\Lambda_{IR}$  is an infrared cutoff to be discussed now. The steps in the calculation that lead to eq. (2.190) are very similar to those that were performed at the end of sec. 2.2.5, i.e. performing an expansion in the ratio of 'external' momentum  $\mathbf{p}$  to a loop momentum to obtain the logarithmic divergence, etc. And similarly to that calculation we obtain an infrared divergence as an artifact of that expansion (one can check that before one performs the expansion the integral is IR finite). Thus, again one has to introduce an IR cutoff which has to be well above the scale that dominates the  $\mathbf{p}$  integration, and therefore depends on the characteristic of  $\tilde{\omega}$  and thus ultimately on the charge distribution that one wants to prescribe. We perform the Fourier integral, and obtain<sup>65</sup>

$$\text{tr}(\hat{T}^a[\Sigma, G]_{\mathbf{xx}}) = \frac{g^2 N}{48\pi^2} (\Delta \omega^a(\mathbf{x})) \ln \left( \frac{\Lambda^2}{\Lambda_{IR}^2} \right). \quad (2.191)$$

Thus, we obtain the following relation between external charge and  $\omega$ :

$$g\rho^a(\mathbf{x}) = \langle \Gamma^a(\mathbf{x}) \rangle = -\Delta \omega^a(\mathbf{x}) \left\{ 1 + \frac{g^2 N}{48\pi^2} \ln \left( \frac{\Lambda^2}{\Lambda_{IR}^2} \right) \right\}. \quad (2.192)$$

To obtain the potential to  $\mathcal{O}(g^4)$  is by no means trivial, because one has also to compute  $\text{Tr}(G^{-1})$  where  $G^{-1}$  is given (implicitly) by eq. (2.170); the task is simplified, however, since we are only interested in the  $\mathcal{O}(g^4)$  contribution to the trace. Similar to sec. 2.3.5 we introduce operators  $\mathbb{G}^{-1}, \mathbb{K}_0, \Sigma, \mathbb{P}^T$ , s.t.

$$\langle \mathbf{z}_1; i_1, a_1 | \mathbb{G}^{-1} | \mathbf{z}_2; i_2, a_2 \rangle = (G^{-1})_{i_1 i_2}^{a_1 a_2}(\mathbf{z}_1, \mathbf{z}_2) \quad (2.193)$$

$$\langle \mathbf{z}_1; i_1, a_1 | \mathbb{K}_0 | \mathbf{z}_2; i_2, a_2 \rangle = (K_0)_{i_1 i_2}^{a_1 a_2}(\mathbf{z}_1, \mathbf{z}_2) \quad (2.194)$$

$$\langle \mathbf{z}_1; i_1, a_1 | \Sigma | \mathbf{z}_2; i_2, a_2 \rangle = (\Sigma \Sigma - \frac{g}{2} (\omega^a \hat{T}^a \Sigma - \Sigma \hat{T}^a \omega^a))_{i_1 i_2}^{a_1 a_2}(\mathbf{z}_1, \mathbf{z}_2) \quad (2.195)$$

$$\langle \mathbf{z}_1; i_1, a_1 | \mathbb{P}^T | \mathbf{z}_2; i_2, a_2 \rangle = \delta^{a_1 a_2} \int \frac{d^3 k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{z}_1 - \mathbf{z}_2)} \mathbf{P}_{i_1 i_2}^T(\mathbf{k}), \quad (2.196)$$

<sup>64</sup>This result can also be found in [HIMV00].

<sup>65</sup>This result can also be found in [HIMV00].

where  $\Sigma$  is proportional to  $g^4$ . Let us also use the notation

$$\langle \mathbf{z}_1; i_1, a_1 | (\mathbb{K}_0)^{-1} | \mathbf{z}_2; i_2, a_2 \rangle = \delta^{a_1 a_2} \int \frac{d^3 k}{(2\pi)^3} e^{i\mathbf{k} \cdot (\mathbf{z}_1 - \mathbf{z}_2)} \frac{1}{\sqrt{\mathbf{k}^2}} \left( \delta_{i_1 i_2} - \frac{\mathbf{k}_{i_1} \mathbf{k}_{i_2}}{\mathbf{k}^2} \right). \quad (2.197)$$

With this we have

$$(\mathbb{K}_0)^{-1} \mathbb{K}_0 = \mathbb{P}^T = \mathbb{K}_0 (\mathbb{K}_0)^{-1}. \quad (2.198)$$

In order to determine the static potential to  $\mathcal{O}(g^4)$  we now have to compute

$$\text{Tr}(\mathbb{G}^{-1}) = \text{Tr} \left( \sqrt{(4\mathbb{K}_0^2 + 16\Sigma)} \right) = 2 \text{Tr} \left( \sqrt{(\mathbb{K}_0^2 + 4\Sigma)} \right) \quad (2.199)$$

to  $\mathcal{O}(g^4)$ . The first term under the square root is of  $\mathcal{O}(g^0)$  whereas the second is of  $\mathcal{O}(g^4)$ . Therefore,  $\text{Tr}(\mathbb{G}^{-1})$  is given as a power series in  $g^4$ . The  $\mathcal{O}(g^4)$  term can hence be obtained as

$$\left. \frac{\partial}{\partial(g^4)} \left( \text{Tr}(\mathbb{G}^{-1}) - 2\text{Tr}(\mathbb{K}_0) \right) \right|_{g=0}, \quad (2.200)$$

where we have subtracted the contribution to the trace that is independent of  $g$  for convenience. We now use a proper-time representation of the square root [Sch51], [KV89], [Zin89]:

$$\sqrt{\lambda_1} - \sqrt{\lambda_2} = - \int_0^\infty \frac{ds}{2\sqrt{\pi s^3}} \left( e^{-s\lambda_1} - e^{-s\lambda_2} \right), \quad (2.201)$$

the 'fluctuation formula', cf. e.g. [AR95],

$$\frac{d}{dx} e^A = \int_0^1 dt e^{tA} \frac{dA}{dx} e^{(1-t)A} \quad (2.202)$$

and the cyclic property of the trace to obtain

$$\begin{aligned} & \left. \frac{\partial}{\partial(g^4)} \left( \text{Tr}(\mathbb{G}^{-1}) - 2\text{Tr}(\mathbb{K}_0) \right) \right|_{g=0} \\ &= \left. \frac{\partial}{\partial(g^4)} \text{Tr} \left( - \int_0^\infty \frac{ds}{2\sqrt{\pi s^3}} \left[ e^{-s\mathbb{G}^{-2}} - e^{-s4\mathbb{K}_0^2} \right] \right) \right|_{g=0} \\ &= \text{Tr} \left( \int_0^\infty \frac{ds}{2\sqrt{\pi s}} \left[ \frac{\partial}{\partial(g^4)} \mathbb{G}^{-2} \right] e^{-s4\mathbb{K}_0^2} \right). \end{aligned} \quad (2.203)$$

Since  $\text{Tr} \left( \left( \frac{\partial}{\partial(g^4)} \mathbb{G}^{-2} \right) \mathbb{P}^T \right) = \text{Tr} \left( \frac{\partial}{\partial(g^4)} \mathbb{G}^{-2} \right)$ , we can carry out the proper-time integration, and obtain

$$\text{Tr}(\mathbb{G}^{-1}) = 2 \text{Tr}(\mathbb{K}_0) + 4 \text{Tr} \left( (\mathbb{K}_0)^{-1} \frac{1}{g^4} \Sigma \right) g^4 + \mathcal{O}(g^8) \quad (2.204)$$

because  $\frac{\partial}{\partial(g^4)} \mathbb{G}^{-2} = \frac{16}{g^4} \Sigma$ . Using eq. (2.189), we can express  $\text{Tr}((\mathbb{K}_0)^{-1} \Sigma)$  as

$$\begin{aligned} & \frac{g^2}{4} \text{tr}_c(\hat{T}^{c_1} \hat{T}^{c_2}) \int \frac{d^3 k}{(2\pi)^3} \frac{d^3 k_2}{(2\pi)^3} \left\{ \tilde{\omega}^{c_1}(\mathbf{k} - \mathbf{k}_2) \tilde{\omega}^{c_2}(\mathbf{k}_2 - \mathbf{k}) \frac{1}{|\mathbf{k}_2|} \left( \frac{|\mathbf{k}| - |\mathbf{k}_2|}{|\mathbf{k}| + |\mathbf{k}_2|} \right) \left( \frac{|\mathbf{k}_2| - |\mathbf{k}|}{|\mathbf{k}| + |\mathbf{k}_2|} + 2 \right) \right. \\ & \quad \left. \times \text{tr}_s(\mathbb{P}^T(\mathbf{k}) \mathbb{P}^T(\mathbf{k}_2)) \right\}, \end{aligned} \quad (2.205)$$

where  $\text{tr}_c$  denotes a colour trace and  $\text{tr}_s$  a trace over the spatial indices. We can now introduce new sets of momenta  $\mathbf{P} = \mathbf{k} - \mathbf{k}_2$ ,  $\mathbf{Q} = \frac{1}{2}(\mathbf{k} + \mathbf{k}_2)$ . Since we are mainly interested in the logarithmic UV divergence, we can expand the part of the integrand that depends on both  $\mathbf{P}$  and  $\mathbf{Q}$  in powers of  $\frac{|\mathbf{P}|}{|\mathbf{Q}|}$ . As discussed above we again have to introduce also an infrared cutoff  $\Lambda_{IR}$ , and end up with<sup>66</sup>

$$\text{Tr}(\mathbb{G}^{-1}) = 2\text{Tr}(\mathbb{K}_0) + 4\frac{Ng^2}{(4\pi)^2} \ln\left(\frac{\Lambda}{\Lambda_{IR}}\right) \int \frac{d^3P}{(2\pi)^3} \mathbf{P}^2 \tilde{\omega}^a(\mathbf{P}) \tilde{\omega}^a(-\mathbf{P}) + \mathcal{O}(g^8). \quad (2.206)$$

Thus, to  $\mathcal{O}(g^4)$ , the contribution to the energy that depends on  $\omega$  is<sup>67</sup>

$$\begin{aligned} E[\omega] - E[\omega = 0] &= -\frac{1}{2} \int d^3x (\nabla_i \omega^a(\mathbf{x})) (\nabla_i \omega^a(\mathbf{x})) + \int d^3x \omega^a(\mathbf{x}) \langle \Gamma^a(\mathbf{x}) \rangle + \frac{1}{4} 4\text{Tr}((\mathbb{K}_0)^{-1} \Sigma) \\ &= \frac{1}{2} \int \frac{d^3p}{(2\pi)^3} \mathbf{p}^2 \tilde{\omega}^a(\mathbf{p}) \tilde{\omega}^a(-\mathbf{p}) \left[ 1 + \frac{Ng^2}{48\pi^2} \ln\left(\frac{\Lambda^2}{\Lambda_{IR}^2}\right) \right]. \end{aligned} \quad (2.207)$$

Here one should note that the size of the infrared cutoff is in both cases ( $\langle \Gamma^a \rangle$  and  $\text{Tr}(\mathbb{G}^{-1})$ ) determined by  $\tilde{\omega}$  and can hence chosen to be identical. This outcome for the energy is not unexpected, since it simply means that the a priori different moments of inertia<sup>68</sup>  $T^{ab}(\mathbf{x}, \mathbf{y})$  and  $I^{ab}(\mathbf{x}, \mathbf{y})$  are in this perturbative calculation identical. In cases where we can treat the cranking Hamiltonian exactly, this has in fact to be the case, and deviations from  $I = T$  can only come into play due to an approximative treatment of the Schrödinger equation. As a last point, we have to relate the energy to external charges. In accordance with [HIMV00], we take  $\langle \Gamma^a(\mathbf{x}) \rangle|_{g=0}$  as definition of our external charge  $\rho_e^a$ ; this allows to express  $\tilde{\omega}$  in terms of  $\tilde{\rho}_e$  as (using eq. (2.182))

$$\tilde{\omega}^a(\mathbf{p}) = \frac{g}{\mathbf{p}^2} \tilde{\rho}_e^a(\mathbf{p}). \quad (2.208)$$

Then the one-loop energy can be written as

$$E[\rho_e] - E[0] = \frac{g^2}{2} \int \frac{d^3p}{(2\pi)^3} \frac{1}{\mathbf{p}^2} \tilde{\rho}_e^a(\mathbf{p}) \tilde{\rho}_e^a(-\mathbf{p}) \left[ 1 + \frac{Ng^2}{48\pi^2} \ln\left(\frac{\Lambda^2}{\Lambda_{IR}^2}\right) \right] + \mathcal{O}(g^8). \quad (2.209)$$

If we compare this result with the result of sec. 2.2 we observe that the cranking treatment does not lead to the correct  $\beta$ -function.

The conclusion one can draw from the  $\mathcal{O}(g^4)$  treatment is that cranking deals with  $\langle \mathbf{\Pi}_i \rangle$  correctly, which is enough for classical quantities; however, beyond that, i.e. on the one-loop level, charges are not correctly coupled to the system any more, and quantities like  $\langle \mathbf{\Pi}_i \mathbf{\Pi}_j \rangle$  are not treated correctly. This conclusion is also suggested by the Kamlah expansion that will be treated in the next section. There, it turns out, the first order - which under certain circumstances is equivalent to cranking [Man75] - also treats only  $\langle \mathbf{\Pi}_i \rangle$  correctly, but not  $\langle \mathbf{\Pi}_i \mathbf{\Pi}_j \rangle$ .

<sup>66</sup>One should keep in mind that  $\omega$  is of  $\mathcal{O}(g^1)$ , cf. eq. (2.175).

<sup>67</sup>The contribution to the energy from the trace term is  $\frac{1}{4}\text{Tr}(\mathbb{G}^{-1})$ .

<sup>68</sup>They are defined by eqs. (2.157, 2.160).

## 2.6 The Kamlah Expansion

In this section we want to present another method to deal with the projector approximately that also has its roots in nuclear physics: the Kamlah expansion. We introduce it by considering the example of ordinary two-dimensional rotation, and then apply the concept to electrodynamics with external charges. Next, we consider Yang-Mills theory without external charges but we have to restrict ourselves to lowest order in perturbation theory, albeit we treat a possible background field to all orders. As a last point we consider how the quasi-Abelian properties of Yang-Mills theory in lowest order of perturbation theory allow for the inclusion of charges to that order.

### 2.6.1 Generalities

In this first section we want to discuss the Kamlah expansion as it is introduced in the context of nuclear physics<sup>69</sup> [Ka68], [Kub72], [Man75], [RS80], [BR86], cf. also [Zeh65], [Zeh67]. In nuclear physics, one is often confronted with the problem that (usually through the restriction of the space of test wave functions to be used in the variational problem) the 'best' variational wave functions (i.e. those with the lowest energy expectation value) are 'deformed'. In other words, the wave functions are not eigenstates of the symmetry operators that commute with the Hamiltonian and form a complete commuting set. An important example for this is given by the Hartree-Fock-Bogoliubov theory, where the states considered do not have a good particle number. In order to remedy this problem, one uses a projector that ensures that the projected states do carry good quantum numbers. In the case of particle number this would be

$$P^n = \int_0^{2\pi} \frac{d\alpha}{(2\pi)} e^{i\alpha(\hat{N}-n)}, \quad (2.210)$$

where  $\hat{N}$  is the particle number operator and  $n$  is the prescribed particle number. Equivalently, we can also consider a system which is deformed in ordinary space and which has to be projected onto states with good angular momentum. For simplicity we will deal with the two dimensional case - where the rotation group is Abelian with generator  $\hat{J}$  - first. In this case we have the projector

$$P^I = \int_0^{2\pi} \frac{d\alpha}{(2\pi)} e^{i\alpha(\hat{J}-I)}. \quad (2.211)$$

We see that the projectors are integral operators, and when computer time was too costly to implement them, one sought for methods that could deal with them approximately. The case which worked particularly well is the case of *strong deformations*. Strongly deformed states  $|\phi\rangle$  are states where

$$|\langle\phi|e^{i\alpha\hat{J}}|\phi\rangle| \quad (2.212)$$

decreases rapidly for increasing  $\alpha$ . This is very useful, since one can argue that

$$|\langle\phi|He^{i\alpha\hat{J}}|\phi\rangle| \quad (2.213)$$

will vanish rapidly for increasing  $\alpha$ , too, but

$$\frac{\langle\phi|He^{i\alpha\hat{J}}|\phi\rangle}{\langle\phi|e^{i\alpha\hat{J}}|\phi\rangle} \quad (2.214)$$

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<sup>69</sup>Also of interest in the case of nuclear physics are [BMR70], [RBM70], [Cor72], and [VSR71]. Applications can be found e.g. in [BMR73], [RMB74]. That the Kamlah expansion can also be used to implement a symmetry-projected Random Phase Approximation was considered in [EMR80b].

is a smooth function of  $\alpha$ . The argument consists basically of noting that, whereas  $\hat{J}$  is a one-particle operator,  $e^{i\alpha\hat{J}}$  is a collective operator that affects arbitrarily large numbers of particles

$$e^{i\alpha\hat{J}} = \underbrace{1}_{0\text{-body operator}} + \underbrace{i\alpha\hat{J}}_{1\text{-body operator}} + \underbrace{\frac{1}{2}(i\alpha\hat{J})^2}_{2\text{-body operator}} + \underbrace{\frac{1}{3!}(i\alpha\hat{J})^3}_{3\text{-body operator}} + \dots, \quad (2.215)$$

$H$  is (in nuclear physics) at most a two-body operator<sup>70</sup>; thus the behaviour w.r.t. increasing  $\alpha$  should be the same whether we consider  $e^{i\alpha\hat{J}}$  or  $He^{i\alpha\hat{J}}$ . One can now argue further that in the matrix element  $\langle\phi|He^{i\alpha\hat{J}}|\phi\rangle$  all degrees of freedom that are not affected by the collective rotation ('internal degrees of freedom') can be integrated out, and that this results in an effective Hamiltonian operator that is an - up to now - unknown function of  $\hat{J}$ , the symmetry generator. For this function it is proposed to use a power series expansion in powers of <sup>71,72</sup>  $(\hat{J} - \langle\hat{J}\rangle)$ , which is plausible, since one does not expect singularities for collective rotations with finite angular momenta. However, this is only useful if we can stop the expansion after a few terms. That this is indeed possible one can see as follows:

- $\langle\phi|e^{i\alpha\hat{J}}|\phi\rangle$  is well localized in  $\alpha$  space; therefore, a broad range of wave functions with good  $\hat{J}$  quantum number have to be added up coherently
- $\langle\phi|(\hat{J} - \langle\hat{J}\rangle)e^{i\alpha\hat{J}}|\phi\rangle$ : each wave function with good  $\hat{J}$  quantum number is now weighted by that quantum number and this begins to destroy the coherence, in other words  $\langle\phi|(\hat{J} - \langle\hat{J}\rangle)e^{i\alpha\hat{J}}|\phi\rangle$  is broader in  $\alpha$  space than  $\langle\phi|e^{i\alpha\hat{J}}|\phi\rangle$
- the higher the power of  $(\hat{J} - \langle\hat{J}\rangle)$ , the broader is the resulting matrix element in  $\alpha$  space, *but* we already know that  $\langle\phi|He^{i\alpha\hat{J}}|\phi\rangle$  is not very much broader in  $\alpha$  space than is  $\langle\phi|e^{i\alpha\hat{J}}|\phi\rangle$ , hence the matrix elements containing higher powers of  $(\hat{J} - \langle\hat{J}\rangle)$  (besides  $e^{i\alpha\hat{J}}$ ) must be suppressed<sup>73</sup>, i.e. the corresponding expansion coefficients must be small. qed.

Thus, we can stop the expansion

$$\langle\phi|He^{i\alpha\hat{J}}|\phi\rangle = \sum_{k=0}^{\infty} A_k \langle\phi|(\hat{J} - \langle\hat{J}\rangle)^k e^{i\alpha\hat{J}}|\phi\rangle \quad (2.216)$$

after a few terms:

$$\langle\phi|H_{approx}e^{i\alpha\hat{J}}|\phi\rangle = \sum_{k=0}^n A_k \langle\phi|(\hat{J} - \langle\hat{J}\rangle)^k e^{i\alpha\hat{J}}|\phi\rangle. \quad (2.217)$$

The  $(n+1)$  coefficients are determined by requiring that  $\langle\phi|He^{i\alpha\hat{J}}|\phi\rangle$  and  $\langle\phi|H_{approx}e^{i\alpha\hat{J}}|\phi\rangle$  along with their first  $n$  derivatives w.r.t.  $\alpha$  are equal at the point  $\alpha = 0$ . One thus ends up with the

<sup>70</sup>A similar terminology can also be constructed for Yang-Mills theory, which will in fact be done in chapter 3. In this terminology the Yang-Mills Hamiltonian also will be at most a two-body operator, i.e. contain up to four creation/annihilation operators.

<sup>71</sup> $\langle\hat{J}\rangle$  is used as an abbreviation for  $\langle\phi|\hat{J}|\phi\rangle$

<sup>72</sup>The idea to expand the Hamiltonian in powers of the symmetry generators, although with a different method to obtain the coefficients, was proposed in [Vil65a],[Vil65b], cf. also [MW69], [MW70].

<sup>73</sup>We assume here that there is no 'conspiracy' between different orders in the expansion, but this seems to be a plausible assumption.

set of equations<sup>74</sup>

$$\langle \phi | H(\hat{J} - \langle \hat{J} \rangle)^m | \phi \rangle = \sum_{k=0}^n A_k \langle \phi | (\hat{J} - \langle \hat{J} \rangle)^{k+m} | \phi \rangle, \quad (2.218)$$

where  $m = 0, \dots, n$ . After we have solved these equations to obtain  $A_i$ , we can insert  $H_{approx} = \sum_{k=0}^n A_k (\hat{J} - \langle \hat{J} \rangle)^k$  into the expression for the projected energy<sup>75</sup>

$$\begin{aligned} E_{approx}^{proj}(I) &= \frac{\langle \phi | H_{approx} \mathbf{P}^I | \phi \rangle}{\langle \phi | \mathbf{P}^I | \phi \rangle} = \int_0^{2\pi} \frac{d\alpha}{2\pi} \frac{\langle \phi | H_{approx} e^{i\alpha \hat{J}} | \phi \rangle}{\langle \phi | \mathbf{P}^I | \phi \rangle} \\ &= \sum_{k=0}^n A_k \int_0^{2\pi} \frac{d\alpha}{2\pi} \frac{\langle \phi | (\hat{J} - \langle \hat{J} \rangle)^k e^{i\alpha \hat{J}} | \phi \rangle}{\langle \phi | \mathbf{P}^I | \phi \rangle} = \sum_{k=0}^n A_k \frac{\langle \phi | (\hat{J} - \langle \hat{J} \rangle)^k \mathbf{P}^I | \phi \rangle}{\langle \phi | \mathbf{P}^I | \phi \rangle}. \end{aligned} \quad (2.219)$$

The advantage of the approach now becomes visible: whereas before we did not know how to evaluate the matrix elements including the projector, it has now become trivial;  $\mathbf{P}^I$  projects onto angular momentum  $I$ . Then  $\hat{J}\mathbf{P}^I = I\mathbf{P}^I$ , and numerator and denominator cancel, which means that we *do not have to calculate a single matrix element containing the projector explicitly*:

$$E^{proj}(I) = \sum_{k=0}^n A_k (I - \langle \hat{J} \rangle)^k. \quad (2.220)$$

In nuclear physics, for most applications  $n$  was taken to be one or two; one then ends up with<sup>76</sup>

$$E^{proj}(I) = \langle H \rangle + \frac{\langle H \Delta \hat{J} \rangle}{\langle (\Delta \hat{J})^2 \rangle} (I - \langle \hat{J} \rangle) \quad (2.221)$$

for  $n = 1$  and

$$E^{proj}(I) = \langle H \rangle - \frac{\langle \Delta \hat{J}^2 \rangle}{2\mathcal{I}_Y} + \frac{\langle \hat{J} \rangle}{\mathcal{I}_{sc}} (I - \langle \hat{J} \rangle) + \frac{1}{2\mathcal{I}_Y} (I - \langle \hat{J} \rangle)^2, \quad (2.222)$$

$$\text{with } \frac{1}{2\mathcal{I}_Y} = \frac{\langle H \Delta \hat{J}^2 \rangle - \langle H \rangle \langle \Delta \hat{J}^2 \rangle}{\langle \Delta \hat{J}^4 \rangle - \langle \Delta \hat{J}^2 \rangle^2} \quad \text{and} \quad \frac{\langle \hat{J} \rangle}{\mathcal{I}_{sc}} = \frac{\langle H \Delta \hat{J} \rangle}{\langle \Delta \hat{J}^2 \rangle} \quad (2.223)$$

for  $n = 2$  [RS80]. We have used the notation  $\Delta \hat{J} = \hat{J} - \langle \hat{J} \rangle$  and abbreviated  $\langle \phi | \dots | \phi \rangle$  by  $\langle \dots \rangle$ . We see that, at first order, we get no corrections to the mean field energy if  $\langle \hat{J} \rangle = I$ , whereas for the expansion to second order, we obtain even then a correction. One can interpret these corrections if one considers a deformed state as being a superposition of different angular momenta; especially, there are components in the wave function that are of higher angular momentum than the angular momentum one projects on. Usually one would assume that higher angular momenta also contain higher kinetic energy that should not be present in the projected

<sup>74</sup>In the field theory case below, the equations will look slightly different; this comes about since we multiply both sides of eq. (2.216) by the analogue of  $e^{-i\alpha I}$ , whereas here, we multiply both sides with  $e^{-i\alpha \langle \hat{J} \rangle}$ ; this should not affect the coefficients  $A_n$  (we will actually see that the coefficients in the field theory case are independent of  $I$ ), it only serves to give more compact formulas here.

<sup>75</sup>Let us draw at this point attention to the following difference in notation between sec. 2.1.6 and here: whereas in sec. 2.1.6  $\langle \dots \rangle$  was thought to include the projection already we have here the projector explicitly. This leads to e.g.  $\langle 1 \rangle_{\text{sec. 2.1.6}} = \langle \mathbf{P} \rangle_{\text{here}}$ .

<sup>76</sup>If we take simply  $n = 0$ , we obviously end up with  $A_0 = \langle H \rangle$  which is reassuring: the lowest order term just gives the unprojected expectation value.

wave function; thus one obtains negative corrections to the ordinary energy expectation value. One notes in passing that the moment of inertia  $1/\mathcal{I}_Y$  is quite different from  $1/\mathcal{I}_{sc}$ ; the latter one is associated with the cranking model. In fact one can show that, if the variational space considered for the cranking calculation contains<sup>77</sup> not only  $|\phi\rangle$  but also  $\Delta\hat{J}|\phi\rangle$ , then the solution of the cranking equations indeed solves also the variational equations derived for the  $n = 1$  Kamlah expansion, and that the Lagrange multiplier of the cranking model has precisely the same form as the first order correction of the Kamlah expansion [Man75].

There are calculations that seem to assume that in practice both moments of inertia are identical,  $\mathcal{I}_Y = \mathcal{I}_{sc}$  [HMVI98], [HIMV00], and that one can determine the moment of inertia  $\mathcal{I}_Y$  from a cranking type calculation. In Yang-Mills theory it turns out that to  $\mathcal{O}(g^0)$  they are indeed identical, but the explicit expressions given above don't give much hope that it stays this way for higher orders in perturbation theory.

If one goes from an Abelian type problem to a non-Abelian problem (like three dimensional angular momentum projection) one immediately has to face some problems [Sor77]; the first one is that a rigid body has two frames of reference (the lab frame and the internal frame), two sets of angular momentum operators and (since the total angular momentum is identical in the intrinsic and in the lab frame) three angular momentum quantum numbers (usually called I,K,M belonging to  $J^2 = I^2, J_3, I_3$ ). The basic ingredient into any projector is then

$$P_{KM}^I = |I, K\rangle\langle I, M|. \quad (2.224)$$

The quantum numbers I,K are those of the state to be observed in the lab frame, whereas M is only seen in the intrinsic frame. This object does not have the properties usually expected of a projector, since it is neither hermitian, nor do we have a relation like  $P^2 = P$ . The obvious remedy cannot be used, since taking  $P_{K=M,M}^I$  would avoid the mathematical problems but would violate rotational symmetry, as an 'intrinsic' state with  $M = 0$  would always lead to a state to be observed in the lab frame with  $K = 0$  [RS80]. One could also ask more physically: if  $M$  is an internal quantum number that has rather little to do with what can be observed in the lab frame, why don't we use

$$P_K^I = \sum_M f_M P_{KM}^I \quad (2.225)$$

as a projector with  $f_M$  as additional variational parameters (cf. e.g. [KO77]) ? In [Ka68] it was argued that one should take all  $f_M$  to be equal to one, but whatever one does, one always ends up with the problem that one has to evaluate matrix elements of operators acting upon projectors that do not carry the quantum numbers that are projected upon; to be concrete, one has e.g. to evaluate

$$\frac{\sum_{M,M'} \langle \psi | \vec{J} P_{MM'}^I | \psi \rangle}{\sum_{M,M'} \langle \psi | P_{MM'}^I | \psi \rangle}. \quad (2.226)$$

One sees clearly that, unlike in the Abelian case, the projector matrix elements do not usually cancel. A number of ways have been devised in the literature to approximately evaluate these sums, but they are not of interest here, since they cannot be transcribed to the field theory case. We only want to point to the fact that the difficulties even in the formulation of the projector do not come into play if we want to project onto a state with  $I = 0$ , since then there is only one projector  $P_{00}^0$  and no factors of  $f$  can be chosen. This is the case of the Yang-Mills projector

<sup>77</sup>The variational space that we use in field theory, consisting of Gaussian wave functionals, is not so large as would be required for this equivalence.

since we have combined the gluonic ( $\Gamma$ ) and the matter ( $\rho$ ) contribution into one set of operators  $\mathcal{G}$  which now are supposed to form an 's-wave'. The problem of non-factorizability of projectors and other operators will nevertheless also haunt us later on, too.

One last comment on the validity of the Kamlah expansion shall be made at this point. It is a priori not clear that it is physically sensible to perform the Kamlah expansion for a local symmetry. In nuclear physics, the very deformed states usually do not come about through a very deformed nucleus in space, but are due to a very large number of participating nucleons. In gauge field theory, one has usually the situation of a very small number of excitations at every point in space. Therefore it is not clear whether it is sensible to use the 'large-deformation' expansion. However, it will turn out that the Kamlah expansion performs very well in the cases we have considered.

### 2.6.2 Application to Electrodynamics

In this section, we want to apply the general principles outlined above to what we call electrodynamics - a quantized electromagnetic field interacting with static sources. It is illuminating since we will see that in marked contrast to nuclear physics, the first and second order expansions are quite different.

#### Kamlah Expansion to First Order

Here one starts from the expression

$$\langle H e^{i \int \phi(\Gamma-\rho)} \rangle = A_0 \langle e^{i \int \phi(\Gamma-\rho)} \rangle + A_1(\mathbf{y}) \langle \{\Gamma(\mathbf{y}) - \langle \Gamma(\mathbf{y}) \rangle\} e^{i \int \phi(\Gamma-\rho)} \rangle, \quad (2.227)$$

where we have used  $\int \phi(\Gamma-\rho)$  as an abbreviation for  $\int d^3z \phi(\mathbf{z})(\Gamma(\mathbf{z}) - \rho(\mathbf{z}))$ . A useful notation that will be used throughout the remainder of this section is

$$\Delta(\mathbf{x}) = \Gamma(\mathbf{x}) - \langle \Gamma(\mathbf{x}) \rangle, \quad \delta(\mathbf{x}) = \rho(\mathbf{x}) - \langle \Gamma(\mathbf{x}) \rangle. \quad (2.228)$$

The coefficient  $A_0$  is determined by setting  $\phi = 0$ :

$$A_0 = \langle H \rangle, \quad (2.229)$$

and for  $A_1(\mathbf{x})$ , we perform the functional derivative  $\delta/\delta\phi(\mathbf{x})$ , and set  $\phi = 0$  afterwards. Inserting the result for  $A_0$  into this equation, and noting that  $\langle H\rho(\mathbf{x}) \rangle = \langle H \rangle \rho(\mathbf{x})$  since  $\rho$  is just a c-number function, we obtain

$$\int A_1(\mathbf{y}) \langle \Delta(\mathbf{y}) \Delta(\mathbf{x}) \rangle = \langle H \Delta(\mathbf{x}) \rangle. \quad (2.230)$$

We introduce the functional inverse  $\Theta^{-1}(\mathbf{x}, \mathbf{y})$  of  $\langle \Delta(\mathbf{x}) \Delta(\mathbf{y}) \rangle$ , s.t.

$$\Theta^{-1}(\mathbf{x}, \mathbf{z}) \langle \Delta(\mathbf{z}) \Delta(\mathbf{y}) \rangle = \delta_{\mathbf{xy}} \quad (2.231)$$

and can now resolve eq. (2.230) to give

$$A_1(\mathbf{y}) = \langle H \Delta(\mathbf{x}) \rangle \Theta^{-1}(\mathbf{x}, \mathbf{y}). \quad (2.232)$$

Inserting this into eq. (2.227), integrating over  $\phi$  to obtain  $\int \mathcal{D}\phi e^{i \int \phi(\Gamma-\rho)} = \mathbf{P}^\rho$  and using  $\Gamma(\mathbf{x})\mathbf{P}^\rho = \rho(\mathbf{x})\mathbf{P}^\rho$ , we obtain for the projected energy functional

$$\frac{\langle H \mathbf{P}^\rho \rangle}{\langle \mathbf{P}^\rho \rangle} = \langle H \rangle + \langle H \Delta(\mathbf{x}) \rangle \Theta^{-1}(\mathbf{x}, \mathbf{y}) \delta(\mathbf{y}). \quad (2.233)$$



Note that the derivation can be carried out for any gauge-invariant few-body operator  $\mathcal{O}$ , since there is nothing special about the Hamiltonian:

$$\boxed{\frac{\langle \mathcal{O} \mathbf{P}^\rho \rangle}{\langle \mathbf{P}^\rho \rangle} = \langle \mathcal{O} \rangle + \langle \mathcal{O} \Delta(\mathbf{x}) \rangle \Theta^{-1}(\mathbf{x}, \mathbf{y}) \delta(\mathbf{y})}. \quad (2.234)$$

This provides a first test of the validity of the first-order Kamlah expansion. We may set  $\mathcal{O} = \Delta(\mathbf{z})$ , and obtain

$$\frac{\langle \Delta(\mathbf{z}) \mathbf{P}^\rho \rangle}{\langle \mathbf{P}^\rho \rangle} = \langle \Delta(\mathbf{z}) \rangle + \underbrace{\langle \Delta(\mathbf{z}) \Delta(\mathbf{x}) \rangle \Theta^{-1}(\mathbf{x}, \mathbf{y}) \delta(\mathbf{y})}_{= \delta_{\mathbf{z}\mathbf{y}}} = \rho(\mathbf{z}) - \langle \Gamma(\mathbf{z}) \rangle, \quad (2.235)$$

or in other words

$$\frac{\langle \Gamma(\mathbf{z}) \mathbf{P}^\rho \rangle}{\langle \mathbf{P}^\rho \rangle} = \rho(\mathbf{z}) \quad (2.236)$$

showing that the expression provided by the first order Kamlah expansion for  $\langle \Gamma(\mathbf{z}) \mathbf{P}^\rho \rangle / \langle \mathbf{P}^\rho \rangle$  is *exact*. It doesn't stay that way, however, if one considers e.g.  $\mathcal{O} = \Delta(\mathbf{z}_1) \Delta(\mathbf{z}_2)$  :

$$\frac{\langle \Delta(\mathbf{z}_1) \Delta(\mathbf{z}_2) \mathbf{P}^\rho \rangle}{\langle \mathbf{P}^\rho \rangle} = \langle \Delta(\mathbf{z}_1) \Delta(\mathbf{z}_2) \rangle + \underbrace{\langle \Delta(\mathbf{z}_1) \Delta(\mathbf{z}_2) \Delta(\mathbf{x}) \rangle \Theta^{-1}(\mathbf{x}, \mathbf{y}) \delta(\mathbf{y})}_{=0} = \langle \Delta(\mathbf{z}_1) \Delta(\mathbf{z}_2) \rangle, \quad (2.237)$$

where we have used that  $\langle \Delta(\mathbf{z}_1) \Delta(\mathbf{z}_2) \Delta(\mathbf{x}) \rangle = 0$ , which is true for every Gaussian state. We see that there are no corrections due to the projector for  $\Delta(\mathbf{z}_1) \Delta(\mathbf{z}_2)$  by the first order Kamlah formula. This gives rise to the expectation that the energy will not be correctly projected, since it contains terms of the type  $\langle \Gamma(\mathbf{x}) \Gamma(\mathbf{y}) \mathbf{P}^\rho \rangle$  (as we will see below, they arise from the kinetic energy).

We now start to evaluate the projected energy. For this it is useful to note that under a variety of assumptions<sup>78</sup>

$$\langle \mathbf{B}_i(\mathbf{x}) \mathbf{B}_j(\mathbf{y}) \Gamma(\mathbf{z}) \rangle = \langle \mathbf{B}_i(\mathbf{x}) \mathbf{B}_j(\mathbf{y}) \rangle \langle \Gamma(\mathbf{z}) \rangle, \quad (2.238)$$

i.e.  $\langle \mathbf{B}_i(\mathbf{x}) \mathbf{B}_j(\mathbf{y}) \Delta(\mathbf{z}) \rangle = 0$ . Physically it is plausible that the magnetic part of the energy should not be affected, since it contains the transversal degrees of freedom only. For the electrical field one obtains

$$\langle \mathbf{\Pi}_i(\mathbf{x}) \mathbf{\Pi}_i(\mathbf{x}) \Gamma(\mathbf{z}) \rangle = 2 \langle \mathbf{\Pi}_i(\mathbf{x}) \Delta(\mathbf{z}) \rangle \langle \mathbf{\Pi}_i(\mathbf{x}) \rangle + \langle \mathbf{\Pi}_i(\mathbf{x}) \mathbf{\Pi}_i(\mathbf{x}) \rangle \langle \Gamma(\mathbf{z}) \rangle, \quad (2.239)$$

which is valid even without integrating over  $\mathbf{x}$ . With this, the first order energy correction is given by

$$\langle H \Delta(\mathbf{z}) \rangle = \langle \mathbf{\Pi}_i(\mathbf{x}) \Delta(\mathbf{z}) \rangle \langle \mathbf{\Pi}_i(\mathbf{x}) \rangle. \quad (2.240)$$

In order to make any further progress, it seems that one has to assume that both  $G^{-1}$  and  $\Sigma$  are translationally invariant; then one can write

$$\langle \mathbf{\Pi}_i(\mathbf{x}) \mathbf{\Pi}_j(\mathbf{y}) \rangle_c = \frac{1}{4} G_{ij}^{-1}(\mathbf{x}, \mathbf{y}) + 4(\Sigma G \Sigma)_{ij}(\mathbf{x}, \mathbf{y}) = \int \frac{d^3 p}{(2\pi)^3} e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} (\tilde{\sigma}_L^{\mathbf{P}} \mathbf{P}_{ij}^{L\mathbf{P}} + \tilde{\sigma}_T^{\mathbf{P}} \mathbf{P}_{ij}^{T\mathbf{P}}) \quad (2.241)$$

<sup>78</sup>Either one may assume that the kernel in the Gaussian wave functional is purely real, i.e.  $\Sigma = 0$ , or that both  $G^{-1}$  and  $\Sigma$  are translation invariant, or that the background field  $\bar{\mathbf{B}}_i = \epsilon_{ijk} \nabla_j \bar{\mathbf{A}}_k$  fulfils the classical equations of motion.

which defines the longitudinal and transversal components  $\tilde{\sigma}_L, \tilde{\sigma}_T$ , and where we have used the abbreviation  $\mathbf{P}_{ij}^{LP}$  for  $\mathbf{p}_i \mathbf{p}_j / \mathbf{p}^2$ ; correspondingly  $\mathbf{P}_{ij}^{TP} = \delta_{ij} - \mathbf{P}_{ij}^{LP}$ . This expression allows an explicit expression for  $\Theta^{-1}(\mathbf{x}, \mathbf{y})$ :

$$\Theta^{-1}(\mathbf{x}, \mathbf{y}) = \int \frac{d^3 p}{(2\pi)^3} e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} \frac{1}{\mathbf{p}^2 \tilde{\sigma}_L^{\mathbf{p}}} \quad (2.242)$$

and thus

$$\begin{aligned} \langle H \Delta(\mathbf{x}_1) \rangle \Theta^{-1}(\mathbf{x}_1, \mathbf{y}) &= \langle \mathbf{\Pi}_i(\mathbf{x}) \rangle \langle \mathbf{\Pi}_i(\mathbf{x}) \Delta(\mathbf{x}_1) \rangle \Theta^{-1}(\mathbf{x}_1, \mathbf{y}) \\ &= \langle \mathbf{\Pi}_i(\mathbf{x}) \rangle \int \frac{d^3 q}{(2\pi)^3} \nabla_j^{\mathbf{x}_1} e^{i\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}_1)} (\tilde{\sigma}_L^{\mathbf{q}} \mathbf{P}_{ij}^{L\mathbf{q}} + \tilde{\sigma}_T^{\mathbf{q}} \mathbf{P}_{ij}^{T\mathbf{q}}) \Theta^{-1}(\mathbf{x}_1, \mathbf{y}) \\ &= \langle \mathbf{\Pi}_i(\mathbf{x}) \rangle \int \frac{d^3 q}{(2\pi)^3} e^{i\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}_1)} \frac{1}{i} \mathbf{q}_j (\tilde{\sigma}_L^{\mathbf{q}} \mathbf{P}_{ij}^{L\mathbf{q}} + \tilde{\sigma}_T^{\mathbf{q}} \mathbf{P}_{ij}^{T\mathbf{q}}) \Theta^{-1}(\mathbf{x}_1, \mathbf{y}) \\ &= \langle \mathbf{\Pi}_i(\mathbf{x}) \rangle \int \frac{d^3 q}{(2\pi)^3} e^{i\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}_1)} \frac{1}{i} \frac{\mathbf{q}_i}{\mathbf{q}^2} (\mathbf{q}^2 \tilde{\sigma}_L^{\mathbf{q}}) \Theta^{-1}(\mathbf{x}_1, \mathbf{y}) \\ &= \langle \mathbf{\Pi}_i(\mathbf{x}) \rangle \int \frac{d^3 q}{(2\pi)^3} \frac{1}{i^2} \frac{\nabla_i^{\mathbf{x}}}{\mathbf{q}^2} e^{i\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}_1)} (\mathbf{q}^2 \tilde{\sigma}_L^{\mathbf{q}}) \Theta^{-1}(\mathbf{x}_1, \mathbf{y}) \\ &= \langle \Gamma(\mathbf{x}) \rangle \left( -G_{\Delta}(\mathbf{x}, \mathbf{z}) \right) \underbrace{\Theta(\mathbf{z}, \mathbf{x}_1) \Theta^{-1}(\mathbf{x}_1, \mathbf{y})}_{=\delta_{\mathbf{z}\mathbf{y}}} \\ &= \langle \Gamma(\mathbf{x}) \rangle \left( -G_{\Delta}(\mathbf{x}, \mathbf{y}) \right). \end{aligned} \quad (2.243)$$

$G_{\Delta}$  denotes the Green's function of the (ordinary) Laplace operator, i.e.  $\nabla_i^{\mathbf{x}} \nabla_i^{\mathbf{x}} G_{\Delta}(\mathbf{x}, \mathbf{y}) = \delta_{\mathbf{x}\mathbf{y}}$ . Thus the projected energy reads

$$\frac{\langle H \mathbf{P}^{\rho} \rangle}{\langle \mathbf{P}^{\rho} \rangle} = \langle H \rangle - \langle \Gamma(\mathbf{x}) \rangle \left( -G_{\Delta}(\mathbf{x}, \mathbf{y}) \right) \left( \langle \Gamma(\mathbf{y}) \rangle - \rho(\mathbf{y}) \right). \quad (2.244)$$

We can make this expression even more transparent if we have a look at<sup>79</sup>  $\langle \mathbf{\Pi}_i^L(\mathbf{x}) \rangle \langle \mathbf{\Pi}_i^L(\mathbf{x}) \rangle$  where  $\mathbf{\Pi}_i^L(\mathbf{x})$  denotes the longitudinal component of  $\mathbf{\Pi}_i(\mathbf{x})$ . One can derive the identity

$$\langle \mathbf{\Pi}_i^L(\mathbf{x}) \rangle \langle \mathbf{\Pi}_i^L(\mathbf{x}) \rangle = \langle \Gamma(\mathbf{x}) \rangle \left( -G_{\Delta}(\mathbf{x}, \mathbf{y}) \right) \langle \Gamma(\mathbf{y}) \rangle, \quad (2.245)$$

and therefore one can write

$$\frac{\langle H \mathbf{P}^{\rho} \rangle}{\langle \mathbf{P}^{\rho} \rangle} = \langle H \rangle^P - \frac{1}{2} \left\{ \langle \Gamma(\mathbf{x}) \rangle \left( -G_{\Delta}(\mathbf{x}, \mathbf{y}) \right) \langle \Gamma(\mathbf{y}) \rangle - 2 \langle \Gamma(\mathbf{x}) \rangle \left( -G_{\Delta}(\mathbf{x}, \mathbf{y}) \right) \rho(\mathbf{y}) \right\}, \quad (2.246)$$

where  $\langle H \rangle^P$  denotes the part of the energy expectation value which is independent of  $\langle \mathbf{\Pi}^L \rangle$ , but which still<sup>80</sup> depends on  $\langle \mathbf{\Pi}^L \mathbf{\Pi}^L \rangle_c$ . Thus  $\langle \Gamma(\mathbf{x}) \rangle$  is determined to be equal to  $\rho(\mathbf{x})$  at the stationary point, giving the correct charge contribution to the energy

$$\frac{1}{2} \rho(\mathbf{x}) \left( -G_{\Delta}(\mathbf{x}, \mathbf{y}) \right) \rho(\mathbf{y}). \quad (2.247)$$

<sup>79</sup>Remember, in a Gaussian state, it makes sense to split  $\langle \mathbf{\Pi}_i(\mathbf{x}) \mathbf{\Pi}_i(\mathbf{x}) \rangle = \langle \mathbf{\Pi}_i(\mathbf{x}) \mathbf{\Pi}_i(\mathbf{x}) \rangle_c + \langle \mathbf{\Pi}_i(\mathbf{x}) \rangle \langle \mathbf{\Pi}_i(\mathbf{x}) \rangle$ .

<sup>80</sup>In formulas this is expressed simply by  $\langle H \rangle^P = \langle H \rangle - \frac{1}{2} \langle \mathbf{\Pi}_i^L(\mathbf{x}) \rangle \langle \mathbf{\Pi}_i^L(\mathbf{x}) \rangle$ .

As we have seen in the section about cranking, at the stationary point,  $\langle \mathbf{\Pi}^L \mathbf{\Pi}^L \rangle_c$  will be zero as well, s.t. the energy will depend only on the transversal degrees of freedom and on the charge density. However, the outcome is quite in contrast to what we expected from the Kamlah expansion initially: since we have computed the projected energy functional, (a) this should be completely independent of the gauge dependent degrees of freedom; thus, it should not depend on  $\langle \mathbf{\Pi}^L \mathbf{\Pi}^L \rangle_c$ , since in order to provide a non-vanishing expectation value  $\langle \mathbf{\Pi}^L \mathbf{\Pi}^L \rangle_c$  the wave functional has to depend on  $\mathbf{A}^L$ ; and (b) the state was assumed to be strongly deformed, but, if we take the first-order formalism seriously, at the stationary point our state is just *not deformed*, since  $\langle \mathbf{\Pi}^L \mathbf{\Pi}^L \rangle_c = 0$ . These problems are overcome by performing the Kamlah expansion to second order. Therefore, we will now turn to this.

### Kamlah Expansion to Second Order

Here one starts from the expression

$$\langle H e^{i \int \phi(\Gamma-\rho)} \rangle = A_0 \langle e^{i \int \phi(\Gamma-\rho)} \rangle + A_1(\mathbf{y}) \langle \{\Gamma(\mathbf{y}) - \langle \Gamma(\mathbf{y}) \rangle\} e^{i \int \phi(\Gamma-\rho)} \rangle + A_2(\mathbf{y}, \mathbf{z}) \langle \{\Gamma(\mathbf{y}) - \langle \Gamma(\mathbf{y}) \rangle\} \{\Gamma(\mathbf{z}) - \langle \Gamma(\mathbf{z}) \rangle\} e^{i \int \phi(\Gamma-\rho)} \rangle. \quad (2.248)$$

The coefficients will be determined in principle as above: one needs three equations, which are obtained by (a) setting  $\phi = 0$ , (b) performing a functional derivative w.r.t.  $\phi(\mathbf{x}_1)$  and setting  $\phi = 0$  afterwards, (c) performing two functional derivatives, w.r.t.  $\phi(\mathbf{x}_1), \phi(\mathbf{x}_2)$  and setting  $\phi = 0$  afterwards. After a bit of manipulation, one obtains

$$A_0 = \langle H \rangle - A_2(\mathbf{y}, \mathbf{z}) \langle \Delta(\mathbf{y}) \Delta(\mathbf{z}) \rangle, \quad (2.249)$$

$$A_1(\mathbf{y}) = (\langle H \Delta(\mathbf{x}_1) \rangle - A_2(\mathbf{y}_1, \mathbf{z}_1) \langle \Delta(\mathbf{y}_1) \Delta(\mathbf{z}_1) \Delta(\mathbf{x}_1) \rangle) \Theta^{-1}(\mathbf{x}_1, \mathbf{y}) \quad (2.250)$$

and for  $A_2$  one obtains an even less pleasant equation

$$\begin{aligned} & \langle H \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle - \langle H \rangle \langle \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle - \langle H \Delta(\mathbf{z}) \rangle \Theta^{-1}(\mathbf{z}, \mathbf{y}) \langle \Delta(\mathbf{y}) \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle \\ &= A_2(\mathbf{y}, \mathbf{z}) \left[ \langle \Delta(\mathbf{y}) \Delta(\mathbf{z}) \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle - \langle \Delta(\mathbf{y}) \Delta(\mathbf{z}) \rangle \langle \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle \right. \\ & \quad \left. - \langle \Delta(\mathbf{y}) \Delta(\mathbf{z}) \Delta(\mathbf{y}_1) \rangle \Theta^{-1}(\mathbf{y}_1, \mathbf{y}_2) \langle \Delta(\mathbf{y}_2) \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle \right]. \end{aligned} \quad (2.251)$$

This simplifies drastically if one exploits some of the factorization features of Gaussian states,

$$\langle \Delta(\mathbf{x}) \Delta(\mathbf{y}) \Delta(\mathbf{z}) \rangle = 0 \quad (2.252)$$

$$\begin{aligned} \langle \Delta(\mathbf{y}) \Delta(\mathbf{z}) \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle &= \langle \Delta(\mathbf{y}) \Delta(\mathbf{z}) \rangle \langle \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle + \langle \Delta(\mathbf{x}_1) \Delta(\mathbf{z}) \rangle \langle \Delta(\mathbf{y}) \Delta(\mathbf{x}_2) \rangle \\ & \quad + \langle \Delta(\mathbf{x}_2) \Delta(\mathbf{z}) \rangle \langle \Delta(\mathbf{x}_1) \Delta(\mathbf{y}) \rangle \end{aligned} \quad (2.253)$$

This allows to simplify eq. (2.251) drastically:

$$\begin{aligned} & \langle H \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle - \langle H \rangle \langle \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle \\ &= A_2(\mathbf{y}, \mathbf{z}) (\langle \Delta(\mathbf{y}) \Delta(\mathbf{x}_1) \rangle \langle \Delta(\mathbf{z}) \Delta(\mathbf{x}_2) \rangle + \langle \Delta(\mathbf{y}) \Delta(\mathbf{x}_2) \rangle \langle \Delta(\mathbf{z}) \Delta(\mathbf{x}_1) \rangle). \end{aligned} \quad (2.254)$$

In order to obtain  $A_2$  explicitly, we can again use  $\Theta^{-1}$ :

$$\begin{aligned} & \left( \langle \Delta(\mathbf{y}) \Delta(\mathbf{x}_1) \rangle \langle \Delta(\mathbf{z}) \Delta(\mathbf{x}_2) \rangle + \langle \Delta(\mathbf{y}) \Delta(\mathbf{x}_2) \rangle \langle \Delta(\mathbf{z}) \Delta(\mathbf{x}_1) \rangle \right) \frac{1}{2} \Theta^{-1}(\mathbf{x}_1, \mathbf{y}_1) \Theta^{-1}(\mathbf{x}_2, \mathbf{y}_2) \\ &= \frac{1}{2} (\delta_{\mathbf{y}\mathbf{y}_1} \delta_{\mathbf{z}\mathbf{y}_2} + \delta_{\mathbf{y}\mathbf{y}_2} \delta_{\mathbf{z}\mathbf{y}_1}). \end{aligned} \quad (2.255)$$

This can be inserted into the expression for  $A_0$ , and since  $\langle[\Gamma(\mathbf{y}), \Gamma(\mathbf{z})]\rangle = 0$  in electrodynamics, we obtain for the projected energy functional (using the notation  $\Delta H = H - \langle H \rangle$ ):

$$\begin{aligned} \frac{\langle H P^\rho \rangle}{\langle P^\rho \rangle} &= \langle H \rangle - \frac{1}{2} \langle \Delta H \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle \Theta^{-1}(\mathbf{x}_1, \mathbf{x}_2) - \langle \Delta H \Delta(\mathbf{x}_1) \rangle \Theta^{-1}(\mathbf{x}_1, \mathbf{y}_1) \langle \Gamma(\mathbf{y}_1) - \rho(\mathbf{y}_1) \rangle \\ &\quad + \frac{1}{2} \langle \Delta H \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle \Theta^{-1}(\mathbf{x}_1, \mathbf{y}_1) \Theta^{-1}(\mathbf{x}_2, \mathbf{y}_2) \langle \Gamma(\mathbf{y}_1) - \rho(\mathbf{y}_1) \rangle \langle \Gamma(\mathbf{y}_2) - \rho(\mathbf{y}_2) \rangle. \end{aligned} \quad (2.256)$$

As in the paragraph above, in the derivation no special property of  $H$  apart from gauge invariance was used, and therefore the expression is valid for every gauge-invariant few-body operator  $\mathcal{O}$ :

$$\begin{aligned} \frac{\langle \mathcal{O} P^\rho \rangle}{\langle P^\rho \rangle} &= \langle \mathcal{O} \rangle - \frac{1}{2} \langle \Delta \mathcal{O} \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle \Theta^{-1}(\mathbf{x}_1, \mathbf{x}_2) \\ &\quad - \langle \Delta \mathcal{O} \Delta(\mathbf{x}_1) \rangle \Theta^{-1}(\mathbf{x}_1, \mathbf{y}_1) \langle \Gamma(\mathbf{y}_1) - \rho(\mathbf{y}_1) \rangle \\ &\quad + \frac{1}{2} \langle \Delta \mathcal{O} \Delta(\mathbf{x}_1) \Delta(\mathbf{x}_2) \rangle \Theta^{-1}(\mathbf{x}_1, \mathbf{y}_1) \Theta^{-1}(\mathbf{x}_2, \mathbf{y}_2) \langle \Gamma(\mathbf{y}_1) - \rho(\mathbf{y}_1) \rangle \langle \Gamma(\mathbf{y}_2) - \rho(\mathbf{y}_2) \rangle. \end{aligned} \quad (2.257)$$

As in the first order case, we now have a look at  $\mathcal{O} = \Delta(\mathbf{z})$  and  $\mathcal{O} = \Delta(\mathbf{z}_1)\Delta(\mathbf{z}_2)$ :

$$\frac{\langle \Delta(\mathbf{z}) P^\rho \rangle}{\langle P^\rho \rangle} \stackrel{eq. (2.257)}{=} \rho(\mathbf{z}) - \langle \Gamma(\mathbf{z}) \rangle \quad (2.258)$$

which is the same result as in the first-order expansion, since all the additional terms due to second order vanish; next

$$\frac{\langle \Delta(\mathbf{z}_1)\Delta(\mathbf{z}_2) P^\rho \rangle}{\langle P^\rho \rangle} \stackrel{eq. (2.257)}{=} \langle \Gamma(\mathbf{z}_1) - \rho(\mathbf{z}_1) \rangle \langle \Gamma(\mathbf{z}_2) - \rho(\mathbf{z}_2) \rangle. \quad (2.259)$$

Thus, in the second-order Kamlah expansion, both  $\langle \Delta(\mathbf{z}) P^\rho \rangle / \langle P^\rho \rangle$  and  $\langle \Delta(\mathbf{z}_1)\Delta(\mathbf{z}_2) P^\rho \rangle / \langle P^\rho \rangle$  are reproduced<sup>81</sup> *exactly*. This gives rise to the hope that the energy, too, will be projected correctly, since it depends both on  $\langle \Gamma(\mathbf{x}) \rangle \langle \Gamma(\mathbf{y}) \rangle$  and on  $\langle \Gamma(\mathbf{x}) \Gamma(\mathbf{y}) \rangle$ . We will now turn to the evaluation of the energy. In addition to the terms we have computed above, we need to compute

<sup>81</sup>A certain pattern seems to emerge here: in the first-order expansion the expectation value of a single Gauss law operator between projected states was corrected, but not those of more operators (we checked the expectation value of  $\Delta(\mathbf{z}_1)\Delta(\mathbf{z}_2)$  in eq. (2.237)). In the second-order expansion the expectation values of up to two Gauss law operators between projected states were corrected, but not those of more operators (it is easy to convince oneself that  $\langle \Delta(\mathbf{z}_1)\Delta(\mathbf{z}_2)\Delta(\mathbf{z}_3) P^\rho \rangle / \langle P^\rho \rangle = -\langle \Delta(\mathbf{z}_1)\Delta(\mathbf{z}_2) \rangle \langle \Gamma(\mathbf{z}_3) - \rho(\mathbf{z}_3) \rangle + \text{permutations}$ ). Thus, we would expect in order to have the expectation values of up to three Gauss law operators corrected we need a third-order expansion etc, although we have not checked this explicitly. To what extent this pattern extends also to other operators is currently not known. The Gauss law operator is in this context obviously useful as a first check on the accuracy of the method, since one knows what to expect of the projected expectation value. One can give a further argument in support of the pattern found here. If we want to project correctly the product of  $n$  Gauss law operators we have to obtain a product of  $n$  charge distributions  $\rho$  from the Kamlah expression for the projected operator. We have seen that the coefficients  $A_i$  are independent of  $\rho$  so the only place where  $\rho$  does appear is in the terms  $(\langle \Gamma \rangle - \rho)^i$  (where for simplicity we haven't written out the product). But the highest power  $i$  that we obtain is equal to the order of the Kamlah expansion, i.e. a Kamlah expansion to second order includes at most terms  $\propto \rho^2$ . Thus the operator  $\Gamma^3$  can never be correctly projected to give  $\rho^3$  in the second order Kamlah expansion and a third order treatment would be called for.

$\langle \mathbf{B}_i(\mathbf{x})\mathbf{B}_j(\mathbf{y})\Gamma(\mathbf{z}_1)\Gamma(\mathbf{z}_2) \rangle$ . If we again take either  $\Sigma = 0$  or  $G^{-1}$  and  $\Sigma$  translationally invariant, the matrix element factorizes,

$$\langle \mathbf{B}_i(\mathbf{x})\mathbf{B}_j(\mathbf{y})\Gamma(\mathbf{z}_1)\Gamma(\mathbf{z}_2) \rangle = \langle \mathbf{B}_i(\mathbf{x})\mathbf{B}_j(\mathbf{y}) \rangle \langle \Gamma(\mathbf{z}_1)\Gamma(\mathbf{z}_2) \rangle \quad (2.260)$$

which is again plausible, since there should be no corrections to the magnetic part of the energy; it depends on the transversal degrees of freedom only. The next ingredient we have to compute for  $\langle \Delta H \Delta(\mathbf{x}_1)\Delta(\mathbf{x}_2) \rangle$  is the electric energy, which gives a rather simple contribution, too. We can evaluate it using the same factorization properties that underly eq. (2.253), and obtain altogether:

$$\langle \Delta H \Delta(\mathbf{x}_1)\Delta(\mathbf{x}_2) \rangle = \langle \Gamma(\mathbf{x}_2)\mathbf{\Pi}_i(\mathbf{x}) \rangle_c \langle \Gamma(\mathbf{x}_1)\mathbf{\Pi}_i(\mathbf{x}) \rangle_c. \quad (2.261)$$

This expression enters the correction of the mean-field energy

$$\frac{1}{2} \langle \Delta H \Delta(\mathbf{x}_1)\Delta(\mathbf{x}_2) \rangle \Theta^{-1}(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{2} \langle \mathbf{P}_{ij}^L(\mathbf{x}_1, \mathbf{x}_2)\mathbf{\Pi}_j(\mathbf{x}_2)\mathbf{\Pi}_i(\mathbf{x}_1) \rangle_c, \quad (2.262)$$

where  $\mathbf{P}_{ij}^L(\mathbf{x}_2, \mathbf{x}_1)$  denotes the longitudinal projector as defined<sup>82</sup> e.g. in eq. (A.16); translation invariance, that has been assumed before, implies that the electrical energy can be written as

$$\frac{1}{2} \langle \mathbf{\Pi}_i(\mathbf{x})\mathbf{\Pi}_i(\mathbf{x}) \rangle = \frac{1}{2} \langle \mathbf{P}_{ji}^L(\mathbf{y}, \mathbf{x})\mathbf{\Pi}_i(\mathbf{x})\mathbf{\Pi}_j(\mathbf{y}) \rangle + \frac{1}{2} \langle \mathbf{P}_{ji}^T(\mathbf{y}, \mathbf{x})\mathbf{\Pi}_j(\mathbf{x})\mathbf{\Pi}_i(\mathbf{y}) \rangle \quad (2.263)$$

and thus the second order Kamlah expansion precisely subtracts off the longitudinal (gauge variant) part of the kernel. The other term needed to compute  $\langle H \mathbf{P}^\rho \rangle / \langle \mathbf{P}^\rho \rangle$  is even simpler,

$$\frac{1}{2} \langle \Delta H \Delta(\mathbf{x}_1)\Delta(\mathbf{x}_2) \rangle \Theta^{-1}(\mathbf{x}_1, \mathbf{y}_1)\Theta^{-1}(\mathbf{x}_2, \mathbf{y}_2) = -G_\Delta(\mathbf{y}_1, \mathbf{y}_2). \quad (2.264)$$

Similar to the first-order discussion, we subtract off the part  $\langle \mathbf{\Pi}_i^L \rangle \langle \mathbf{\Pi}_i^L \rangle$  (thus completing  $\langle \mathbf{P}_{ji}^L \mathbf{\Pi}_i \mathbf{\Pi}_j \rangle_c$  to  $\langle \mathbf{P}_{ji}^L \mathbf{\Pi}_i \mathbf{\Pi}_j \rangle$ ) and add it back in afterwards. This gives a concise formula for the projected energy:

$$\boxed{\frac{\langle H \mathbf{P}^\rho \rangle}{\langle \mathbf{P}^\rho \rangle} = \langle H \rangle - \frac{1}{2} \langle \mathbf{P}_{ij}^L \mathbf{\Pi}_i \mathbf{\Pi}_j \rangle + \frac{1}{2} \rho(\mathbf{x}) \left( -G_\Delta(\mathbf{x}, \mathbf{y}) \right) \rho(\mathbf{y}).} \quad (2.265)$$

Note how different the outcome is from the first-order calculation: the projected energy is completely independent of the longitudinal parts of the electric field (both the expectation value and the correlator), and in turn they cannot be determined variationally. In the wave functional, the longitudinal parts are totally undetermined, which is what one wants since their value is prescribed by the projector. Thus we can conclude that, at least in electrodynamics, the second order Kamlah expansion is mandatory for a consistent formalism.

One amusing point might be noted at the end of this section; if one restricts the dimensionality of space-time to (1+1), there are no transversal components of  $\mathbf{A}$ ,  $\mathbf{\Pi}$ ; thus the projection to second order as carried out by the Kamlah expansion leaves behind only the interaction of static charges<sup>83</sup>.

<sup>82</sup>In this context there is no problem with the other definitions eqs. (A.17, A.18).

<sup>83</sup>Though we have not checked explicitly (by replacing Fourier integrals by sums etc), eq. (2.265) seems to suggest strongly that if we consider the theory on a compact spatial manifold in (1+1) dimensions, we would also keep - in addition to the energy of the charges - the spatially constant part of  $\mathbf{\Pi}$  (since this part is annihilated by the derivatives in the longitudinal projector, and is thus not subtracted), just as one would expect.

### 2.6.3 Application to Yang-Mills Theory

After the experience with the Kamlah expansion in electrodynamics, we want to try to apply it also to the Yang-Mills case. We will see, however, that we cannot incorporate charges as simply as in electrodynamics, and an explicit computation does not transcend the lowest order in perturbation theory (although the external field is treated to all orders). However, the outcome will be natural in view of the previous discussion of perturbative fulfilment of Gauss' law of sec. 2.4.

In order to discuss why we cannot include charges, the first order in the Kamlah expansion will be enough; we won't consider the first order any further than necessary for this purpose, since its shortcomings were already obvious in the discussion of the electrodynamic case. Again we start from the expression

$$\langle H e^{-i \int \varphi^a \mathcal{G}^a} \rangle = A_0 \langle e^{-i \int \varphi^a \mathcal{G}^a} \rangle + A_1^a(\mathbf{y}) \langle \Delta^a(\mathbf{y}) e^{-i \int \varphi^a \mathcal{G}^a} \rangle \quad (2.266)$$

where we have used the abbreviation  $\Delta^a(\mathbf{x}) = \Gamma^a(\mathbf{x}) - \langle \Gamma^a(\mathbf{x}) \rangle$ ; later on, we will also use<sup>84</sup>  $\delta^a(\mathbf{x}) = \rho^a(\mathbf{x}) - \langle \Gamma^a(\mathbf{x}) \rangle$ . In contrast to the previous section,  $\delta^a(\mathbf{x})$  is now an *operator*. As before, we obtain two equations to determine  $A_0, A_1$ :

$$\langle H \rangle = A_0, \quad (2.267)$$

$$\langle H \mathcal{G}^b(\mathbf{x}) \rangle = A_0 \langle H \mathcal{G}^b(\mathbf{x}) \rangle + A_1^a(\mathbf{y}) \langle \Delta^a(\mathbf{y}) \mathcal{G}^b(\mathbf{x}) \rangle. \quad (2.268)$$

In the following, we make the ansatz that our state  $|\rangle$  has the form  $|\text{fermion}\rangle|\text{YM}\rangle$ ; this is actually a restriction, since the most general state would obviously consist of a superposition of such states, but then the following formulas would become intractable. We then obtain<sup>85</sup>

$$\langle H \rangle = \langle \text{YM} | H | \text{YM} \rangle, \quad (2.269)$$

$$\langle H \mathcal{G}^b(\mathbf{x}) \rangle = -\langle \text{YM} | H \Gamma^b(\mathbf{x}) | \text{YM} \rangle + \langle \text{YM} | H | \text{YM} \rangle \langle f | \rho^b(\mathbf{x}) | f \rangle. \quad (2.270)$$

At this point we again introduce the functional inverse of  $\langle \text{YM} | \Delta^a(\mathbf{x}) \Delta^b(\mathbf{y}) | \text{YM} \rangle$ ,  $(\Theta^{-1})^{ab}(\mathbf{x}, \mathbf{y})$ , s.t.

$$(\Theta^{-1})^{ab}(\mathbf{x}, \mathbf{y}) \langle \text{YM} | \Delta^c(\mathbf{z}) \Delta^b(\mathbf{y}) | \text{YM} \rangle = \delta^{ab} \delta_{\mathbf{xy}}. \quad (2.271)$$

With its help, we can solve eq. (2.268) for  $A_1$ , and inserting both the expression for  $A_0$  and  $A_1$  into eq. (2.266), we obtain

$$\langle H e^{-i \int \varphi^a \mathcal{G}^a} \rangle = \langle H \rangle \langle e^{-i \int \varphi^a \mathcal{G}^a} \rangle + \langle \text{YM} | H \Gamma^a(\mathbf{x}) | \text{YM} \rangle (\Theta^{-1})^{ab}(\mathbf{x}, \mathbf{y}) \langle \Delta^b(\mathbf{y}) e^{-i \int \varphi^a \mathcal{G}^a} \rangle. \quad (2.272)$$

We may now integrate both sides over all configurations  $\varphi$  with trivial topology using the correct Haar measure. This results in

$$\langle H P^\rho \rangle = \langle H \rangle \langle P^\rho \rangle + \langle \text{YM} | H \Gamma^a(\mathbf{x}) | \text{YM} \rangle (\Theta^{-1})^{ab}(\mathbf{x}, \mathbf{y}) \langle \delta^b(\mathbf{y}) P^\rho \rangle, \quad (2.273)$$

<sup>84</sup>Here, a little care has to be taken w.r.t. the placement of  $g$ s. If we use 'perturbative scaling', i.e. the same scaling as in sec. 2.4, the generator of gauge transformations in the gluonic sector is not  $-\Gamma^a$ , but  $-\frac{1}{g}\Gamma^a$ . Thus the projector is in principle  $\int \mathcal{D}\varphi e^{-i \int g \varphi^a \mathcal{G}^a} = \int \mathcal{D}\varphi e^{i \int \varphi^a (\Gamma^a - g \rho^a)}$ . However, this explicit scaling will only be used later on when we have already done away with the charges; we use the 'non-perturbative scaling' while we are developing most of the formalism, and re-install explicit factors of  $g$  later on.

<sup>85</sup>The mass term of the fermions has been dropped from the Hamiltonian, since the mass depends only on the number of external charges, which is kept constant during the variational calculation.

where we have used that  $\Gamma^a(\mathbf{x})\mathcal{P}^\rho = \rho^a(\mathbf{x})\mathcal{P}^\rho$ . Here we see already that the results of electrodynamics do not generalize straightforwardly: there the fermionic states could be chosen as eigenstates of *all* charge operators. In Yang-Mills theory this is not possible (apart from non-charged states<sup>86</sup>), and therefore we cannot write

$$\langle \delta^b(\mathbf{y})\mathcal{P}^\rho \rangle = \langle \delta^b(\mathbf{y}) \rangle \langle \mathcal{P}^\rho \rangle. \quad (2.274)$$

Thus, we cannot get rid of all the projector integrals simply by considering the normalized projected energy expectation value  $\langle H\mathcal{P}^\rho \rangle / \langle \mathcal{P}^\rho \rangle$ . This, however, was the main appeal of the Kamlah expansion, and in order to rescue as much as possible of it, we will consider only uncharged states in the following: states that satisfy  $\langle f | \rho^a(\mathbf{x}) = 0$  and  $\rho^a(\mathbf{x}) | f \rangle = 0$ .

We will now turn to the second order Kamlah expansion. While determining the coefficients  $A_0, \dots, A_2$ , we still work with general (possibly charged) states; it will turn out that the coefficients are actually independent of whether we have a charged state or not. Thus we start from

$$\langle H e^{-i \int \varphi^a \mathcal{G}^a} \rangle = A_0 \langle e^{-i \int \varphi^a \mathcal{G}^a} \rangle + A_1^a(\mathbf{y}) \langle \Delta^a(\mathbf{y}) e^{-i \int \varphi^a \mathcal{G}^a} \rangle + A_2^{ab}(\mathbf{y}, \mathbf{z}) \langle \Delta^a(\mathbf{y}) \Delta^b(\mathbf{z}) e^{-i \int \varphi^a \mathcal{G}^a} \rangle. \quad (2.275)$$

It seems to be quite sensible to assume that  $A_2^{ab}(\mathbf{y}, \mathbf{z})$  should be symmetric under interchange of all indices, i.e.  $A_2^{ab}(\mathbf{y}, \mathbf{z}) = A_2^{ba}(\mathbf{z}, \mathbf{y})$ , since (a) most of  $\Delta^a(\mathbf{y})\Delta^b(\mathbf{z})$  is symmetric apart from  $\Gamma^a(\mathbf{y})\Gamma^b(\mathbf{z})$ , (b) the antisymmetric part of  $\Delta^a(\mathbf{y})\Delta^b(\mathbf{z})$  is  $-\frac{i}{2} f^{abc} \Gamma^c(\mathbf{y}) \delta_{\mathbf{y}\mathbf{z}}$  and should therefore rather be assigned to the term multiplying  $A_1$  from a systematic point of view. From eq. (2.275) we obtain three equations:

$$\langle H \rangle = A_0 + A_2^{ab}(\mathbf{y}, \mathbf{z}) \langle \Delta^a(\mathbf{y}) \Delta^b(\mathbf{z}) \rangle, \quad (2.276)$$

$$\begin{aligned} \langle H \mathcal{G}^c(\mathbf{x}) \rangle &= A_0 \langle \mathcal{G}^c(\mathbf{x}) \rangle + A_1^a(\mathbf{y}) \langle \Delta^a(\mathbf{y}) \mathcal{G}^c(\mathbf{x}) \rangle \\ &\quad + A_2^{ab}(\mathbf{y}, \mathbf{z}) \langle \Delta^a(\mathbf{y}) \Delta^b(\mathbf{z}) \mathcal{G}^c(\mathbf{x}) \rangle \end{aligned} \quad (2.277)$$

$$\begin{aligned} \langle H \frac{1}{2} \{ \mathcal{G}^{c_1}(\mathbf{x}_1), \mathcal{G}^{c_2}(\mathbf{x}_2) \} \rangle &= A_0 \langle \frac{1}{2} \{ \mathcal{G}^{c_1}(\mathbf{x}_1), \mathcal{G}^{c_2}(\mathbf{x}_2) \} \rangle + A_1^a(\mathbf{y}) \langle \Delta^a(\mathbf{y}) \frac{1}{2} \{ \mathcal{G}^{c_1}(\mathbf{x}_1), \mathcal{G}^{c_2}(\mathbf{x}_2) \} \rangle \\ &\quad + A_2^{ab}(\mathbf{y}, \mathbf{z}) \langle \Delta^a(\mathbf{y}) \Delta^b(\mathbf{z}) \frac{1}{2} \{ \mathcal{G}^{c_1}(\mathbf{x}_1), \mathcal{G}^{c_2}(\mathbf{x}_2) \} \rangle \end{aligned} \quad (2.278)$$

where in the last equation, eq. (2.278), we have used the abbreviation  $\{ \mathcal{G}^{c_1}(\mathbf{x}_1), \mathcal{G}^{c_2}(\mathbf{x}_2) \} = \mathcal{G}^{c_1}(\mathbf{x}_1) \mathcal{G}^{c_2}(\mathbf{x}_2) + \mathcal{G}^{c_2}(\mathbf{x}_2) \mathcal{G}^{c_1}(\mathbf{x}_1)$ . We then can - again - express  $A_0, A_1$  in terms of  $A_2$  and unprojected expectation values; the equation for  $A_2$  is very similar to eq. (2.251) in the electrodynamic calculation, but here it is even worse, since  $[\Delta^a(\mathbf{x}), \Delta^b(\mathbf{y})] \neq 0$ . Since we want to continue to perform analytic calculations, we first have to restrict ourselves to Gaussian states (as in electrodynamics). However, we have to make a second approximation, which is more severe: we will restrict the Gauss law operator to its  $\mathcal{O}(g^0)$  part<sup>87</sup>:

$$\Gamma^a(\mathbf{x}) = \hat{\mathbf{D}}_i^{ab}(\mathbf{x}) \Pi_i^b(\mathbf{x}) = (\hat{\mathbf{D}}_i^{ab}(\mathbf{x}) - g f^{acb} \mathbf{a}_i^c(\mathbf{x})) \Pi_i^b(\mathbf{x}) = \bar{\Gamma}^a(\mathbf{x}) - g f^{acb} \mathbf{a}_i^c(\mathbf{x}) \Pi_i^b(\mathbf{x}) = \bar{\Gamma}^a(\mathbf{x}) + \mathcal{O}(g), \quad (2.279)$$

<sup>86</sup>Of course, there is also another exception from the rule, namely if we have constructed our external charges s.t. they form a local colour singlet; with objects that transform under the fundamental representation of the gauge group this is possible only if the charges are localized at the same space point, which is quite useless for practical purposes such as calculating the static inter-quark potential.

<sup>87</sup>We use the same scalings as indicated in footnote 40 in sec. 2.3.4. We start with the 'non-perturbative scaling' and then replace  $\mathbf{A} \rightarrow \bar{\mathbf{A}} + g\mathbf{a}$ .

i.e.  $\bar{\Gamma}^a(\mathbf{x}) = \hat{\mathbf{D}}_i^{ab}(\mathbf{x})\mathbf{\Pi}_i^b(\mathbf{x})$ . This then will allow to use factorizability in a fashion identical to the case of electrodynamics:

$$\langle \bar{\Delta}^a(\mathbf{x})\bar{\Delta}^b(\mathbf{y})\bar{\Delta}^c(\mathbf{z}) \rangle = 0, \quad (2.280)$$

$$\begin{aligned} \langle \bar{\Delta}^a(\mathbf{y})\bar{\Delta}^b(\mathbf{z})\bar{\Delta}^{c_1}(\mathbf{x}_1)\bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle &= \langle \bar{\Delta}^a(\mathbf{y})\bar{\Delta}^b(\mathbf{z}) \rangle \langle \bar{\Delta}^{c_1}(\mathbf{x}_1)\bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle \\ &+ \langle \bar{\Delta}^{c_1}(\mathbf{x}_1)\bar{\Delta}^b(\mathbf{z}) \rangle \langle \bar{\Delta}^a(\mathbf{y})\bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle \\ &+ \langle \bar{\Delta}^{c_2}(\mathbf{x}_2)\bar{\Delta}^b(\mathbf{z}) \rangle \langle \bar{\Delta}^{c_1}(\mathbf{x}_1)\bar{\Delta}^a(\mathbf{y}) \rangle, \end{aligned} \quad (2.281)$$

where we have introduced the notation  $\bar{\Delta}^a(\mathbf{x}) = \bar{\Gamma}^a(\mathbf{x}) - \langle \bar{\Gamma}^a(\mathbf{x}) \rangle$ . However, this approximation has consequences; the first one is that we have reduced the non-Abelian  $SU(N)$  symmetry to an Abelian  $U(1)^{(N^2-1)}$  symmetry, since:

$$[\bar{\Gamma}^a(\mathbf{x}), \bar{\Gamma}^b(\mathbf{y})] = 0. \quad (2.282)$$

The second one has to do with the admissible background fields  $\bar{\mathbf{A}}$ ; it is clear that we cannot expect accuracy of the energy expectation value to order higher than  $\mathcal{O}(g^0)$ ; thus we approximate the Hamiltonian by its  $\mathcal{O}(g^0)$  contribution<sup>88</sup>. The kinetic energy remains unchanged, but the magnetic energy is simplified quite dramatically if we insert the decomposition  $\mathbf{A}_i^a(\mathbf{x}) = \bar{\mathbf{A}}_i^a(\mathbf{x}) + g\mathbf{a}_i^a(\mathbf{x})$  into  $\frac{1}{g^2}\mathbf{B}_i^a(\mathbf{x})\mathbf{B}_i^a(\mathbf{x})$  and neglect all terms of higher order than  $g^0$ :

$$\begin{aligned} &\frac{1}{g^2}\mathbf{B}_i^a(\mathbf{x})\mathbf{B}_i^a(\mathbf{x}) \\ &= \frac{1}{g^2}\bar{\mathbf{B}}_i^a(\mathbf{x})\bar{\mathbf{B}}_i^a(\mathbf{x}) + \frac{2}{g}\bar{\mathbf{B}}_i^a(\mathbf{x})\epsilon_{ij_1k_1}(\hat{\mathbf{D}}_{j_1}^{ac_1}(\mathbf{x})\delta_{\mathbf{xz}_1})\mathbf{a}_{k_1}^{c_1}(\mathbf{z}_1) \end{aligned} \quad (2.283)$$

$$\begin{aligned} &+ \left( \epsilon_{ij_1k_1}(\hat{\mathbf{D}}_{j_1}^{ac_1}(\mathbf{x})\delta_{\mathbf{xz}_1})\epsilon_{ij_2k_2}(\hat{\mathbf{D}}_{j_2}^{ac_2}(\mathbf{x})\delta_{\mathbf{xz}_2}) - \bar{\mathbf{B}}_i^a(\mathbf{x})f^{ac_1c_2}\epsilon_{ik_1k_2}\delta_{\mathbf{xz}_1}\delta_{\mathbf{xz}_2} \right) \mathbf{a}_{k_1}^{c_1}(\mathbf{z}_1)\mathbf{a}_{k_2}^{c_2}(\mathbf{z}_2). \\ &= \frac{1}{g^2}\bar{\mathbf{B}}_i^a(\mathbf{x})\bar{\mathbf{B}}_i^a(\mathbf{x}) + \frac{2}{g}J_{k_1}^{c_1}(\mathbf{x}; \mathbf{z}_1)\mathbf{a}_{k_1}^{c_1}(\mathbf{z}_1) + M_{k_1k_2}^{c_1c_2}(\mathbf{x}; \mathbf{z}_1, \mathbf{z}_2)\mathbf{a}_{k_1}^{c_1}(\mathbf{z}_1)\mathbf{a}_{k_2}^{c_2}(\mathbf{z}_2). \end{aligned} \quad (2.284)$$

For eqs. (2.283, 2.284) to be valid we don't have to integrate over  $\mathbf{x}$ . The restriction on  $\bar{\mathbf{A}}$  comes about from the requirement that the approximated Hamiltonian should commute with the approximated Gauss law operator, otherwise the (implicit) assumption of the Kamlah expansion - that in the beginning the Hamiltonian commutes with the projector - is incorrect. That one can obtain a non-trivial condition at all results from the fact that, to  $\mathcal{O}(g^0)$  of the commutator of the full quantities, one gets also a cross term from the  $\mathcal{O}(g^{-1})$  part of  $\mathbf{B}^2$  with the  $\mathcal{O}(g^1)$  part of  $\Gamma$ . Thus we can express the requirement of gauge invariance of the approximated Hamiltonian in two different ways: (a) the term of order  $g^{-1}$  in eq. (2.284) should vanish, since then there can be no cross term with the  $\mathcal{O}(g^1)$  contribution to  $\Gamma$ . With a partial integration, we see that this condition can be written as

$$\epsilon_{ij_1k_1}\hat{\mathbf{D}}_{j_1}^{c_1a}(\mathbf{x})\bar{\mathbf{B}}_i^a(\mathbf{x}) = -\hat{\mathbf{D}}_{j_1}^{c_1a}(\mathbf{x})F_{j_1k_1}^a(\mathbf{x}), \quad (2.285)$$

which is nothing but the classical equation of motion eq. (1.16), since  $F$  is the field strength tensor. (b) the commutator  $\frac{1}{g^2}[\mathbf{B}^2, \bar{\Gamma}]$  should vanish. We can compute the commutator and obtain

$$\frac{1}{g^2}[\mathbf{B}_i^a(\mathbf{x})\mathbf{B}_i^a(\mathbf{x}), \bar{\Gamma}^b(\mathbf{y})] = 2\hat{\mathbf{D}}_{l_1}^{bb_1}(\mathbf{y})M_{l_1k_2}^{b_1c_2}(\mathbf{x}; \mathbf{y}, \mathbf{z}_2)\mathbf{a}_{k_2}^{c_2}(\mathbf{z}_2) \stackrel{!}{=} 0, \quad (2.286)$$

<sup>88</sup>This approximation is also sensible from another point of view: the  $\mathcal{O}(g^0)$  contribution of the Hamiltonian is at most quadratic in the operators  $\mathbf{A}$  and  $\mathbf{\Pi}$  and from the case of electrodynamics one expects that the second-order Kamlah expansion treats correctly only (projected) expectation values of up to two operators, cf. footnote 81.



where we have used the fact that  $M$  is symmetric under interchange of all its indices. This is of course equivalent to condition (a), and thus to the requirement of the background field fulfilling the classical equations of motion<sup>89</sup>. This form will be useful later on.

We now use the factorization properties to compute  $A_2$  (or, if we hadn't required  $A_2$  to be symmetric from the outset, the symmetric part of  $A_2$ ; but since the  $\bar{\Gamma}$ s commute anyway, the distinction does not play a role):

$$A_2^{d_1 d_2}(\mathbf{y}_1, \mathbf{y}_2) = \frac{1}{2} [\langle H \bar{\Delta}^{c_1}(\mathbf{x}_1) \bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle - \langle H \rangle \langle \bar{\Delta}^{c_1}(\mathbf{x}_1) \bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle] (\Theta^{-1})^{c_1 d_1}(\mathbf{x}_1, \mathbf{y}_1) (\Theta^{-1})^{c_2 d_2}(\mathbf{x}_2, \mathbf{y}_2). \quad (2.287)$$

With this, we can give now explicitly the projected, normalized energy functional to second order in the Kamlah expansion:

$$\begin{aligned} \frac{\langle HP \rangle}{\langle P \rangle} &= \langle H \rangle - \frac{1}{2} \langle \Delta H \bar{\Delta}^{c_1}(\mathbf{x}_1) \bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle (\Theta^{-1})^{c_2 c_1}(\mathbf{x}_2, \mathbf{x}_1) \\ &\quad - \langle \Delta H \bar{\Delta}^{c_1}(\mathbf{x}_1) \rangle (\Theta^{-1})^{c_1 c_2}(\mathbf{x}_1, \mathbf{x}_2) \langle \Gamma^{c_2}(\mathbf{x}_2) \rangle \\ &\quad + \frac{1}{2} \langle \Delta H \bar{\Delta}^{c_1}(\mathbf{x}_1) \bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle (\Theta^{-1})^{c_1 d_1}(\mathbf{x}_1, \mathbf{y}_1) (\Theta^{-1})^{c_2 d_2}(\mathbf{x}_2, \mathbf{y}_2) \langle \Gamma^{d_1}(\mathbf{y}_1) \rangle \langle \Gamma^{d_2}(\mathbf{y}_2) \rangle. \end{aligned} \quad (2.288)$$

As in the case of electrodynamics, we may here also insert  $\bar{\Gamma}$  into the Kamlah expansion<sup>90</sup> instead of  $H$ . If we do this, the terms analogous to the second and the fourth term in eq. (2.288) (with  $H$  replaced by  $\bar{\Gamma}^a$ ) are zero, and the terms analogous to the first and third term cancel, so that we obtain the correct result  $\langle \bar{\Gamma}^a P \rangle = 0$ . The computation can also be carried out for  $\langle \bar{\Gamma}^a \bar{\Gamma}^b P \rangle / \langle P \rangle$ , and one obtains also the correct result, namely 0; the term analogous to the second term gives  $-\langle \bar{\Delta}^a \bar{\Delta}^b \rangle$ , whereas the terms analogous to the third and fourth term add up to give  $-\langle \bar{\Gamma}^a \rangle \langle \bar{\Gamma}^b \rangle$ , thus cancelling (together with the term analogous to the second) the term analogous to the first term.

In order to be able to compute the projected energy functional to  $\mathcal{O}(g^0)$ , we now need the following ingredients:

$$\langle \Delta(\mathbf{\Pi}_i^a(\mathbf{x}) \mathbf{\Pi}_i^a(\mathbf{x})) \bar{\Delta}^{c_1}(\mathbf{x}_1) \rangle = 2 \langle \mathbf{\Pi}_i^a(\mathbf{x}) \bar{\Delta}^{c_1}(\mathbf{x}_1) \rangle \langle \mathbf{\Pi}_i^a(\mathbf{x}) \rangle, \quad (2.289)$$

$$\langle \Delta(\mathbf{\Pi}_i^a(\mathbf{x}) \mathbf{\Pi}_i^a(\mathbf{x})) \bar{\Delta}^{c_1}(\mathbf{x}_1) \bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle = 2 \langle \mathbf{\Pi}_i^a(\mathbf{x}) \bar{\Delta}^{c_1}(\mathbf{x}_1) \rangle \langle \mathbf{\Pi}_i^a(\mathbf{x}) \bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle, \quad (2.290)$$

$$\langle \Delta(\mathbf{B}_i^a(\mathbf{x}) \mathbf{B}_i^a(\mathbf{x})) \bar{\Delta}^{c_1}(\mathbf{x}_1) \rangle = 0, \quad (2.291)$$

$$\begin{aligned} \langle \mathbf{B}_i^a(\mathbf{x}) \mathbf{B}_i^a(\mathbf{x}) \bar{\Gamma}^{c_1}(\mathbf{x}_1) \bar{\Gamma}^{c_2}(\mathbf{x}_2) \rangle &= -\frac{1}{2} \int d^3x \hat{\mathbf{D}}_{l_1}^{c_1 d_1}(\mathbf{x}_1) \hat{\mathbf{D}}_{l_2}^{c_2 d_2}(\mathbf{x}_2) M_{l_1 l_2}^{d_1 d_2}(\mathbf{x}; \mathbf{x}_1, \mathbf{x}_2) \\ &= 0, \end{aligned} \quad (2.292)$$

where we have set  $\Sigma$  to zero here and the remaining computations of this section. Also the expression  $\int d^3x \hat{\mathbf{D}}_{l_1}^{c_1 d_1}(\mathbf{x}_1) \hat{\mathbf{D}}_{l_2}^{c_2 d_2}(\mathbf{x}_2) M_{l_1 l_2}^{d_1 d_2}(\mathbf{x}; \mathbf{x}_1, \mathbf{x}_2)$  requires a bit of special attention: there is no integration over  $\mathbf{x}_1, \mathbf{x}_2$  although they appear more than once, but we have to integrate over  $\mathbf{x}$ , although it seems to appear only once (but this is an artifact of the notation introduced in eq. (2.284)). The last identity eq. (2.292) is true since we had to restrict the allowed background fields to fulfil the classical equations as discussed above. In addition, we need a simple expression for  $\Theta^{-1}$ ; in the electrodynamics calculation we saw that we had to assume translational invariance

<sup>89</sup>In the electrodynamical case there is no  $\mathcal{O}(g^1)$  contribution to the Gauss law operator and hence the whole discussion is not necessary.

<sup>90</sup>This is due to the fact that  $\bar{\Gamma}^a$  is gauge-invariant w.r.t. gauge transformations carried out by  $e^{i\varphi^a \bar{\Gamma}^a}$ .

of  $G, \Sigma$ . Here we'll need something similar, namely

$$\begin{aligned} (G^{-1})_{ij}^{ab}(\mathbf{x}, \mathbf{y}) &= (\Pi_L)_{i_1}^{ac_1}(\mathbf{x}, \mathbf{x}_1)(G^{-1})_{i_1 i_2}^{c_1 c_2}(\mathbf{x}_1, \mathbf{x}_2)(\Pi_L)_{i_2 j}^{c_2 b}(\mathbf{x}_2, \mathbf{y}) \\ &\quad + (\Pi_T)_{i_1}^{ac_1}(\mathbf{x}, \mathbf{x}_1)(G^{-1})_{i_1 i_2}^{c_1 c_2}(\mathbf{x}_1, \mathbf{x}_2)(\Pi_T)_{i_2 j}^{c_2 b}(\mathbf{x}_2, \mathbf{y}) \\ &= (G_{LL}^{-1})_{ij}^{ab}(\mathbf{x}, \mathbf{y}) + (G_{TT}^{-1})_{ij}^{ab}(\mathbf{x}, \mathbf{y}) \end{aligned} \quad (2.293)$$

with the (generalized) longitudinal projector<sup>91</sup>

$$(\Pi_L)_{ij}^{ab}(\mathbf{x}, \mathbf{y}) = \hat{\mathbf{D}}_i^{ac}(\mathbf{x})G_{\Delta}^{cd}(\mathbf{x}, \mathbf{y})\hat{\mathbf{D}}_j^{db}(\mathbf{y}), \quad \text{where } (\hat{\mathbf{D}}\hat{\mathbf{D}})^{ac}(\mathbf{x})G_{\Delta}^{cb}(\mathbf{x}, \mathbf{y}) = \delta^{ab}\delta_{\mathbf{xy}}, \quad (2.294)$$

(no integration over  $\mathbf{x}, \mathbf{y}$ ) and the (generalized) transversal projector  $(\Pi_T)_{ij}^{ab}(\mathbf{x}, \mathbf{y}) = \delta^{ab}\delta_{ij}\delta_{\mathbf{xy}} - (\Pi_L)_{ij}^{ab}(\mathbf{x}, \mathbf{y})$ . Thus, we don't want to allow for cross terms  $\Pi_L G^{-1} \Pi_T, \Pi_T G^{-1} \Pi_L$  being non-zero. For the explicit construction of  $\Theta^{-1}$  this has the advantage that one can invert the longitudinal and transversal parts individually:

$$(G_{LL}^{-1})_{ij}^{ab}(\mathbf{x}, \mathbf{y})(G_{LL})_{jk}^{bc}(\mathbf{y}, \mathbf{z}) = (\Pi_L)_{ik}^{ac}(\mathbf{x}, \mathbf{z}) \quad \text{and} \quad (G_{TT}^{-1})_{ij}^{ab}(\mathbf{x}, \mathbf{y})(G_{TT})_{jk}^{bc}(\mathbf{y}, \mathbf{z}) = (\Pi_T)_{ik}^{ac}(\mathbf{x}, \mathbf{z}). \quad (2.295)$$

We now want to relate the inverse of  $\hat{\mathbf{D}}_i \hat{\mathbf{D}}_j (G^{-1})$  to  $\hat{\mathbf{D}}_i \hat{\mathbf{D}}_j G$ : we start with the observation that, since  $G_{LL}^{-1} = \Pi_L G^{-1} \Pi_L$ , we can write (no integration over  $\mathbf{x}, \mathbf{z}$ )

$$(G_{LL}^{-1})_{ij}^{ab}(\mathbf{x}, \mathbf{z}) = \hat{\mathbf{D}}_i^{ac_1}(\mathbf{x})\hat{\mathbf{D}}_j^{bc_2}(\mathbf{z})(H_L)^{c_1 c_2}(\mathbf{x}, \mathbf{z}) \quad (2.296)$$

and correspondingly (again no integration over  $\mathbf{x}, \mathbf{z}$ )

$$(G_{LL})_{ij}^{ab}(\mathbf{x}, \mathbf{z}) = \hat{\mathbf{D}}_i^{ac_1}(\mathbf{x})\hat{\mathbf{D}}_j^{bc_2}(\mathbf{z})(K_L)^{c_1 c_2}(\mathbf{x}, \mathbf{z}), \quad (2.297)$$

where  $H_L, K_L$  are auxiliary functions that have the important characteristic that they don't carry spatial indices. From the requirement  $\int d^3 y (G_{LL}^{-1})_{ij}^{ab}(\mathbf{x}, \mathbf{y})(G_{LL})_{jk}^{bc}(\mathbf{y}, \mathbf{z}) = (\Pi_L)_{ik}^{ac}(\mathbf{x}, \mathbf{z})$  we obtain

$$G_{\Delta}^{a_1 c_1}(\mathbf{x}, \mathbf{y}) = \int d^3 z \left( (\hat{\mathbf{D}}\hat{\mathbf{D}})^{b_2 b_1}(\mathbf{z})(H_L)^{a_1 b_1}(\mathbf{x}, \mathbf{z}) \right) (K_L)^{b_2 c_1}(\mathbf{z}, \mathbf{y}). \quad (2.298)$$

If on the other hand we start from the defining equation of  $\Theta^{-1}$

$$\int d^3 y \left( \frac{1}{4} \hat{\mathbf{D}}_i^{ab_1}(\mathbf{x})\hat{\mathbf{D}}_j^{bb_2}(\mathbf{y})(G^{-1})_{ij}^{b_1 b_2}(\mathbf{x}, \mathbf{y}) \right) (\Theta^{-1})^{bc}(\mathbf{y}, \mathbf{z}) = \delta^{ac}\delta_{\mathbf{xz}} \quad (2.299)$$

we end up with

$$4G_{\Delta}^{a_1 c_1}(\mathbf{x}, \mathbf{y}) = \int d^3 z \left( (\hat{\mathbf{D}}\hat{\mathbf{D}})^{b_2 b_1}(\mathbf{z})(H_L)^{a_1 b_1}(\mathbf{x}, \mathbf{z}) \right) (\Theta^{-1})^{b_2 c_1}(\mathbf{z}, \mathbf{y}). \quad (2.300)$$

From the comparison of eq. (2.300) with eq. (2.298), we obtain

$$(\Theta^{-1})^{b_2 c_1}(\mathbf{z}, \mathbf{y}) = 4(K_L)^{b_2 c_1}(\mathbf{z}, \mathbf{y}) \quad (2.301)$$

and thus conclude

$$\boxed{\hat{\mathbf{D}}_i^{bb_1}(\mathbf{x})\hat{\mathbf{D}}_j^{cb_2}(\mathbf{y})(\Theta^{-1})^{b_1 b_2}(\mathbf{x}, \mathbf{y}) = 4(G_{LL})_{ij}^{bc}(\mathbf{x}, \mathbf{y})}, \quad (2.302)$$

<sup>91</sup>Some properties of generalized projectors are given in appendix A.6.

where again we don't integrate over  $\mathbf{x}, \mathbf{y}$ . We can now compute the correction terms to the Kamlah expansion very easily, using the fact that e.g.  $\langle \mathbf{\Pi}_i^a(\mathbf{x}) \bar{\Delta}^b(\mathbf{y}) \rangle = \hat{\mathbf{D}}_j^{bc}(\mathbf{y})(G_{LL}^{-1})_{ij}^{ac}(\mathbf{x}, \mathbf{y})$ ,

$$\begin{aligned}
 \text{first term :} & \quad \langle \Delta(\mathbf{\Pi}_i^a(\mathbf{x}) \mathbf{\Pi}_i^a(\mathbf{x})) \bar{\Delta}^{c_1}(\mathbf{x}_1) \bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle (\Theta^{-1})^{c_1 c_2}(\mathbf{x}_1, \mathbf{x}_2) \\
 & = 2(\Pi_L)_{i_2 i_1}^{c_2 c_1}(\mathbf{x}_2, \mathbf{x}_1) \langle \mathbf{\Pi}_{i_1}^{c_1}(\mathbf{x}_1) \mathbf{\Pi}_{i_2}^{c_2}(\mathbf{x}_2) \rangle_c \\
 \text{second term :} & \quad \langle \mathbf{\Pi}_i^a(\mathbf{x}) \mathbf{\Pi}_i^a(\mathbf{x}) \bar{\Delta}^{c_1}(\mathbf{x}_1) \rangle (\Theta^{-1})^{c_1 c_2}(\mathbf{x}_1, \mathbf{x}_2) \langle \bar{\Gamma}^{c_2}(\mathbf{x}_2) \rangle \\
 & = 2(\Pi_L)_{i_2 i_1}^{c_2 c_1}(\mathbf{x}_2, \mathbf{x}_1) \langle \mathbf{\Pi}_{i_1}^{c_1}(\mathbf{x}_1) \rangle \langle \mathbf{\Pi}_{i_2}^{c_2}(\mathbf{x}_2) \rangle \\
 \text{third term :} & \quad \langle \Delta(\mathbf{\Pi}_i^a(\mathbf{x}) \mathbf{\Pi}_i^a(\mathbf{x})) \bar{\Delta}^{c_1}(\mathbf{x}_1) \bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle (\Theta^{-1})^{c_1 d_1}(\mathbf{x}_1, \mathbf{y}_1) (\Theta^{-1})^{c_2 d_2}(\mathbf{x}_2, \mathbf{y}_2) \langle \bar{\Gamma}^{d_1}(\mathbf{y}_1) \rangle \langle \bar{\Gamma}^{d_2}(\mathbf{y}_2) \rangle \\
 & = 2(\Pi_L)_{i_2 i_1}^{c_2 c_1}(\mathbf{x}_2, \mathbf{x}_1) \langle \mathbf{\Pi}_{i_1}^{c_1}(\mathbf{x}_1) \rangle \langle \mathbf{\Pi}_{i_2}^{c_2}(\mathbf{x}_2) \rangle.
 \end{aligned}$$

This gives an overall correction to the electric energy of

$$-\frac{1}{2} \int d^3 x_1 d^3 x_2 (\Pi_L)_{i_2 i_1}^{c_2 c_1}(\mathbf{x}_2, \mathbf{x}_1) \langle \mathbf{\Pi}_{i_1}^{c_1}(\mathbf{x}_1) \mathbf{\Pi}_{i_2}^{c_2}(\mathbf{x}_2) \rangle \quad (2.303)$$

Thus, the electrical energy neither contains  $\hat{\mathbf{D}}\bar{\mathbf{e}}$  nor the (generalized) longitudinal component of  $G^{-1}$ . Since by requirement of approximate gauge invariance the magnetic energy is transversal as well, this is true for the total energy, and to  $\mathcal{O}(g^0)$ , we can write

$$\boxed{
 \begin{aligned}
 \frac{\langle HP \rangle}{\langle P \rangle} & = \frac{1}{2} \int d^3 x_1 d^3 x_2 (\Pi_T)_{i_2 i_1}^{c_2 c_1}(\mathbf{x}_2, \mathbf{x}_1) \langle \mathbf{\Pi}_{i_1}^{c_1}(\mathbf{x}_1) \mathbf{\Pi}_{i_2}^{c_2}(\mathbf{x}_2) \rangle \\
 & + \frac{1}{2} \int d^3 x \left\{ \frac{1}{g^2} \bar{\mathbf{B}}_i^a(\mathbf{x}) \bar{\mathbf{B}}_i^a(\mathbf{x}) + \text{tr}(MG_{\mathbf{xy}})|_{\mathbf{y} \rightarrow \mathbf{x}} \right\},
 \end{aligned}
 } \quad (2.304)$$

where we use  $M$  as it was defined in sec. 2.3.5, s.t.  $\text{tr}(MG_{\mathbf{xy}}) = \text{tr}((\hat{\mathbf{D}}(\mathbf{x})\hat{\mathbf{D}}(\mathbf{x}) - \hat{\mathbf{B}}(\mathbf{x}))G_{\mathbf{xy}})$ . Writing the kinetic energy also in terms of  $G^{-1}$  and  $\bar{\mathbf{e}}$ , the energy is given as

$$\begin{aligned}
 E_{\text{proj}} = \frac{\langle HP \rangle}{\langle P \rangle} & = \frac{1}{2} \int d^3 x_1 d^3 x_2 \{ (\Pi_T)_{i_2 i_1}^{c_2 c_1}(\mathbf{x}_2, \mathbf{x}_1) \bar{\mathbf{e}}_{i_1}^{c_1}(\mathbf{x}_1) \bar{\mathbf{e}}_{i_2}^{c_2}(\mathbf{x}_2) \} + \frac{1}{8} \text{Tr}(G_{TT}^{-1}) \\
 & + \frac{1}{2} \int d^3 x \left\{ \frac{1}{g^2} \bar{\mathbf{B}}_i^a(\mathbf{x}) \bar{\mathbf{B}}_i^a(\mathbf{x}) + \text{tr}(MG_{\mathbf{xy}})|_{\mathbf{y} \rightarrow \mathbf{x}} \right\}.
 \end{aligned} \quad (2.305)$$

We see that the projected energy is in fact independent of the (generalized) longitudinal components of  $\bar{\mathbf{e}}$  and  $G^{-1}$ . This is what we would expect from the projector: we treat it to  $\mathcal{O}(g^0)$ , and we obtain an energy functional that is compatible with the energy functional of a state that is annihilated to  $\mathcal{O}(g^0)$  by the Gauss law operator. Perturbation theory thus seems not to invalidate the treatment of the Kamlah expansion. It is interesting to note that eq. (2.305) is (at least formally) identical to the improved energy functional obtained in [HIMV00] in the case of magnetic background fields, to the same order in perturbation theory as considered here. One difference, however, should be noted: in our treatment the condition that  $\bar{\mathbf{A}}$  has to satisfy the classical equations of motion (and thus  $M$  has to be transversal in the generalized sense) occurred naturally due to the requirement that the approximated Hamiltonian should still commute with the approximated Gauss law operator, whereas in [HIMV00] it seems to be simply assumed that  $M$  is transversal in the generalized sense. In the application considered in [HIMV00], the Savvidy vacuum, the condition is of course fulfilled. In other cases, as e.g. the constant magnetic field stemming from a non-commuting gauge potential [HL94], [Gie99], this need not be the case.

As a last topic in this section we want to consider the value of the energy if we consider it at the stationary point of  $\bar{\mathbf{e}}$  and  $G$ . Since eq. (2.305) is very similar to the expression of the energy that we obtained in sec. 2.3.4, the treatment may basically adopted from there.

We first consider  $\bar{\mathbf{e}}$ :

$$\frac{\delta}{\delta \bar{\mathbf{e}}_i^a(\mathbf{x})} E_{\text{proj}} = \int d^3 x_1 \{ (\Pi_T)_{ii_1}^{ac_1}(\mathbf{x}, \mathbf{x}_1) \bar{\mathbf{e}}_{i_1}^{c_1}(\mathbf{x}_1) \} \stackrel{!}{=} 0, \quad (2.306)$$

thus the transversal component of  $\bar{\mathbf{e}}$  has to be zero at the stationary point. Next we consider  $G_{TT}$  (since  $M$  is transversal, the magnetic energy also contains only  $G_{TT}$ ). For the variation w.r.t.  $G_{TT}$  we need a relation<sup>92</sup> analogous to eq. (2.125)

$$\frac{\delta}{\delta (G_{TT})_{i_1 i_2}^{a_1 a_2}(\mathbf{z}_1, \mathbf{z}_2)} \text{Tr}(G^{-1}) = -(G_{TT}^{-1} G_{TT}^{-1})_{i_1 i_2}^{a_1 a_2}(\mathbf{z}_1, \mathbf{z}_2). \quad (2.307)$$

With intermediate steps analogous to eqs. (2.127-2.129) we end up with

$$E_{\text{proj}}[\bar{\mathbf{A}}] = \frac{1}{4} \text{Tr}(G_{TT}^{-1}) + \frac{1}{2g^2} \int d^3 x \bar{\mathbf{B}}_i^a(\mathbf{x}) \bar{\mathbf{B}}_i^a(\mathbf{x}) \quad (2.308)$$

$$= \frac{1}{2} \text{Tr} \left( (\hat{\mathbf{D}} \hat{\mathbf{D}} - \hat{\mathbf{B}})^{\frac{1}{2}} \right) + \frac{1}{2g^2} \int d^3 x \bar{\mathbf{B}}_i^a(\mathbf{x}) \bar{\mathbf{B}}_i^a(\mathbf{x}). \quad (2.309)$$

Thus we see that at the stationary point, the difference to the naive treatment of eq. (2.131) lies only in the requirement that here  $\bar{\mathbf{A}}$  has to satisfy the classical equations of motion. The important point of the Kamlah expansion is, however, that the energy functional depends only on the transversal degrees of freedom even away from the stationary point.

#### 2.6.4 Treatment of Charges to Lowest Order in $g$

Here we only want to insert an additional point that is inspired by the observation that, in the low-order perturbative treatment, the gauge group  $SU(N)$  is reduced to a direct product of  $U(1)$  groups. In that case one can obviously also require the charged states to be simultaneous eigenstates of all charge operators, and can therefore factorize

$$\langle \delta^b(\mathbf{y}) \mathbf{P}^\rho \rangle = \delta^b(\mathbf{y}) \langle \mathbf{P}^\rho \rangle, \quad (2.310)$$

where the  $\delta^b(\mathbf{y})$  on the RHS is no longer an operator but simply a c-number function. At this point, we should make clear that in the perturbative scaling that has been used here,  $\delta$  reads

$$\delta^a(\mathbf{x}) = g\rho^a(\mathbf{x}) - \langle \Gamma^a(\mathbf{x}) \rangle, \quad (2.311)$$

since the Gauss law implies  $\mathcal{G}^a| \rangle = (-\frac{1}{g}\Gamma^a + \rho^a)| \rangle = 0 \rightarrow \Gamma^a| \rangle = g\rho^a| \rangle$ . For this kind of quasi-Abelian charges, we can immediately obtain the projected energy to second order in the Kamlah expansion by replacing  $\langle \Gamma^a \rangle$  by  $\langle \Gamma^a \rangle - g\rho^a$  in eq. (2.288):

$$\begin{aligned} \frac{\langle H \mathbf{P}^\rho \rangle}{\langle \mathbf{P} \rangle} &= \langle H \rangle - \frac{1}{2} \langle \Delta H \bar{\Delta}^{c_1}(\mathbf{x}_1) \bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle \Theta^{c_2 c_1}(\mathbf{x}_2, \mathbf{x}_1) \\ &\quad - \langle \Delta H \bar{\Delta}^{c_1}(\mathbf{x}_1) \rangle \Theta^{c_2 c_1}(\mathbf{x}_2, \mathbf{x}_1) \left( \langle \Gamma^{c_2}(\mathbf{x}_2) \rangle - g\rho^{c_2}(\mathbf{x}_2) \right) \\ &\quad + \frac{1}{2} \langle \Delta H \bar{\Delta}^{c_1}(\mathbf{x}_1) \bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle \Theta^{c_1 d_1}(\mathbf{x}_1, \mathbf{y}_1) \Theta^{c_2 d_2}(\mathbf{x}_2, \mathbf{y}_2) \times \\ &\quad \left( \langle \Gamma^{d_1}(\mathbf{y}_1) \rangle - g\rho^{d_1}(\mathbf{y}_1) \right) \left( \langle \Gamma^{d_2}(\mathbf{y}_2) \rangle - g\rho^{d_2}(\mathbf{y}_2) \right). \end{aligned} \quad (2.312)$$

<sup>92</sup>As was discussed in sec. 2.5.5, a derivative w.r.t. the transversal components can be implemented by a derivative w.r.t. the full  $G$ , but acting with transversal projectors from the left and right on this functional derivative.

We see that it differs from the energy projected onto the chargeless sector by

$$\begin{aligned}
& -g \left\{ \left( \langle \Delta H \bar{\Delta}^{c_1}(\mathbf{y}_1) \bar{\Delta}^{c_2}(\mathbf{y}_2) \rangle \Theta^{c_1 d_1}(\mathbf{y}_1, \mathbf{x}_1) \Theta^{c_2 d_2}(\mathbf{y}_2, \mathbf{x}_2) \langle \Gamma^{d_1}(\mathbf{x}_1) \rangle \right) \right. \\
& \quad \left. - \langle \Delta H \bar{\Delta}^{c_1}(\mathbf{x}_1) \rangle \Theta^{c_1 c_2}(\mathbf{x}_1, \mathbf{x}_2) \right\} \rho^{c_2}(\mathbf{x}_2) \\
& + \frac{g^2}{2} \langle \Delta H \bar{\Delta}^{c_1}(\mathbf{x}_1) \bar{\Delta}^{c_2}(\mathbf{x}_2) \rangle \Theta^{c_1 d_1}(\mathbf{x}_1, \mathbf{y}_1) \Theta^{c_2 d_2}(\mathbf{x}_2, \mathbf{y}_2) \rho^{d_1}(\mathbf{y}_1) \rho^{d_2}(\mathbf{y}_2).
\end{aligned} \tag{2.313}$$

The first term can be easily calculated to give<sup>93</sup> *zero*, thus there is no term linear in  $\rho$  that contributes to the energy, whereas the second term simplifies to

$$-\frac{g^2}{2} \int d^3 y_1 d^3 y_2 \rho^{d_1}(\mathbf{y}_1) G_{\Delta}^{d_1 d_2}(\mathbf{y}_1, \mathbf{y}_2) \rho^{d_2}(\mathbf{y}_2). \tag{2.314}$$

We see that in lowest order perturbation theory, the charges interact via a potential given by the (negative of the) Green's function of the background field-covariant Laplacian. Two comments are in order: first, since the Green's function depends on the background field, the variational equations for  $\mathbf{A}$  are not independent of the charge distribution. This is a bit different from the electrodynamical case where radiation (transversal terms) and charges were completely decoupled. Second, we see that obtaining the  $\beta$  function from corrections to the Coulomb potential (which would result for  $\bar{\mathbf{A}} = 0$ ) is on this level of approximation not possible; it seems almost surprising that we obtained the correct lowest order potential, since our projection scheme only attempts to give the correct energy to  $\mathcal{O}(g^0)$ . For the first quantum corrections to the interquark potential, we would need the energy up to  $\mathcal{O}(g^4)$ .

## 2.7 Treatment of the Savvidy Problem

In this section we want to illustrate the general considerations we have presented before by the specific example of the Savvidy vacuum.

In this section, we want to illustrate the calculation of the projected energy to  $\mathcal{O}(g^0)$  that was performed above in general terms for a more specific example. The example we are going to examine is well-known in the literature, and has also been treated in calculations that started from different assumptions<sup>94</sup>, but ended up with expressions for the energy to be computed that are identical to our eq. (2.309). The case we want to consider is the Savvidy vacuum [Sav77],

<sup>93</sup>We have already indicated above that the two apparently very different moments of inertia are identical in perturbation theory; this is the point where one observes this most clearly. For the evaluation of the expressions used here, we have used a different form of the longitudinal projector,  $(\Pi_L)_{i_2 i_1}^{c_2 c_1}(\mathbf{x}_2, \mathbf{x}_1) = -\left( \hat{\mathbf{D}}_{i_2}^{c_2 b_2}(\mathbf{x}_2) \hat{\mathbf{D}}_{i_1}^{c_1 b_1}(\mathbf{x}_1) G_{\Delta}^{b_1 b_2}(\mathbf{x}_1, \mathbf{x}_2) \right)$ , where again we don't integrate over  $\mathbf{x}_1, \mathbf{x}_2$ .

<sup>94</sup>Kerman and Vautherin [KV89] did not attach very much importance to violations of (exact) gauge invariance, although they already indicated that one should use a projector, and that the projector could be approximately evaluated as in nuclear physics. They gave also a local expression for the corrections, which looks remarkably similar to what one would get if one performed a Kamlah expansion not to the Hamiltonian but to the Hamiltonian density, and would restrict oneself to a purely local expansion; in other words, one would expand  $\mathcal{H}(\mathbf{x})$  only in powers of  $\Gamma^a(\mathbf{x})$ . If one performs such studies in electrodynamics, it turns out that for translationally invariant kernels  $G^{-1}$ , corrections from a local Kamlah expansion are generically zero, and do not subtract longitudinal parts as they should. Anyway, [KV89] neglect these corrections with the argument: '*Because the method is variational the corrections (13) are expected to be small and improve the energy. They are omitted in the following discussion.*' They also argued that gauge invariance would imply that the fulfillment of the classical equations of motion would result in  $\hat{\mathbf{D}}M = 0$ . Somehow they seem not to make a point of the fact that the state they used was gauge invariant

[MS78], where one considers a homogeneous (quasi-Abelian) magnetic background field generated by a vector potential

$$\bar{\mathbf{A}}_i^a(\mathbf{x}) = x_1 B \delta^{a3} \delta_{i2} \quad (2.315)$$

which leads to a magnetic field

$$\bar{\mathbf{B}}_i^a = \delta_{i3} \delta^{a3} B. \quad (2.316)$$

This background field certainly satisfies the classical equation of motion and hence can be used in our calculation. We will follow [KV89] in our presentation; thus we restrict ourselves to the SU(2) case, and also set both  $\bar{e}$  and  $\Sigma$  to zero in this calculation. Furthermore, we use a special notation in the remainder of this section: instead of denoting components of vectors by  $_{1,2,3}$ , we denote them here by  $_{x,y,z}$ . The position vector  $\mathbf{x}$  has the components  $(x, y, z)$ .

We have in the course of this thesis not talked very much about renormalization. In Yang-Mills theory in the Schrödinger picture, it is usually assumed<sup>95</sup> that it is sufficient to renormalize the coupling constant and to normal order the Hamiltonian, thereby subtracting the (infinite) energy of the perturbative vacuum. We will do this by only considering the difference between the expectation value of the Hamiltonian in a state with background field  $\bar{\mathbf{A}}$  and a state with background field 0. For both cases, we will solve the variational equation for  $G_{TT}^{-1}$  and consider the energy expectation value in dependence of  $\bar{\mathbf{A}}$  only, i.e. we compute the effective potential depending on  $\bar{\mathbf{A}}$ . For this, we have to compute the trace of  $G_{TT}^{-1}$  with the equation of motion for  $G_{TT}^{-1}$ :  $G_{TT}^{-1}(\bar{\mathbf{A}})G_{TT}^{-1}(\bar{\mathbf{A}}) = 4M(\bar{\mathbf{A}})$ , where  $M(\bar{\mathbf{A}})$  is defined in eqs. (2.283, 2.284). The fact that we compute only the difference between two traces, namely  $\text{tr}(G_{TT}^{-1}(\bar{\mathbf{A}})) - \text{tr}(G_{TT}^{-1}(0))$ , is reflected in our calculation by dropping all contributions to the trace of the square root of  $M$  that do not depend on the parameter  $B$ . We start out by trying to diagonalize  $M$  explicitly. First, we perform a partial integration w.r.t.  $x$ , and obtain as the operator to diagonalize

$$M_{ij}^{ab}(\mathbf{x}) = \epsilon_{ii_1 k} \hat{\mathbf{D}}_{i_1}^{ac}(\mathbf{x}) \epsilon_{ki_2 j} \hat{\mathbf{D}}_{i_2}^{cb}(\mathbf{x}) - \epsilon_{ijk} f^{acb} \bar{\mathbf{B}}_j^c(\mathbf{x}). \quad (2.317)$$

One can make some progress if one interprets  $i\epsilon_{ijk}$  as the generators of the adjoint (spin-1) representation of the rotation group  $S_i$ , and  $if^{abc}$  as the generators of the adjoint representation of the colour group. This becomes useful in two different ways: in the case of colour, we can use a different basis of generators that is connected to the basis  $if^{abc}$  by a unitary transformation (thus not changing the trace), namely the so-called *Cartan-Weyl basis* in which the generators of the Cartan subgroup are diagonal. In our case,  $\Lambda_{ab}^3$  (generated by the unitary transformation

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(annihilated by the Gauss law operator) to the order in  $g$  that was sufficient at least for the one-loop part of their investigations. The treatment of Heinemann et al. [HMVI98],[HIMV00], was already discussed above following eq. (2.305). Another interesting treatment of the Savvidy vacuum in the Schrödinger picture can be found in [Lae01]. A useful reference in this context is also [Mul85].

<sup>95</sup>The discussion of renormalization in this context is often based on the so-called *Schrödinger functional* which is identical to the Feynman propagation kernel of sec. 2.2 with time in the latter taken to be imaginary. The first one to consider the renormalization of the Schrödinger functional was Symanzik [Sym81] who considered massless  $\phi^4$  theory, where he proved the existence of the Schrödinger representation to all orders in perturbation theory. A short account of the work of Symanzik where also the language of wave functionals is used can be found in [Lus85]. In these works additional counterterms that result from the presence of boundaries at time  $t = 0$  and  $t = T$  appear. In [LNWW92] it is argued that in the case of Yang-Mills theories these additional terms cannot appear since there are no gauge invariant terms of the right canonical dimensions, and this claim is verified up to one-loop order explicitly. The case of QCD (also to one-loop order) has been considered in [Sin95] where it turned out that a multiplicative renormalization of the quark boundary fields is necessary, i.e. for vanishing quark fields at the boundary only counterterms for quark masses and a coupling constant renormalization are necessary.

from  $if^{ab3}$ ) is of special interest:

$$\Lambda_{ab}^3 = \begin{pmatrix} 1 & & \\ & 0 & \\ & & -1 \end{pmatrix}. \quad (2.318)$$

With this, the equivalently transformed  $\epsilon_{i_1 k} \hat{\mathbf{D}}_{i_1}^{ac}(x)$  can be written as

$$i(S_{i_1})_{ik} \hat{\mathbf{D}}_{i_1}^{ac}(x) = i \begin{pmatrix} (S_l \nabla_l + S_y x B)_{ik} & & \\ & (S_l \nabla_l)_{ik} & \\ & & (S_l \nabla_l - S_y x B)_{ik} \end{pmatrix} \quad (2.319)$$

and with this, the whole operator  $M$  decomposes into three blocks; thus, we have already completed the diagonalization in colour space. Each block has in addition a very similar structure; therefore in the following we will only consider a 'generic' block and put in a parameter  $e_a$  that may be either 1, 0,  $-1$  depending on which block we are considering at the moment:

$$i(S_{i_1})_{ik} \hat{\mathbf{D}}_{i_1}^{ac}(x) \rightarrow (S_l \nabla_l + e_a S_y B)_{ik}. \quad (2.320)$$

Since we interpret  $S_i$  as spin matrices, it is useful to use  $S_z$  and linear combinations of  $S_x, S_y$  as raising and lowering operators,  $S_{\pm} = S_x \pm iS_y$ . Then one can rewrite<sup>96</sup>

$$(S_l \nabla + e_a S_y B)_{ik} = S_z \nabla_z - \sqrt{\frac{B}{2}}(a^\dagger S_+ - a S_-) \quad (2.321)$$

with  $a = \frac{1}{\sqrt{2B}}(\nabla_x + i\nabla_y + e_a x B)$ . Furthermore, we have

$$[a, a^\dagger] = e_a. \quad (2.322)$$

In the following, we will first concentrate on the case  $e_a = 1$ . Since apart from  $\nabla_y$  the  $a$  operators look very much like annihilation operators for the harmonic oscillator problem, this motivates us to consider the functions

$$u_{n, k_y, k_z, s}(x, y, z, \sigma) = e^{ik_y y + ik_z z} \psi_n(x - \frac{k_y}{B}) \chi_s(\sigma), \quad (2.323)$$

where  $\psi_n(x)$  is the harmonic oscillator wave function with  $n$  nodes and  $\chi_s(\sigma)$  is an eigenstate of  $S_z$ , as a possible set of basis wave functions. Acting on these functions with  $a$ , the relation to the harmonic oscillator will become even clearer:

$$\begin{aligned} a u_{n, k_y, k_z, s}(x, y, z, \sigma) &= e^{ik_y y + ik_z z} \chi_s(\sigma) \frac{1}{\sqrt{2B}} (\nabla_x + B(x - \frac{k_y}{B})) \psi_n(x - \frac{k_y}{B}) \\ &\stackrel{x - \frac{k_y}{B} = x'}{=} e^{ik_y y + ik_z z} \chi_s(\sigma) \frac{1}{\sqrt{2B}} (\nabla_{x'} + Bx') \psi_n(x'). \end{aligned}$$

If we compare this with the annihilation operator for an oscillator with oscillator length  $x_0$

$$b = \frac{x_0}{\sqrt{2}} (\nabla_x + \frac{1}{x_0^2} x) \quad (2.324)$$

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<sup>96</sup>From here on, we will always assume  $B > 0$ , since otherwise the formulas would become too clumsy, containing instead of  $B$  always  $|B|$ .

we see that  $a$  acts as an annihilation operator for an oscillator with oscillator length  $x_0 = 1/\sqrt{B}$ . We can conclude

$$au_{n,k_y,k_z,s}(x,y,z,\sigma) = \sqrt{n}u_{n-1,k_y,k_z,s}(x,y,z,\sigma), \quad (2.325)$$

$$a^\dagger u_{n,k_y,k_z,s}(x,y,z,\sigma) = \sqrt{n+1}u_{n+1,k_y,k_z,s}(x,y,z,\sigma). \quad (2.326)$$

The spin operators  $S_\pm$  also only permute the  $us$ . Since  $\chi_s$  are taken to be eigenstates of  $S_z$ :

$$S_\pm u_{n,k_y,k_z,s}(x,y,z,\sigma) = \sqrt{2-s(s\pm 1)}u_{n,k_y,k_z,s\pm 1}(x,y,z,\sigma). \quad (2.327)$$

Thus, if  $(S_l \nabla + e_a S_y B)_{ik}|_{e_a=+1}$  acts upon  $u$ , the first term  $S_z \nabla_z$  leaves both  $n, s$  unchanged, whereas  $S_+ a^\dagger$  changes both  $n, s \rightarrow (n+1), (s+1)$ , and similarly  $S_- a$ :  $n, s \rightarrow (n-1), (s-1)$ . We see that the operator  $(S_l \nabla_l + e_a S_y B)_{ik}|_{e_a=+1}$  does not change  $N = n - s$ , thus we have made a further step towards diagonalizing  $M$ . Quite identical considerations can be made for  $e_a = -1$ ; only the following things will change: as a basis it will be more useful to use

$$u'_{n,k_y,k_z,s}(x,y,z,\sigma) = e^{ik_y y + ik_z z} \psi_n(x + \frac{k_y}{B}) \chi_s(\sigma). \quad (2.328)$$

It will turn out that here,  $a^\dagger$  acts as an annihilation operator, and  $a$  as a creation operator, and last the conserved number is not  $n - s$  but  $N' = n + s$ . After this short interlude, we return to the case  $N = n - s$ . In the following we will always consider  $N$  to be fixed. Then the matrix elements

$$\begin{aligned} \langle k'_y, k'_z, n', s' | (-iS_i \hat{\mathbf{D}}_i) | k_y, k_z, n, s \rangle &= sk_z \delta_{nn'} \delta_{k_y k'_y} \delta_{k_z k'_z} \delta_{ss'} \\ &+ i\sqrt{\frac{B}{2}} \left( \sqrt{n+1} \sqrt{2-s(s+1)} \delta_{n+1, n'} \delta_{k_y k'_y} \delta_{k_z k'_z} \delta_{s+1, s'} \right. \\ &\quad \left. - \sqrt{n} \sqrt{2-s(s-1)} \delta_{n-1, n'} \delta_{k_y k'_y} \delta_{k_z k'_z} \delta_{s-1, s'} \right) \end{aligned} \quad (2.329)$$

can be factored into a matrix  $K'(N)_{ss'}$  that depends on  $N$  and has its rows and columns labelled by  $s, s'$  and a product of three  $\delta$  functions<sup>97</sup>. Also the abbreviation  $p = k_z/\sqrt{B}$  will be used in the following:

$$K'(N)_{ss'} = \sqrt{B} \begin{pmatrix} p & -i\sqrt{N+1} & 0 \\ i\sqrt{N+1} & 0 & -i\sqrt{N} \\ 0 & i\sqrt{N} & -p \end{pmatrix}. \quad (2.330)$$

With the help of this  $K'(N)$ , matrix elements of  $M$  between the states  $u$  can be written as

$$\begin{aligned} \langle k'_y, k'_z, n', s' | M | k_y, k_z, n, s \rangle &= \delta_{k_y k'_y} \delta_{k_z k'_z} \delta_{NN'} (K'(N) K'(N) + \begin{pmatrix} -B & & \\ & 0 & \\ & & B \end{pmatrix})_{ss'} \\ &= K(N)_{ss'} \delta_{k_y k'_y} \delta_{k_z k'_z} \delta_{NN'}. \end{aligned} \quad (2.331)$$

Thus the only thing left to do is to diagonalize the matrix  $K(N)$ :

$$K(N) = B \begin{pmatrix} p^2 + N & -ip\sqrt{N+1} & -\sqrt{N(N+1)} \\ ip\sqrt{N+1} & 2N+1 & ip\sqrt{N} \\ -\sqrt{N(N+1)} & -ip\sqrt{N} & p^2 + N + 1 \end{pmatrix}. \quad (2.332)$$

<sup>97</sup> $\delta_{NN'}$  is actually only a Kronecker- $\delta$ ;



This can be greatly simplified, since  $K(N)$  turns out to be the square of a much simpler matrix  $P(N)$  times  $B$ , i.e. with

$$P(N) = \begin{pmatrix} 0 & \sqrt{N} & ip \\ \sqrt{N} & 0 & -\sqrt{N+1} \\ -ip & -\sqrt{N+1} & 0 \end{pmatrix} \quad (2.333)$$

we have

$$K(N) = BP(N)P(N). \quad (2.334)$$

The characteristic polynomial for  $P$  is  $\det(P - \lambda \mathbb{1}) = \lambda(\lambda^2 - (p^2 + 2N + 1))$ , resulting in the eigenvalues

$$\lambda_0 = 0 \quad \text{and} \quad \lambda_{1,2} = \pm \sqrt{p^2 + 2N + 1}. \quad (2.335)$$

This results in the eigenvalues of  $K(N)$ :

$$k_0 = 0 \quad \text{and} \quad k_{1,2} = B(p^2 + 2N + 1) = k_z^2 + B(2N + 1). \quad (2.336)$$

That one zero mode should appear is desired and results from the fact that  $\hat{\mathbf{D}}M = 0$ . The discussion up to now is valid only for  $N \geq 1$ , since only then do  $s, s'$  span their whole range  $-1, 0, 1$ . For  $N = 0$  there are only two possible combinations of  $n, s$ :  $n = 1, s = 1$ ;  $n = 0, s = 0$ ; for  $N = -1$  there is only one possibility  $n = 0; s = 1$ . We will discuss both cases individually:

$$K(0) = B \begin{pmatrix} p^2 & -ip \\ ip & 1 \end{pmatrix}. \quad (2.337)$$

The characteristic polynomial  $\det(K(0) - k \mathbb{1})$  is given by  $k(k - (p^2 + 1))$ , resulting in eigenvalues  $k_0 = 0, k_1 = k_z^2 + B$ .

For the case  $N = -1$  the matrix is only one-dimensional, resulting in the eigenvalue  $k_0 = k_z^2 - B$ , thus leading to a mode with a *negative* eigenvalue in the region  $-B < k_z < B$ , resulting in an imaginary contribution to the energy. Note that the three modes for  $N = 0, -1$  together again have one zero mode, just as was the case for the other values of  $N$ . We can now also determine the spectrum for the case  $e_a = -1$ . For all  $N \geq 1$  the same construction as for the case  $e_a = 1$  works, only in the matrix corresponding to eq.(2.333) one has to interchange  $N$  and  $N + 1$ . The eigenvalues, however, are identical. For  $N = 0$  one has to interchange 1 and  $p^2$  in the matrix  $K(0)$  leaving the resulting eigenvalues invariant, and for  $N = -1$  both expressions are identical. For  $e_a = 0$ , the eigenvalues are independent of  $B$  (they are easily determined, and are given by  $0, |\mathbf{k}|, |\mathbf{k}|$ ), and will thus be dropped as we have explained above.

In order to perform the calculation of  $\text{tr}(G_{TT}^{-1}(\bar{\mathbf{A}})) - \text{tr}(G_{TT}^{-1}(0))$ , we use a proper-time representation of the square root [Cea88]:

$$\sqrt{\lambda} = - \int_0^\infty \frac{ds}{\sqrt{\pi s}} \frac{d}{ds} e^{-s\lambda} \quad (2.338)$$

which is an exact identity. The regularization will be imposed when we sum over all eigenvalues ' $\lambda$ ' by replacing the lower boundary of the integral by  $1/\Lambda^2$ . When we sum over all states, we have to take into account that the states that we have calculated above are degenerate (e.g. the energies are independent of  $k_2$ ). Since the problem we have analyzed is (in the end) identical to the Landau levels in a constant magnetic field, we can take the degeneracy factor directly from

[LL88]. We put the system in a box, and require that the centre<sup>98</sup> of the harmonic oscillator wave function shall be inside the box. This results in a degeneracy factor

$$\frac{L^2 B}{2\pi}, \quad (2.339)$$

where  $L$  denotes the length of the box. The sum over  $k_3$  will be replaced by the integral  $\frac{L}{2\pi} \int dk_3$ , so that the total prefactor is  $VB/(2\pi)^2$  where  $V = L^3$  is the total spatial volume. We now have to take into account two contributions separately: first the contribution from the modes that give a real energy over the whole  $k_3$  range. They give a contribution

$$\begin{aligned} & -\frac{VB}{(2\pi)^2} \int_{1/\Lambda^2}^{\infty} \frac{ds}{\sqrt{\pi s}} \frac{d}{ds} e^{-sB} \coth(sB) \int_{-\infty}^{\infty} dk_3 e^{-sk_3^2} \\ & \approx \frac{VB^2}{(2\pi)^2} \left( \frac{3}{4} \frac{\Lambda^4}{B^2} - \frac{1}{2} \frac{\Lambda^2}{B} + \frac{5}{12} \ln\left(\frac{B}{\Lambda^2}\right) + \text{UV finite terms} \right). \end{aligned} \quad (2.340)$$

The second contribution comes from the mode that gives for  $|k_3| < \sqrt{B}$  an imaginary contribution to the energy; if we consider the real part of the energy we obtain<sup>99</sup>

$$-\frac{VB}{(2\pi)^2} \int_{1/\Lambda^2}^{\infty} \frac{ds}{\sqrt{\pi s}} \frac{d}{ds} e^{sB} \int_{\sqrt{B}}^{\infty} dk_3 e^{-sk_3^2} \approx \frac{VB^2}{(2\pi)^2} \left( \frac{1}{2} \frac{\Lambda^2}{B} + \frac{1}{2} \ln\left(\frac{B}{\Lambda^2}\right) + \text{UV finite terms} \right). \quad (2.341)$$

Thus, if we add the two contributions, the  $B$ -dependent quadratic divergences cancel, and the logarithmic terms add up; dropping the  $B$ -dependent quartic divergence (or more properly, cancelling it against the contribution from  $G_{TT}^{-1}(0)$ ), we have left

$$\frac{VB^2}{(4\pi)^2} \frac{11}{3} \ln\left(\frac{B}{\Lambda^2}\right). \quad (2.342)$$

This is the contribution from the block with  $e_a = 1$ . An identical contribution comes from the block with  $e_a = -1$ ; in the expression for the energy, the trace (of  $M$ ) had a factor  $(1/2)$  in front, so we obtain as the one-loop contribution to the energy the well-known result [KV89]:

$$\frac{VB^2}{(4\pi)^2} \frac{11N}{6} \ln\left(\frac{B}{\Lambda^2}\right) \quad (2.343)$$

with  $N = 2$ . The total energy up to one loop,  $E^{1\text{-loop}}$ , contains in addition to the one-loop contribution also the classical term

$$E^{1\text{-loop}} = \frac{(VB^2)}{2} \left[ \frac{1}{g^2} - \frac{11N}{48\pi^2} \ln\left(\frac{\Lambda^2}{B}\right) \right]. \quad (2.344)$$

We can now introduce the renormalized coupling via

$$\frac{1}{g_R^2} = \frac{1}{g^2} - \frac{11N}{48\pi^2} \ln\left(\frac{\Lambda^2}{\mu^2}\right) \quad (2.345)$$

<sup>98</sup>The centre is not at 0, but is shifted by  $k_y/B$ .

<sup>99</sup>A factor of 2 appears since we have to consider  $k_3 > \sqrt{B}$  and  $k_3 < -\sqrt{B}$ .

at the scale  $\mu$ , consistent with the standard one-loop  $\beta$ -function (e.g. [PS95]):

$$\beta = \mu \frac{\partial g_R}{\partial \mu} = -\frac{1}{(4\pi)^2} \frac{11N}{3} g_R^3. \quad (2.346)$$

This allows us to give a cut-off free expression of the energy to one loop:

$$E^{1\text{-loop}} = \frac{(VB^2)}{2} \left[ \frac{1}{g_R^2} + \frac{11N}{48\pi^2} \ln\left(\frac{B}{\mu^2}\right) \right], \quad (2.347)$$

which is the standard (Savvidy) result [Sav77], [MS78]. A last comment should be made with regard to the imaginary part of the energy that has not been taken into account. It is easily calculable and no regularization has to be used, since it is finite. We obtain

$$\frac{VB}{(2\pi)^2} \int_{-\sqrt{B}}^{\sqrt{B}} dk_3 \left( \pm i \sqrt{B - k_3^2} \right) = \pm i \frac{VB^2}{8\pi}. \quad (2.348)$$

The sign seems to be undetermined; however, even though the interpretation of the imaginary part, which also appears in the path integral formalism, as a measure of the strength of vacuum decay has been questioned<sup>100</sup>, see e.g. [Sch82], [Gie99], in a Hamiltonian framework (where energy eigenstates vary in time like  $e^{-iEt}$ ), a positive imaginary part seems to be undesirable, since it would lead to an exponential increase of the norm, which is not compatible with the requirements of unitarity.

## 2.8 Summary and Conclusions

Let us shortly summarize what has been achieved in this chapter, and which problems remain. We started this chapter by considering the projector onto physical states including external charges. This projector was cast into a compact form by introducing an extra Hilbert space for the external (fermionic) charges, and using the insight that the time component of the (fermionic) colour current is the generator of gauge transformations of the external charges. Then we briefly considered the calculation by Kogan and Kovner [KK95], since one way of approaching the problem of evaluating the projector integral was presented there: [KK95] considered the projection integral as an effective non-linear, non-local  $\sigma$ -model. We also presented some criticism of their notion of gauge invariance.

Then we considered the work of Testa and Rossi [TR80a], [TR80b] on the projected Feynman propagation kernel. They gave a method to calculate the static inter-quark potential to one-loop order including the effects of the projector. This was a calculation of interest, since Testa and Rossi gave a systematic way of approaching the influence of the projector, whereas Kogan and Kovner always stayed - wherever they used perturbation theory - at lowest order.

Then we turned again to the main theme of this chapter, namely variational calculation with Gaussian states. We gave an interpretation of the parameters that appear in the most general Gaussian state, discussed its factorization property, and drew the connection to the work of

<sup>100</sup>It was argued that the imaginary eigenvalue was an artifact of the one-loop approximation, since for (covariantly) constant magnetic field, the quartic term in the exponent of the Euclidean path integral is strictly negative, thus making an integral that is divergent in one-loop approximation actually convergent in the 'full' theory [Flo83]. One can also study the energy transfer from the magnetic background field to gluons, and one obtains - in contrast to an electric background field in QED coupled to fermions - no energy transfer [Gie99]. Thus, if the Savvidy vacuum is unstable, the instability is not mediated by creation of charged gluons according to these arguments.

[CJT74], where it was shown that the choice of Gaussian states corresponds to the Hartree-Fock approximation. Then we simplified our considerations even further to the leading order in perturbation theory, and considered the energy at the stationary point w.r.t. all parameters except for the background vector potential. It turns out that the energy has the one-loop form that was to be expected. Up to this point, we ignored the requirements of gauge invariance under small gauge transformations that the wave functionals have to satisfy. Therefore, we studied in a next step what form a polynomial that is multiplied to the Gaussian wave functional must take, if we want the complete state to be annihilated by the Gauss law operator to a given order in  $g$ . We have to conclude, however, that annihilation for arbitrary gauge fields is possible only to lowest order in  $g$ . For higher orders, we need in addition a gauge condition that restricts us to a hypersurface in configuration space where Gauss' law can be satisfied.

We then turned to two approximation schemes for the projector on physical states. The first one is based on the time-dependent variational principle, and on the physical idea that, if we have a deformed state (i.e. a state that is not gauge-invariant), this state has to rotate in colour space, and - by considering time-averages - will thereby restore gauge invariance. We studied this approach both for electrodynamics and Yang-Mills theory, where again we considered the inter-quark potential to  $\mathcal{O}(g^4)$ . For electrodynamics the cranking procedure reproduced nicely the Coulomb potential, but for the Yang-Mills case we failed to obtain the correct  $\beta$ -function.

We then turned to the Kamlah expansion, which is an expansion of the expectation value of the Hamiltonian between projected states in powers of the generator of the symmetry. This is a technique successfully employed in nuclear physics, but it is not clear that the same can be done in a field theory with a *local* symmetry since the applicability in nuclear physics is based on the fact that the states are strongly deformed, which comes about usually from many particles participating in that deformed state. We tried the Kamlah expansion first for electrodynamics with external charges, where we found that the first order of the Kamlah expansion is inconsistent with the assumptions, since at the stationary point we find a state that is not deformed. Going to second order, however, we found exactly the properties that we expect of a projected energy functional, namely that it is independent of the longitudinal parts of the  $(\mathbf{\Pi} \mathbf{\Pi})$  correlation function and the longitudinal part of the expectation value of  $\mathbf{\Pi}$ , and therefore the correct Coulomb energy appears in the projected energy. This result motivated us to also consider Yang-Mills theory in this framework but again we restricted ourselves to lowest order in  $g$ . Since we have approximated both the Gauss law operator and the Hamiltonian, we obtain consistency conditions from the requirement that the approximated Hamiltonian still commutes with the approximated Gauss law operator. Effectively, this restricts the choice of possible background fields to those which satisfy the classical equations of motion. This condition makes the operator that multiplies the part of the potential energy quadratic in  $\mathbf{A}$  transversal w.r.t. the covariant derivative in the background field. Since the projection subtracts off the longitudinal part of the electrical energy, we end up with an energy functional that is independent of the longitudinal parts of the parameters of the Gaussian wave functional. At the stationary point of all parameters save the background vector potential, the energy functional looks precisely like the one-loop functional that we obtain in the mean field considerations without taking into account the projector. Of course, this is so only formally, since on the one hand the consistency condition alluded to above ensures that the energy depends only on the transversal degrees of freedom (thereby reducing three polarization states to two), and, on the other hand, the longitudinal parts of the parameters in the Gaussian wave functional are undetermined - instead of being set to zero - as one would expect from a projected energy functional. We then also considered how external charges can be included into the Kamlah expansion. Up to now, we have been able to

allow for them only to lowest order in perturbation theory, since only then the charges can be treated in a quasi-Abelian manner.

As a last point, we considered as a simple application the calculation of the one-loop energy of a constant magnetic background field. We obtained the result that is known in the literature, namely the Savvidy result.

To put it all in a nutshell: variational calculations in Yang-Mills theories that try to take into account the requirement of Gauss' law have up to now only been possible in combination with perturbation theory, and usually been restricted to Gaussian states. These are limitations we have not been able to overcome. However, we have added with the Kamlah expansion a new way of approximately evaluating the projector. Three investigations seem worthwhile:

first, one has to investigate whether the Kamlah expansion is a truly non-perturbative expansion or whether at some stage an implicit expansion in powers of  $g$  takes place. In this context, one should also investigate further the 'pattern' found in our discussion on electrodynamics, namely that one seems to need the Kamlah expansion to  $n^{\text{th}}$  order to project correctly terms containing  $n$  operators. If this would be true in general, one would need the fourth-order Kamlah expansion for a correct projection of the full Yang-Mills Hamiltonian.

Second, one should try to find out whether the Kamlah expansion can be carried out also to higher orders in perturbation theory since this would lift the restriction to background fields that satisfy the classical equations of motion. This should be considered also in the presence of external charges, which up to now can only be dealt with classically. If that can be done successfully, one should face the problem of computing the one-loop contribution to the inter-quark potential. If this reproduces the standard results, one could also try in a third investigation a non-perturbative evaluation of the second-order Kamlah expansion (provided the Kamlah expansion is truly non-perturbative and a second-order treatment is sufficient), although this will be a quite difficult task, since in our evaluation we relied strongly on the factorization properties; these, however, cannot be applied so easily in a non-perturbative framework, since the full Gauss law operator contains products of two operators at the same point in space.

Thus, renormalization problems, which we have ignored completely (apart from sec. 2.7 on the Savvidy vacuum), will have to be taken into account in a non-perturbative manner before one can perform such a non-perturbative evaluation of the projected energy functional.

Of course, when considering such non-perturbative extensions one should keep in mind that the restriction to Gaussian states has tied us already to the Hartree-Fock approximation, which is basically the two-loop approximation of the total quantum energy.

## Chapter 3

# Generalized Random Phase Approximation

### 3.1 Introduction

In this chapter, we study the generalized Random Phase Approximation (gRPA) for bosonic systems in the presence of condensates. The main motivation for this study is drawn from the experience in nuclear physics that symmetries broken by a mean-field treatment are restored in the Random Phase Approximation.

We start our studies by recalling the formulation of the generalized Random Phase Approximation based on the time-dependent variational principle, since this is the approach followed in the literature in the case of field theory. Then we turn to the operator formulation which is more common in nuclear physics, since in this formulation it is easier to see how conservation laws of the full theory translate into conservation laws in the generalized Random Phase Approximation. For a certain class of Hamiltonians, we will show that the two approaches indeed give an identical spectrum, and obtain a correspondence between quantities associated with the 'fluctuations' in the two different approaches. We also study in some detail the problem of zero modes, i.e. solutions of the gRPA equations with zero excitation energy.

We then consider the question of conservation laws in the operator approach and find that, under certain conditions, conservation laws of the full theory can also be translated to conservation laws in the approximate treatment of the generalized RPA, especially if the corresponding symmetries are broken in the mean-field treatment, i.e. the mean-field ground state is deformed. In this case, conservation laws of the full theory imply (if the symmetry generator is a one-body operator) that the gRPA equations have zero mode solutions.

As a last point in this chapter, we study how the mean-field energy is modified in the presence of zero modes due to deformations, and compute the moment-of-inertia which is used to give a transparent expression of this energy modification.

### 3.2 Generalized RPA from the Time-Dependent Variational Principle

In this section we present the approach to the Random Phase Approximation via the time-dependent variational principle as pioneered by Kerman *et al.* We show that it leads to equations of motion of coupled harmonic oscillators.

In this section, we will set up the Random Phase Approximation via the time-dependent variational principle, following Kerman *et al* [KK76], [KL95], [KL98]. We don't want to deal with a specific theory at the moment, we will only require the Hamiltonian to be of the form

$$H = \frac{1}{2}\pi_i^2 + V[\phi_i], \quad (3.1)$$

where  $\phi_i$  are a set of fields, and  $\pi_i$  are the canonical momenta conjugate to  $\phi_i$ , in the field (coordinate) representation under consideration

$$\pi_i = \frac{1}{i} \frac{\delta}{\delta \phi_i} \quad (3.2)$$

and  $i$  is a super-index, containing a position variable  $\mathbf{x}$ , and all other indices required (like colour, spatial etc). The Einstein summation convention is adopted, implying sums over all discrete and integrals over all continuous variables.  $V[\phi]$  is a functional of the field operators, in the following referred to as 'potential'.

The states that we consider as trial states for the time-dependent variational principle are the most general time-dependent Gaussian states (we only indicate the time-variable explicitly,  $i, j$  are super-indices):

$$\psi[\phi, t] = \exp \left( -(\phi - \bar{\phi}(t))_i \left( \frac{1}{4} G^{-1}(t) - i \Sigma(t) \right)_{ij} (\phi - \bar{\phi}(t))_j + i \bar{\pi}_i(t) (\phi - \bar{\phi}(t))_i \right). \quad (3.3)$$

The meaning of the parameters becomes clear by considering expectation values:

$$\langle \psi(t) | \phi_i | \psi(t) \rangle = \bar{\phi}_i(t) \quad ; \quad \langle \psi(t) | \phi_i \phi_j | \psi(t) \rangle = \bar{\phi}_i(t) \bar{\phi}_j(t) + G_{ij}(t) \quad (3.4)$$

$$\langle \psi(t) | \pi_i | \psi(t) \rangle = \bar{\pi}_i(t) \quad ; \quad \langle \psi(t) | \pi_i \pi_j | \psi(t) \rangle = \bar{\pi}_i \bar{\pi}_j + \frac{1}{4} G_{ij}^{-1}(t) + 4(\Sigma(t) G(t) \Sigma(t))_{ij}. \quad (3.5)$$

We can now compute the action of the time-dependent variational principle as defined in eq. (1.109)

$$S = \int dt \langle \psi(t) | i \partial_t - H | \psi(t) \rangle \quad (3.6)$$

and obtain

$$S = \int dt \left\{ \left[ \bar{\pi}_i(t) \dot{\bar{\phi}}_i(t) - \text{tr}(\dot{\Sigma} G) + \frac{i}{4} \text{tr}(\dot{G}^{-1} G) \right] - \mathcal{H}(t) [\bar{\phi}, \bar{\pi}, G, \Sigma] \right\} \quad (3.7)$$

with

$$\mathcal{H}(t) = \langle \psi(t) | H | \psi(t) \rangle. \quad (3.8)$$

We can now add a total time derivative<sup>1</sup> that does not change the equations of motion, and obtain for the action

$$S = \int dt (\Sigma_{ij}(t) \dot{G}_{ij}(t) + \bar{\pi}_i(t) \dot{\bar{\phi}}_i(t) - \mathcal{H}(t)), \quad (3.9)$$

which shows that  $\Sigma$  is to be considered as the canonical momentum conjugate to  $G$ , and  $\bar{\pi}$  that of  $\bar{\phi}$ . The parameters of the wave functional are now determined via Hamilton's classical equations of motion:

$$\dot{\bar{\phi}}_i(t) = \frac{\delta \mathcal{H}}{\delta \bar{\pi}_i} \quad ; \quad \dot{\bar{\pi}}_i(t) = -\frac{\delta \mathcal{H}}{\delta \bar{\phi}_i} \quad (3.10)$$

$$\dot{G}_{ij}(t) = \frac{\delta \mathcal{H}}{\delta \Sigma_{ij}} \quad ; \quad \dot{\Sigma}_{ij}(t) = -\frac{\delta \mathcal{H}}{\delta G_{ij}}. \quad (3.11)$$

<sup>1</sup>Its form can e.g. be found in [KL95] as (here only symbolically)  $\frac{d}{dt}(-\frac{i}{4} \log(G^{-1}) - \Sigma G)$ .

However, in general it will be much too complicated to solve these equations, therefore we now consider a two-step procedure

1. look for static solutions to the equations of motion
2. consider small fluctuations around these static solutions.

The static solutions are (obviously) determined via

$$\dot{\bar{\phi}}_i(t) = 0 ; \quad \dot{\bar{\pi}}_i(t) = 0 ; \quad \dot{\bar{G}}_{ij}(t) = 0 ; \quad \dot{\bar{\Sigma}}_{ij}(t) = 0. \quad (3.12)$$

But these are nothing but the equations resulting from the Rayleigh-Ritz principle:

$$\frac{\delta \mathcal{H}}{\delta \bar{\pi}_i} = 0 ; \quad \frac{\delta \mathcal{H}}{\delta \bar{\phi}_i} = 0 ; \quad \frac{\delta \mathcal{H}}{\delta \bar{\Sigma}_{ij}} = 0 ; \quad \frac{\delta \mathcal{H}}{\delta \bar{G}_{ij}} = 0. \quad (3.13)$$

Thus, for a static solution of the time-dependent variational principle, the parameters are those which minimize the energy. This should not really come as a surprise, since for a static state  $\psi[\phi]$ , the action reduces just to minus the energy times the respective time interval under consideration. For the next step, we decompose the general, time-dependent parameters into the static solution plus a time-dependent contribution that later on is considered to be small, e.g. for  $\bar{\phi}$ :

$$\bar{\phi}_i(t) = \bar{\phi}_{i,s} + \delta \bar{\phi}_i(t), \quad (3.14)$$

where  $\bar{\phi}_{i,s}$  denotes the static solution<sup>2</sup>, and  $\delta \bar{\phi}_i(t)$  the 'small' time-dependent part. We insert this decomposition into the equations of motion eqs. (3.10, 3.11), and obtain

$$\begin{aligned} \delta \dot{\bar{\phi}}_i(t) &= \frac{\delta \mathcal{H}}{\delta \bar{\pi}_i} [\bar{\phi}_s + \delta \bar{\phi}(t), \bar{\pi}_s + \delta \bar{\pi}(t), G_s + \delta G(t), \Sigma_s + \delta \Sigma(t)] \\ &= \frac{\delta \mathcal{H}}{\delta \bar{\pi}_i} [\bar{\phi}_s, \bar{\pi}_s, G_s, \Sigma_s] \\ &\quad + \frac{\delta^2 \mathcal{H}}{\delta \bar{\pi}_j \delta \bar{\pi}_i} [\bar{\phi}_s, \bar{\pi}_s, G_s, \Sigma_s] \delta \bar{\pi}_j + \frac{\delta^2 \mathcal{H}}{\delta \bar{\phi}_j \delta \bar{\pi}_i} [\bar{\phi}_s, \bar{\pi}_s, G_s, \Sigma_s] \delta \bar{\phi}_j \\ &\quad + \frac{\delta^2 \mathcal{H}}{\delta G_{jk} \delta \bar{\pi}_i} [\bar{\phi}_s, \bar{\pi}_s, G_s, \Sigma_s] \delta G_{jk} + \frac{\delta^2 \mathcal{H}}{\delta \Sigma_{jk} \delta \bar{\pi}_i} [\bar{\phi}_s, \bar{\pi}_s, G_s, \Sigma_s] \delta \Sigma_{jk} \\ &\quad + \mathcal{O}(\delta^2). \end{aligned} \quad (3.15)$$

Now the meaning of  $\delta \phi$ , etc. being small is clarified: in the equations of motion terms of higher than linear order are neglected (in the action, it would be terms of higher than quadratic order). The first contribution  $\frac{\delta \mathcal{H}}{\delta \bar{\pi}_i} [\bar{\phi}_s, \bar{\pi}_s, G_s, \Sigma_s]$  vanishes by virtue of the static equations of motion eqs. (3.12, 3.13). The same construction can be carried out for all four parameter types  $(\bar{\phi}, \bar{\pi}, \Sigma, G)$ , and the resulting equations of motion can be nicely summarized as follows:

$$\begin{pmatrix} \delta \dot{\bar{\phi}} \\ \delta \dot{\bar{\pi}} \\ \delta \dot{\bar{G}} \\ \delta \dot{\bar{\Sigma}} \end{pmatrix} = \begin{pmatrix} \frac{\delta^2 \mathcal{H}}{\delta \bar{\pi} \delta \bar{\phi}} & \frac{\delta^2 \mathcal{H}}{\delta \bar{\pi} \delta \bar{\pi}} & \frac{\delta^2 \mathcal{H}}{\delta \bar{\pi} \delta G} & \frac{\delta^2 \mathcal{H}}{\delta \bar{\pi} \delta \Sigma} \\ -\frac{\delta^2 \mathcal{H}}{\delta \bar{\phi} \delta \bar{\phi}} & -\frac{\delta^2 \mathcal{H}}{\delta \bar{\phi} \delta \bar{\pi}} & -\frac{\delta^2 \mathcal{H}}{\delta \bar{\phi} \delta G} & -\frac{\delta^2 \mathcal{H}}{\delta \bar{\phi} \delta \Sigma} \\ \frac{\delta^2 \mathcal{H}}{\delta \Sigma \delta \bar{\phi}} & \frac{\delta^2 \mathcal{H}}{\delta \Sigma \delta \bar{\pi}} & \frac{\delta^2 \mathcal{H}}{\delta \Sigma \delta G} & \frac{\delta^2 \mathcal{H}}{\delta \Sigma \delta \Sigma} \\ -\frac{\delta^2 \mathcal{H}}{\delta G \delta \bar{\phi}} & -\frac{\delta^2 \mathcal{H}}{\delta G \delta \bar{\pi}} & -\frac{\delta^2 \mathcal{H}}{\delta G \delta G} & -\frac{\delta^2 \mathcal{H}}{\delta G \delta \Sigma} \end{pmatrix} \begin{pmatrix} \delta \bar{\phi} \\ \delta \bar{\pi} \\ \delta G \\ \delta \Sigma \end{pmatrix} \quad (3.16)$$

<sup>2</sup>In other words, if we evaluate the first derivative  $\frac{\delta \mathcal{H}}{\delta \bar{\pi}_i}$  for  $\bar{\pi} = \bar{\pi}_s$ , it is zero, and correspondingly for  $\bar{\phi}, G, \Sigma$ .



and can be made even more transparent if one introduces an auxiliary matrix

$$\begin{pmatrix} \delta\dot{\bar{\phi}} \\ \delta\dot{\bar{\pi}} \\ \delta\dot{G} \\ \delta\dot{\Sigma} \end{pmatrix} = \begin{pmatrix} 0 & 1 & & \\ -1 & 0 & & \\ & & 0 & 1 \\ & & -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta^2\mathcal{H}}{\delta\phi\delta\phi} & \frac{\delta^2\mathcal{H}}{\delta\phi\delta\bar{\pi}} & \frac{\delta^2\mathcal{H}}{\delta\phi\delta G} & \frac{\delta^2\mathcal{H}}{\delta\phi\delta\Sigma} \\ \frac{\delta^2\mathcal{H}}{\delta\bar{\pi}\delta\phi} & \frac{\delta^2\mathcal{H}}{\delta\bar{\pi}\delta\bar{\pi}} & \frac{\delta^2\mathcal{H}}{\delta\bar{\pi}\delta G} & \frac{\delta^2\mathcal{H}}{\delta\bar{\pi}\delta\Sigma} \\ \frac{\delta^2\mathcal{H}}{\delta G\delta\phi} & \frac{\delta^2\mathcal{H}}{\delta G\delta\bar{\pi}} & \frac{\delta^2\mathcal{H}}{\delta G\delta G} & \frac{\delta^2\mathcal{H}}{\delta G\delta\Sigma} \\ \frac{\delta^2\mathcal{H}}{\delta\Sigma\delta\phi} & \frac{\delta^2\mathcal{H}}{\delta\Sigma\delta\bar{\pi}} & \frac{\delta^2\mathcal{H}}{\delta\Sigma\delta G} & \frac{\delta^2\mathcal{H}}{\delta\Sigma\delta\Sigma} \end{pmatrix} \begin{pmatrix} \delta\bar{\phi} \\ \delta\bar{\pi} \\ \delta G \\ \delta\Sigma \end{pmatrix}, \quad (3.17)$$

where  $\frac{\delta^2\mathcal{H}}{\delta A\delta B} = \frac{\delta^2\mathcal{H}}{\delta A\delta B}[\bar{\phi}_s, \bar{\pi}_s, G_s, \Sigma_s]$ . At this point it becomes clear what determines the spectrum of small fluctuations around a static mean-field solution: it's the *stability matrix* of this static mean-field solution. Eqs. (3.17) are usually called the generalized RPA equations. Up to now, the only assumption that has been used was the assumption of  $\psi$  being a Gaussian state. But we have also restricted the choice of Hamiltonians that we want to consider by eq. (3.1). This restriction will allow to carry the calculation a bit further.  $\mathcal{H}$  depends only via  $\langle\pi^2\rangle$  on both  $\bar{\pi}$  and  $\Sigma$ ,  $V[\phi]$  only depends on  $\bar{\phi}$  and  $G$ . Thus for all Hamiltonians that we are considering, we have the kinetic energy written as

$$\langle\psi|\frac{1}{2}\pi_i^2|\psi\rangle = \frac{1}{2}\bar{\pi}_i\bar{\pi}_i + \frac{1}{8}\text{tr}(G^{-1}) + 2\text{tr}(\Sigma G\Sigma), \quad (3.18)$$

where  $\text{tr}$  denotes the trace over the super-indices. The static solutions  $\bar{\pi}_{i,s}, \Sigma_{ij,s}$  are determined via

$$\frac{\delta\mathcal{H}}{\delta\bar{\pi}_i} = 0, \quad \frac{\delta\mathcal{H}}{\delta\Sigma_{ij}} = 0 \quad (3.19)$$

and result in

$$\bar{\pi}_{i,s} = 0, \quad \Sigma_{ij,s} = 0. \quad (3.20)$$

This information, together with the knowledge that  $V[\phi]$  does neither depend on  $\bar{\pi}$  nor on  $\Sigma$ , determines a number of second derivatives:

$$\begin{aligned} \frac{\delta^2\mathcal{H}}{\delta\bar{\pi}\delta\phi} &= 0, & \frac{\delta^2\mathcal{H}}{\delta\Sigma\delta\phi} &= 0, & \frac{\delta^2\mathcal{H}}{\delta G\delta\bar{\pi}} &= 0, & \frac{\delta^2\mathcal{H}}{\delta\bar{\pi}_i\delta\bar{\pi}_j} &= \delta_{ij}, \\ \frac{\delta^2\mathcal{H}}{\delta\Sigma\delta\bar{\pi}} &= 0, & \frac{\delta^2\mathcal{H}}{\delta\bar{\pi}\delta G} &= 0, & \frac{\delta^2\mathcal{H}}{\delta\Sigma\delta G} &= 0, & \frac{\delta^2\mathcal{H}}{\delta\Sigma\delta\Sigma} &= (G\mathbb{1}), \end{aligned} \quad (3.21)$$

where we have used the abbreviation

$$(G\mathbb{1})_{ij;kl} = 2\frac{\delta}{\delta\Sigma_{ij}}\frac{\delta}{\delta\Sigma_{kl}}\text{tr}(\Sigma G\Sigma) = G_{ki}\delta_{lj} + G_{kj}\delta_{li} + G_{jl}\delta_{ki} + G_{li}\delta_{kj}. \quad (3.22)$$

These results can be used to simplify eq. (3.16):

$$\begin{pmatrix} \delta\dot{\bar{\phi}} \\ \delta\dot{\bar{\pi}} \\ \delta\dot{G} \\ \delta\dot{\Sigma} \end{pmatrix} = \begin{pmatrix} 0 & \mathbb{1} & 0 & 0 \\ -\frac{\delta^2\mathcal{H}}{\delta\phi\delta\phi} & 0 & -\frac{\delta^2\mathcal{H}}{\delta\phi\delta G} & 0 \\ 0 & 0 & 0 & (G\mathbb{1}) \\ -\frac{\delta^2\mathcal{H}}{\delta G\delta\phi} & 0 & -\frac{\delta^2\mathcal{H}}{\delta G\delta G} & 0 \end{pmatrix} \begin{pmatrix} \delta\bar{\phi} \\ \delta\bar{\pi} \\ \delta G \\ \delta\Sigma \end{pmatrix}, \quad (3.23)$$

with  $(\mathbb{1})_{ij} = \delta_{ij}$ . By taking the derivative of eq. (3.23) with respect to time, and reinserting eq. (3.23), one obtains two sets of partially decoupled equations

$$\begin{pmatrix} \delta\ddot{\bar{\phi}} \\ \delta\ddot{G} \end{pmatrix} = - \begin{pmatrix} \frac{\delta^2\mathcal{H}}{\delta\phi\delta\phi} & \frac{\delta^2\mathcal{H}}{\delta\phi\delta G} \\ (G\mathbb{1})\frac{\delta^2\mathcal{H}}{\delta G\delta\phi} & (G\mathbb{1})\frac{\delta^2\mathcal{H}}{\delta G\delta G} \end{pmatrix} \begin{pmatrix} \delta\bar{\phi} \\ \delta G \end{pmatrix} \quad (3.24)$$

$$\text{and} \quad \begin{pmatrix} \delta\ddot{\bar{\pi}} \\ \delta\ddot{\Sigma} \end{pmatrix} = - \begin{pmatrix} \frac{\delta^2\mathcal{H}}{\delta\phi\delta\phi} & \frac{\delta^2\mathcal{H}}{\delta\phi\delta G}(G\mathbb{1}) \\ \frac{\delta^2\mathcal{H}}{\delta G\delta\phi} & \frac{\delta^2\mathcal{H}}{\delta G\delta G}(G\mathbb{1}) \end{pmatrix} \begin{pmatrix} \delta\bar{\pi} \\ \delta\Sigma \end{pmatrix}. \quad (3.25)$$

If we now make the *ansatz* of a harmonic time-dependence

$$\begin{pmatrix} \delta\phi_i(t) \\ \delta G_{ij}(t) \end{pmatrix} = \begin{pmatrix} \delta\phi_i(0) \\ \delta G_{ij}(0) \end{pmatrix} \cos(\omega t + \delta_1) \quad \text{and} \quad \begin{pmatrix} \delta\pi_i(t) \\ \delta\Sigma_{ij}(t) \end{pmatrix} = \begin{pmatrix} \delta\pi_i(0) \\ \delta\Sigma_{ij}(0) \end{pmatrix} \cos(\omega t + \delta_2) \quad (3.26)$$

we obtain the 'eigenvalue' equations

$$\begin{pmatrix} \frac{\delta^2\mathcal{H}}{\delta\phi\delta\phi} & \frac{\delta^2\mathcal{H}}{\delta\phi\delta G} \\ (G\mathbb{1})\frac{\delta^2\mathcal{H}}{\delta G\delta\phi} & (G\mathbb{1})\frac{\delta^2\mathcal{H}}{\delta G\delta G} \end{pmatrix} \begin{pmatrix} \delta\bar{\phi} \\ \delta G \end{pmatrix} = \omega^2 \begin{pmatrix} \delta\bar{\phi} \\ \delta G \end{pmatrix} \quad (3.27)$$

$$\text{and} \quad \begin{pmatrix} \frac{\delta^2\mathcal{H}}{\delta\phi\delta\phi} & \frac{\delta^2\mathcal{H}}{\delta\phi\delta G}(G\mathbb{1}) \\ \frac{\delta^2\mathcal{H}}{\delta G\delta\phi} & \frac{\delta^2\mathcal{H}}{\delta G\delta G}(G\mathbb{1}) \end{pmatrix} \begin{pmatrix} \delta\bar{\pi} \\ \delta\Sigma \end{pmatrix} = \omega^2 \begin{pmatrix} \delta\bar{\pi} \\ \delta\Sigma \end{pmatrix}. \quad (3.28)$$

In analysing properties of the generalized RPA equations eqs. (3.27, 3.28) it is often simpler to study the Hamiltonian they are derived from than to study the equations themselves. In this context one can imagine eq. (3.23) to originate from a Hamiltonian<sup>3</sup>  $H$ :

$$H = \frac{1}{2}(\delta\pi \ \delta\Sigma) \begin{pmatrix} \mathbb{1} & 0 \\ 0 & (G\mathbb{1}) \end{pmatrix} \begin{pmatrix} \delta\pi \\ \delta\Sigma \end{pmatrix} + \frac{1}{2}(\delta\phi \ \delta G) \begin{pmatrix} \frac{\delta^2\mathcal{H}}{\delta\phi\delta\phi} & \frac{\delta^2\mathcal{H}}{\delta\phi\delta G} \\ \frac{\delta^2\mathcal{H}}{\delta G\delta\phi} & \frac{\delta^2\mathcal{H}}{\delta G\delta G} \end{pmatrix} \begin{pmatrix} \delta\phi \\ \delta\Sigma \end{pmatrix}. \quad (3.29)$$

This evidently is the Hamiltonian of a set of coupled oscillators. The important point is that the signs of the eigenvalues of the decoupled oscillators are determined by the reduced stability matrix<sup>4</sup> containing only second derivatives w.r.t. to  $\bar{\phi}$  and  $G$  (We assume here that  $(G\mathbb{1})$  is positive definite and since  $(G\mathbb{1})$  is only multiplied by objects symmetric in their two indices, e.g.  $\delta\Sigma_{ij} = \delta\Sigma_{ji}$ , this boils down to assuming that  $G$  is positive definite. This is a sensible assumption connected to the normalizability of  $\psi[\phi]$  and will be discussed further in sec. 3.3.1). An interesting observation can be made immediately: usually  $\frac{\delta^2\mathcal{H}}{\delta\phi\delta G}$  will be only non-zero if there is a condensate<sup>5</sup> in the system. Thus if we don't have a condensate, the equations for the one- and two-particle content<sup>6</sup> decouple, and, since in a system without condensate  $G$  will usually be translation invariant, we can see by considering the Fourier transformed quantities<sup>7</sup> that  $1/\tilde{g}(\mathbf{p})$  just describes the energy spectrum of single-particle excitations with momentum  $\mathbf{p}$ , where  $\tilde{g}(\mathbf{p})$  is defined by the following procedure. We introduce the Fourier transform  $\tilde{G}(\mathbf{p}, \mathbf{q})$  by

$$G(\mathbf{x}, \mathbf{y}) = \int \frac{d^3p}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{x}} \tilde{G}(\mathbf{p}, \mathbf{q}) e^{-i\mathbf{q}\cdot\mathbf{y}}. \quad (3.30)$$

If we now require that  $G$  shall be translation invariant, i.e.  $G(\mathbf{x}, \mathbf{y}) = G(\mathbf{x} - \mathbf{y})$ , we obtain for  $\tilde{G}(\mathbf{p}, \mathbf{q})$

$$\tilde{G}(\mathbf{p}, \mathbf{q}) = (2\pi)^3 \delta(\mathbf{p} - \mathbf{q}) \tilde{g}(\mathbf{p}). \quad (3.31)$$

This defines  $\tilde{g}(\mathbf{p})$ .

<sup>3</sup>They originate by the canonical equations of motion, e.g.  $\delta\bar{\pi} = -\delta H/\delta(\delta\bar{\phi})$ .

<sup>4</sup>The problem of coupled oscillators is well-known, cf. [Gold91], [FK92]. If the reduced stability matrix is a positive matrix (and thus our mean field vacuum is indeed a minimum), all the eigenvalues will be positive, and thus all oscillator frequencies will be real.

<sup>5</sup>in other words, if  $\bar{\phi} \neq 0$

<sup>6</sup>We will see in sec. 3.3 that in a creation/annihilation operator formalism  $\delta\bar{\phi}, \delta\bar{\pi}$  are connected to the amplitudes of operators containing one creation/annihilation operator, whereas  $\delta G, \delta\Sigma$  are connected to the amplitudes containing two creation/annihilation operators.

<sup>7</sup>Since  $G$  is translationally invariant, we can separate a total-momentum conserving  $\delta$  function.

### 3.3 Operator Approach to the Generalized Random Phase Approximation

In this section we take a different route to the generalized Random Phase Approximation (gRPA, generalized RPA). In the long run, this approach has the advantage that one can show more easily the special role of symmetry generators that fall into the general class of one-body operators. The formalism is a bit more complicated and in closer resemblance to the formalism usually employed in many-body calculations. In a first step, one introduces creation and annihilation (*c/a*) operators. Then all operators relevant to the problem at hand (especially the Hamiltonian) can be expressed with the help of these *c/a* operators. In the next step the Schrödinger equation is rewritten into an equation containing only vacuum expectation values of commutators (so-called 'equation of motion'). The two basic approximations of the gRPA are introduced that allow to reduce the 'equation of motion' into a generalized eigenvalue equation. Two alternative versions of the second basic approximation are considered. The second of these alternatives, called the quasi-boson approximation, allows to rewrite the gRPA equations in a form that makes the equivalence of the gRPA Hamiltonian to a collection of harmonic oscillators obvious. The special role of symmetry generators is emphasized. The deviations of the gRPA energy from the mean-field energy are presented and the special role of the 'zero modes' is discussed.

#### 3.3.1 Creation and Annihilation Operators

In this section we will take a different route<sup>8</sup> to the generalized Random Phase Approximation (gRPA, generalized RPA) than in the previous section. In order to allow close comparison to the section before, we will again consider Hamiltonians of the form

$$H = \frac{1}{2}\pi_i^2 + V[\phi], \quad (3.32)$$

where  $\pi_i$  is the canonical momentum conjugate to  $\phi_i$ , in the field representation under consideration

$$\pi_i = \frac{1}{i} \frac{\delta}{\delta \phi_i} \quad (3.33)$$

and  $i$  is a super-index, containing a position variable  $\mathbf{x}$ , and all other indices required (like colour, spatial etc). The Einstein summation convention is adopted, implying sums over all discrete and integrals over all continuous variables.  $V[\phi]$  is functional of the field operator, in the following referred to as 'potential'.

The states we are considering here are a bit different though, since the basis of this approach is the *stationary* Schrödinger equation. We start therefore from the most general *time-independent* Gaussian state ( $i, j$  are super-indices):

$$\psi[\phi] = \exp \left( -(\phi - \bar{\phi})_i \left( \frac{1}{4}G^{-1} - i\Sigma \right)_{ij} (\phi - \bar{\phi})_j + i\bar{\pi}_i (\phi - \bar{\phi})_i \right). \quad (3.34)$$

The only difference between eq. (3.34) and eq. (3.3) is that in the latter the parameters  $\bar{\phi}, \bar{\pi}, G, \Sigma$  are time-dependent and in the former they are not. A Gaussian state allows the explicit construction of creation and annihilation operators as linear combinations of  $\phi_i$  and  $\pi_i$ :

$$a_i^\dagger = U_{ij} \left\{ \left( \frac{1}{2}G_{jk}^{-1} + 2i\Sigma_{jk} \right) (\phi - \bar{\phi})_k - i(\pi - \bar{\pi})_j \right\}, \quad (3.35)$$

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<sup>8</sup>In nuclear physics, this is the standard approach [MW69], [RS80], cf. also [Sol76], [MR85], [Tho60a], [Tho60b], [BET61], [TV62], [MW70]. An interesting discussion is also given by [Nes64]. That it may also be used in the boson case was indicated, although only very briefly, in [KT97].

$$a_i = U_{ij} \left\{ \left( \frac{1}{2} G_{jk}^{-1} - 2i \Sigma_{jk} \right) (\phi - \bar{\phi})_k + i (\pi - \bar{\pi})_j \right\}, \quad (3.36)$$

where  $U$  is (implicitly) defined via the relation

$$U_{ij} U_{jk} = G_{ik} \quad (3.37)$$

and could also be called the square root of  $G$ . A short excursion on the existence and the implicit assumption of reality of  $U$  is in order here: since  $G_{ik}$  is a symmetric matrix (matrix is used in the generalized sense s.t. also continuous indices are allowed) one can always diagonalize it. Therefore one can also always write down a  $U$  as given above. However,  $G$  has to satisfy another condition, namely all of its eigenvalues have to be strictly positive, since otherwise one will run into two kinds of problems: if  $G$  has a zero eigenvalue  $G^{-1}$  does not exist and the matrix element of  $\langle \pi^2 \rangle$  will be infinite. This can certainly not be tolerated<sup>9</sup>. Moreover, if  $G$  has a negative eigenvalue,  $\psi[\phi]$  is not even normalizable, since in the direction of the negative eigenvalue  $\psi[\phi]$  will explode exponentially for increasing values of  $\phi$ . Thus, all eigenvalues of  $G$  must be strictly positive, therefore  $U$  can be chosen to be real.

The normalization of the creation/annihilation operators is fixed by the usual bosonic commutation relations

$$[a_i, a_j^\dagger] = \delta_{ij}. \quad (3.38)$$

Since  $a_i, a_i^\dagger$  are just given via linear combinations of  $\phi$  and  $\pi$ , one can invert these relations to obtain  $\phi, \pi$  in terms of  $a, a^\dagger$  and the parameters of the Gaussian wave functional we started with:

$$\phi_i = \bar{\phi}_i + U_{ij} (a_j + a_j^\dagger) \quad (3.39)$$

$$\pi_i = \bar{\pi}_i + 2i \left( \left( \frac{1}{4} G_{ik}^{-1} - i \Sigma_{ik} \right) U_{kj} a_j^\dagger - \left( \frac{1}{4} G_{ik}^{-1} + i \Sigma_{ik} \right) U_{kj} a_j \right). \quad (3.40)$$

One should note that the dependence of the canonical operators on the parameters of the wave functional we choose is only seeming, since the creation and annihilation operators depend implicitly on these parameters as well. If one inserts eqs. (3.36, 3.35) into eqs. (3.39, 3.40) one obtains an identity  $\phi = \phi, \pi = \pi$ . In a practical sense, however, we have transferred information that is contained in the wave functional to the operators, since in the following we will only use that  $a_i \psi[\phi] = 0$ . All parameter dependence that usually comes about by calculating matrix elements now enters the formulas via normal ordering.

Since we have now a representation of the canonical operators in terms of  $a, a^\dagger$ , *all* operators permissible in a canonical system can be expressed in terms of  $a, a^\dagger$ , especially the Hamiltonian which for obvious reasons is central to the following calculations.

### 3.3.2 Hamiltonian in $c/a$ Representation

We have required the Hamiltonian to have a certain structure (cf. eq. (3.32)). The Hamiltonian there resolves naturally into a kinetic energy  $\frac{1}{2} \pi^2$  and a potential term  $V[\phi]$  which is a functional of  $\phi$  only. It is very useful to normal-order these expressions to make further progress. In the

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<sup>9</sup>A rather long discussion on zero modes and existence of certain integrals can be found in chapter 2, footnote 36.

course of this, one makes the useful observation that one can write the kinetic energy as :

$$\begin{aligned}
\frac{1}{2}\pi_i^2 &= \frac{1}{2}(\bar{\pi}_i^2 + \frac{1}{4}\text{Tr}(G^{-1}) + 4\text{Tr}(\Sigma G \Sigma)) \\
&+ \left(\frac{\delta}{\delta\bar{\pi}_{k_1}}\langle\frac{1}{2}\pi_i^2\rangle\right)\left(\frac{i}{2}U_{k_1j_1}^{-1}\left(a_{j_1}^\dagger - a_{j_1}\right) + 2\Sigma_{k_1l_1}U_{l_1j_1}\left(a_{j_1}^\dagger + a_{j_1}\right)\right) \\
&+ \left(\frac{\delta}{\delta G_{k_1k_2}}\langle\frac{1}{2}\pi_i^2\rangle\right)U_{k_1j_1}U_{k_2j_2}\left(a_{j_1}^\dagger a_{j_2}^\dagger + a_{j_1}a_{j_2} + 2a_{j_1}^\dagger a_{j_2}\right) \\
&+ \left(\frac{\delta}{\delta\Sigma_{k_1k_2}}\langle\frac{1}{2}\pi_i^2\rangle\right)U_{k_1j_1}^{-1}U_{k_2j_2}^{-1}\frac{i}{4}\left(a_{j_1}^\dagger a_{j_2}^\dagger - a_{j_1}a_{j_2}\right) \\
&+ \left(\frac{1}{4}G_{j_1j_2}^{-1} + \frac{i}{2}\left(U^{-1}\Sigma U - U\Sigma U^{-1}\right)_{j_1j_2}\right)2a_{j_1}^\dagger a_{j_2},
\end{aligned} \tag{3.41}$$

where Tr is a trace over the super-indices. A similar result can be found for the potential part (except that it is independent of  $\Sigma$  and  $\bar{\pi}$ ). In appendix D we will demonstrate that the potential can be decomposed into c/a operators s.t. the prefactors can be written as functional derivatives of the expectation value of the potential between Gaussian states, and the c/a operators always appear in a fixed structure<sup>10</sup>. In the following we will restrict ourselves to the contributions to  $V$  with up to four c/a operators, since the terms containing higher numbers of c/a operators do not contribute<sup>11</sup> to the gRPA matrices that will be introduced in eq. (3.57):

$$\begin{aligned}
V[\phi] &= \langle V[\phi] \rangle \\
&+ \left(\frac{\delta}{\delta\phi_{k_1}}\langle V[\phi] \rangle\right)U_{k_1j_1}\left(a_{j_1}^\dagger + a_{j_1}\right) \\
&+ \left(\frac{\delta}{\delta G_{k_1k_2}}\langle V[\phi] \rangle\right)U_{k_1j_1}U_{k_2j_2}\left(a_{j_1}^\dagger a_{j_2}^\dagger + a_{j_1}a_{j_2} + 2a_{j_1}^\dagger a_{j_2}\right) \\
&+ \frac{1}{3}\left(\frac{\delta}{\delta\phi_{k_1}}\frac{\delta}{\delta G_{k_2k_3}}\langle V[\phi] \rangle\right)U_{k_1j_1}U_{k_2j_2}U_{k_3j_3} \\
&\quad \times \left(a_{j_1}^\dagger a_{j_2}^\dagger a_{j_3}^\dagger + 3a_{j_1}^\dagger a_{j_2}^\dagger a_{j_3} + 3a_{j_1}^\dagger a_{j_2} a_{j_3} + a_{j_1} a_{j_2} a_{j_3}\right) \\
&+ \frac{1}{6}\left(\frac{\delta}{\delta G_{k_1k_2}}\frac{\delta}{\delta G_{k_3k_4}}\langle V[\phi] \rangle\right)U_{k_1j_1}U_{k_2j_2}U_{k_3j_3}U_{k_4j_4} \\
&\quad \times \left(a_{j_1}^\dagger a_{j_2}^\dagger a_{j_3}^\dagger a_{j_4}^\dagger + 4a_{j_1}^\dagger a_{j_2}^\dagger a_{j_3}^\dagger a_{j_4} + 6a_{j_1}^\dagger a_{j_2}^\dagger a_{j_3} a_{j_4} \right. \\
&\quad \left. + 4a_{j_1}^\dagger a_{j_2} a_{j_3} a_{j_4} + a_{j_1} a_{j_2} a_{j_3} a_{j_4}\right).
\end{aligned} \tag{3.42}$$

<sup>10</sup>e.g. if in the potential there are terms that contain two creation operators, or two annihilation operators or one creation/ one annihilation operator, they can always be written as *factor*  $\times (a_i^\dagger a_j^\dagger + a_i a_j + 2a_i^\dagger a_j)$ , and similarly for all other terms that contain a fixed sum of creation and annihilation operators. For the kinetic terms things are a bit different, but we have given the decomposition of the only allowed kinetic term in eq. (3.41).

<sup>11</sup>That this is true can be seen by usage of Wick's theorem and the so-called *second gRPA approximation*  $a| \rangle = 0$  that will be introduced in sec. 3.3.4.

By adding the expressions eq. (3.41, 3.42) together, one observes that the Hamiltonian has a very simple schematic structure<sup>12</sup> :

$$\begin{aligned}
\hat{H} = & \langle \hat{H} \rangle \\
& + \left( \frac{\delta}{\delta \phi_{k_1}} \langle \hat{H} \rangle \right) U_{k_1 j_1} \left( a_{j_1}^\dagger + a_{j_1} \right) \\
& + \left( \frac{\delta}{\delta \bar{\pi}_{k_1}} \langle \hat{H} \rangle \right) \left( \frac{i}{2} U_{k_1 j_1}^{-1} \left( a_{j_1}^\dagger - a_{j_1} \right) + 2 \Sigma_{k_1 l} U_{l j_1} \left( a_{j_1}^\dagger + a_{j_1} \right) \right) \\
& + \left( \frac{\delta}{\delta G_{k_1 k_2}} \langle \hat{H} \rangle \right) U_{k_1 j_1} U_{k_2 j_2} \left( a_{j_1}^\dagger a_{j_2}^\dagger + a_{j_1} a_{j_2} + 2 a_{j_1}^\dagger a_{j_2} \right) \\
& + \left( \frac{\delta}{\delta \Sigma_{k_1 k_2}} \langle \hat{H} \rangle \right) U_{k_1 j_1}^{-1} U_{k_2 j_2}^{-1} \frac{i}{4} \left( a_{j_1}^\dagger a_{j_2}^\dagger - a_{j_1} a_{j_2} \right) \\
& + \left( \frac{1}{4} G_{j_1 j_2}^{-1} + \frac{i}{2} \left( U^{-1} \Sigma U - U \Sigma U^{-1} \right)_{j_1 j_2} \right) 2 a_{j_1}^\dagger a_{j_2} \\
& + \frac{1}{3} \left( \frac{\delta}{\delta \phi_{k_1}} \frac{\delta}{\delta G_{k_2 k_3}} \langle \hat{H} \rangle \right) U_{k_1 j_1} U_{k_2 j_2} U_{k_3 j_3} \left( a_{j_1}^\dagger a_{j_2}^\dagger a_{j_3}^\dagger + 3 a_{j_1}^\dagger a_{j_2}^\dagger a_{j_3} + 3 a_{j_1}^\dagger a_{j_2} a_{j_3} + a_{j_1} a_{j_2} a_{j_3} \right) \\
& + \frac{1}{6} \left( \frac{\delta}{\delta G_{k_1 k_2}} \frac{\delta}{\delta G_{k_3 k_4}} \langle \hat{V} \rangle \right) U_{k_1 j_1} U_{k_2 j_2} U_{k_3 j_3} U_{k_4 j_4} \left( a_{j_1}^\dagger a_{j_2}^\dagger a_{j_3}^\dagger a_{j_4}^\dagger + 4 a_{j_1}^\dagger a_{j_2}^\dagger a_{j_3}^\dagger a_{j_4} + 6 a_{j_1}^\dagger a_{j_2}^\dagger a_{j_3} a_{j_4} \right. \\
& \qquad \qquad \qquad \left. + 4 a_{j_1}^\dagger a_{j_2} a_{j_3} a_{j_4} + a_{j_1} a_{j_2} a_{j_3} a_{j_4} \right).
\end{aligned} \tag{3.43}$$

Up to now, we have taken an arbitrary Gaussian as a reference state: we have defined our creation/annihilation operators relative to that state - nothing else. Eq. (3.43) is exactly the same as  $H$  given in eq. (3.32). However, it is obvious from eq. (3.43) that the Hamiltonian greatly simplifies if we choose a specific reference state: a state that is a stationary point of the energy functional under variation of the parameters  $\bar{\phi}, \bar{\pi}, G, \Sigma$  - in other words, a state that satisfies the Rayleigh-Ritz variational principle<sup>13</sup>.

### 3.3.3 Reformulation of the Schrödinger Equation

Now we want to reformulate the Schrödinger equation in such a way that it can be written in terms of matrix elements of commutators, since this form will be useful for formulating the generalized RPA. We assume that  $|\nu\rangle$  is an *exact* eigenstate of the full Hamiltonian, and that it is created from the *exact* vacuum  $|0\rangle$  by the operator<sup>14</sup>  $Q_\nu^\dagger$ . Thus

$$H Q_\nu^\dagger |0\rangle = E_\nu Q_\nu^\dagger |0\rangle. \tag{3.44}$$

If we denote the vacuum energy by  $E_0$ , we can write this equivalently with a commutator:

$$[H, Q_\nu^\dagger] |0\rangle = (E_\nu - E_0) Q_\nu^\dagger |0\rangle. \tag{3.45}$$

We may multiply both sides of the equation with an arbitrary operator  $\delta Q$ , and obtain an expectation value by multiplying from the left with  $\langle 0|$ :

$$\langle 0 | \delta Q [H, Q_\nu^\dagger] | 0 \rangle = (E_\nu - E_0) \langle 0 | \delta Q Q_\nu^\dagger | 0 \rangle. \tag{3.46}$$

<sup>12</sup>One should note that in all save the last term, the derivatives are taken of  $\langle \hat{H} \rangle$  whereas in the last term the derivative is taken of  $\langle V \rangle$ . The importance of this will become clear in sec. 3.3.10.

<sup>13</sup>One should note that we required the same in the time-dependent approach, when we decomposed the time-dependent parameters  $\bar{\phi}(t), \bar{\pi}(t), G(t), \Sigma(t)$  into a static part and small fluctuations. The equations for the static part were identical to the Rayleigh-Ritz equations.

<sup>14</sup>It is clear that, since  $Q^\dagger$  are creation operators, when acting to the left they annihilate the vacuum:  $\langle 0 | Q^\dagger = 0$ .

By subtracting zero on both sides<sup>15</sup> we obtain an equation that only contains expectation values of commutators:

$$\langle 0 | [\delta Q, [H, Q_\nu^\dagger]] | 0 \rangle = (E_\nu - E_0) \langle 0 | [\delta Q, Q_\nu^\dagger] | 0 \rangle. \quad (3.47)$$

Using this equation as a starting point to derive the (generalized) RPA is known in nuclear physics as the *equations of motion method* [RS80].

### 3.3.4 Excitation Operators

The operators  $Q_\nu^\dagger$  are called *excitation operators* in the following. The *first gRPA approximation*<sup>16</sup> deals with the class of allowed operators. In nuclear physics it is quite reasonable to assume that the lowest excited state above a Hartree-Fock ground state consists of a particle-hole excitation. This results in the so-called Tamm-Dancoff approximation. In the generalized RPA one assumes that one has a correlated ground state, s.t. not only the creation of a hole and a particle, but also their destruction is a possible excitation. In Yang-Mills theory it is by far not so clear what structure the lowest excitation will have; we have thus taken the two following guiding principles:

1. We already have a formulation of the generalized RPA from the time-dependent variational principle; we know therefore that the choice of the class of operators that we allow should lead to equations where the excitation spectrum is closely related to the stability matrix of the mean-field problem. Therefore, even if the class of operators will look a bit strange at first sight, it will lead to a well-posed and not so unreasonable problem: one looks at the small fluctuations around the mean-field solution.
2. The principal goal of the Random Phase Approximation is the restoration of symmetries that are violated at the mean-field level. The procedure works, generally speaking, in the following way: assume that the system under consideration should be symmetric under a symmetry generated by an operator  $\Gamma$ . The ground state should thus be annihilated by  $\Gamma$ . In the mean-field approximation this symmetry shall be violated, therefore

$$\Gamma | \text{MF} \rangle \neq 0. \quad (3.48)$$

The gRPA equations can be formulated as

$$[H_B, Q_\nu^\dagger] = (E_\nu - E_0) Q_\nu^\dagger \quad (3.49)$$

as we will see later on, cf. eq. (3.88).  $H_B$  denotes the Hamiltonian in the so-called *quasi-boson approximation*. This approximation will be treated in more detail in sec. 3.3.6. Since we are able to show that under quite general conditions,

$$[H, \Gamma] = 0 \rightarrow [H_B, \Gamma_B] = 0 \quad (3.50)$$

<sup>15</sup>On the LHS, we write zero as  $0 = \langle 0 | [H, Q_\nu^\dagger] \delta Q | 0 \rangle$ , whereas on the RHS, we write zero as  $(E_\nu - E_0) \langle 0 | Q_\nu^\dagger \delta Q | 0 \rangle$ , cf. footnote 14.

<sup>16</sup>A short note on linguistic usage is in order here: in the derivation of the gRPA equations we make two prominent approximations, the first one on the class of allowed excitation operators, the second one on the ground state. These approximations are called 'first' and 'second gRPA approximation', whereas the terms 'gRPA', 'generalized RPA' and 'generalized Random Phase Approximation' are used to denote the whole procedure as it is laid down in this section. This naming seems useful even though the term 'approximation' appears twice if one expands 'RPA' to 'Random Phase Approximation' in the term 'RPA approximation'.

( $\Gamma_B$  denotes the quasi-boson approximation of  $\Gamma$ ; it will be defined below in sec. 3.3.6), and we know that all excitations in the generalized RPA are automatically orthogonal, we only have to choose the class of excitation operators in such a way that the generator of the symmetry that is broken on the mean-field level *belongs to the class of excitation operators under consideration* for the formulation of generalized RPA. Then we have restored the symmetry in the sense that, even though

$$\Gamma_B|\text{MF}\rangle \neq 0, \quad (3.51)$$

$\Gamma_B$  creates an excitation that is orthogonal to all other (physical) excitations<sup>17</sup>.

To put it all in a nut-shell: one looks at the Gauss law operator, determines its structure, and keeps the class of excitation operators so large that the Gauss law operator belongs to this class. All the concepts and claims will become clear and be proved in what follows. After this rather long motivation, we will consider excitation operators of the following form<sup>19</sup>:

$$Q_\nu^\dagger = \frac{1}{2} \sum_{mi} \left( \tilde{X}_{mi}^\nu a_m^\dagger a_i + X_{mi}^\nu a_m^\dagger a_i^\dagger - Y_{mi}^\nu a_m a_i \right) + \sum_n \left( \tilde{Z}_m^\nu a_m^\dagger - Z_m^\nu a_m \right). \quad (3.52)$$

In the following<sup>20</sup>, we will call  $\tilde{X}, X, Y, Z, \tilde{Z}$  *amplitudes*. In order to obtain a solvable problem, we want to obtain a set of equations that contain the amplitudes, some given matrices, and the energy difference  $E_\nu - E_0$ . To this end, the (up to now arbitrary) operators  $\delta Q$  will be utilized, together with the *second gRPA approximation*. We choose  $\delta Q$  in such a way that the different amplitudes are extracted individually on the RHS of eq. (3.47). It will be useful to consider  $\delta Q \in \{a_i, a_i^\dagger, a_i^\dagger a_j, a_i a_j, a_i^\dagger a_j^\dagger\}$ , and compute the commutators  $[\delta Q, Q_\nu^\dagger]$ :

$$\begin{aligned} \left[ a_j, Q_\nu^\dagger \right] &= \frac{1}{2} \sum_i \left( \tilde{X}_{ji}^\nu a_i + X_{\{ji\}}^\nu a_i^\dagger \right) + \tilde{Z}_j^\nu \\ \left[ a_j^\dagger, Q_\nu^\dagger \right] &= \frac{1}{2} \sum_i \left( \tilde{X}_{ij}^\nu a_i^\dagger + Y_{\{ji\}}^\nu a_i \right) + Z_j^\nu \\ \left[ a_n^\dagger a_j, Q_\nu^\dagger \right] &= \frac{1}{2} \sum_i \left( \tilde{X}_{ji}^\nu a_n^\dagger a_i - \tilde{X}_{ni}^\nu a_i^\dagger a_j + X_{\{ji\}}^\nu a_n^\dagger a_i^\dagger + Y_{\{ji\}}^\nu a_n a_i \right) + \tilde{Z}_j^\nu a_n^\dagger + Z_n^\nu a_j \\ \left[ a_n^\dagger a_j^\dagger, Q_\nu^\dagger \right] &= -\frac{1}{2} \sum_i \left( \tilde{X}_{in}^\nu a_i^\dagger a_j^\dagger + \tilde{X}_{ij}^\nu a_i^\dagger a_n^\dagger - Y_{\{jn\}}^\nu - Y_{\{in\}}^\nu a_j^\dagger a_i - Y_{\{ij\}}^\nu a_n^\dagger a_i \right) - Z_n^\nu a_j^\dagger - Z_j^\nu a_n^\dagger \\ \left[ a_n a_j, Q_\nu^\dagger \right] &= \frac{1}{2} \sum_i \left( \tilde{X}_{ji}^\nu a_n a_i + \tilde{X}_{ni}^\nu a_j a_i + X_{\{jn\}}^\nu + X_{\{ji\}}^\nu a_i^\dagger a_n - Y_{\{ni\}}^\nu a_i^\dagger a_j \right) + \tilde{Z}_n^\nu a_j + \tilde{Z}_j^\nu a_n \end{aligned} \quad (3.53)$$

<sup>17</sup>This is a certain abuse of language, since the excitation 'created by  $\Gamma_B$ ' is not created by  $\Gamma_B$  by acting upon the gRPA ground state<sup>18</sup>|RPA) (that is in fact annihilated by  $\Gamma_B$ ) in the same way as the other excitations are created by acting with  $Q_\nu^\dagger$  upon the gRPA ground state. However, as we will discuss in secs. 3.3.9 and 3.5, one can construct a coordinate conjugate  $\Theta_B$  to  $\Gamma_B$ , and the states  $|\gamma\rangle = \exp(i\gamma\Theta_B)|\text{RPA}\rangle$  are the states that we call 'excitations generated by  $\Gamma_B$ '. That these states are indeed orthogonal to the all other (physical) excitations follows from the fact that  $[Q_\nu^\dagger, \Theta_B] = 0$  (as follows from the considerations of sec. 3.3.7):  $\langle \text{RPA} | Q_\nu \exp(i\gamma\Theta_B) | \text{RPA} \rangle = \langle \text{RPA} | \exp(i\gamma\Theta_B) Q_\nu | \text{RPA} \rangle = 0$ .

<sup>18</sup>The gRPA ground state is defined by the fact that it is annihilated by all  $Q_\nu$  and the symmetry generators (that are given as one-body operators) that don't annihilate the mean-field vacuum.

<sup>19</sup>The Gauss law operator in creation/annihilation formulation is given in appendix C.4.2.

<sup>20</sup> $Q_\nu^\dagger$  does not contain an  $aa^\dagger$  term. This is due to the fact that  $aa^\dagger$  is distinguished from  $a^\dagger a$  (which is included) only by a constant. However, this constant would lead to a non-vanishing expectation value of  $Q_\nu^\dagger$  between mean-field vacua, in view of the second gRPA approximation a situation certainly not desirable for an excitation operator (all other terms contained in  $Q_\nu^\dagger$  vanish between mean-field vacua!). One could also argue on a formal level that the way the generalized RPA is derived here does not allow to determine any constant parts of  $Q_\nu^\dagger$ , so if we cannot determine a constant, we shouldn't put it into our ansatz in the first place. Another point of view that is based on the quasi-boson approximation can be found in footnote 27.



with  $X_{\{ij\}}$  defined as  $X_{\{ij\}} = X_{ij} + X_{ji}$ , and correspondingly for  $Y_{\{ij\}}$ . The *second gRPA approximation* states that in the case of expectation values of commutators, the exact vacuum state shall be replaced by the mean-field vacuum state; in the rest of this chapter,  $|\rangle$  denotes the mean-field vacuum with the property  $a|\rangle = 0$ . Then the equations simplify drastically, and we obtain:

$$\begin{array}{lcl} \langle [a_j, Q_\nu^\dagger] \rangle & = & \tilde{Z}_j^\nu \quad \langle [a_j^\dagger, Q_\nu^\dagger] \rangle = Z_j^\nu \\ \langle [a_n^\dagger a_j^\dagger, Q_\nu^\dagger] \rangle & = & \frac{1}{2} Y_{\{jn\}}^\nu \quad \langle [a_n a_j, Q_\nu^\dagger] \rangle = \frac{1}{2} X_{\{jn\}}^\nu \\ \langle [a_n^\dagger a_j, Q_\nu^\dagger] \rangle & = & 0, \end{array} \quad (3.54)$$

where we have used the notation  $\langle |\dots| \rangle = \langle \dots \rangle$ . Two things are remarkable: first, quite simple  $\delta Q$  are sufficient to extract (within the second gRPA approximation) the amplitudes on the RHS of eq.(3.47). Second, it is impossible (even if one uses arbitrarily complicated operators) to extract the amplitude  $\tilde{X}^\nu$  if one wants to use the second gRPA approximation:

$$\langle |[\delta Q, a^\dagger a]|\rangle = \langle |\delta Q a^\dagger \underbrace{a}_{=0} \rangle - \langle |a^\dagger \underbrace{a \delta Q}_{=0} \rangle = 0. \quad (3.55)$$

In the context of the quasi-boson approximation, this will be elucidated from a different angle (see below). To accommodate this fact we restrict the class of excitation operators further<sup>21,22</sup> to those that do not contain terms of the form  $a^\dagger a$ :

$$Q_\nu^\dagger = \frac{1}{2} \sum_{mi} \left( X_{mi}^\nu a_m^\dagger a_i^\dagger - Y_{mi}^\nu a_m a_i \right) + \sum_m \left( \tilde{Z}_m^\nu a_m^\dagger - Z_m^\nu a_m \right). \quad (3.56)$$

With the  $\delta Q$ s defined above we now have to compute the LHS of eq. (3.47). For this purpose we introduce a number of matrices

$$\begin{array}{ll} A_{njmi} = \langle [a_n^\dagger a_j^\dagger, [H, a_m^\dagger a_i^\dagger]] \rangle, & B_{njmi} = \langle [a_n^\dagger a_j^\dagger, [H, a_m a_i]] \rangle, \\ C_{njm} = \langle [a_n^\dagger a_j^\dagger, [H, a_m^\dagger]] \rangle, & D_{njm} = \langle [a_n^\dagger a_j^\dagger, [H, a_m]] \rangle, \\ E_{nm} = \langle [a_n^\dagger, [H, a_m^\dagger]] \rangle, & F_{nm} = \langle [a_n^\dagger, [H, a_m]] \rangle, \end{array} \quad (3.57)$$

and study their properties under interchange of labels. This will allow to reduce the number of independent entries of the LHS of eq. (3.47). The basic tools for this study will be the Jacobi identity and the second gRPA approximation, i.e.  $a|\rangle = 0$ . We will also frequently use that  $[a, a] = [a^\dagger, a^\dagger] = 0$ .

<sup>21</sup>The same structure, albeit with  $Z = \tilde{Z} = 0$ , is used in nuclear physics if one performs a quasi-particle RPA starting from a Hartree-Fock-Bogoliubov calculation [RS80].

<sup>22</sup>It may be possible that instead of using  $Q_\nu^\dagger$  in the form given in eq. (3.56) one could also use a two-step process that starts with a Bogoliubov transformation  $b_\mu = \sum_m (\tilde{Z}_m^\mu a_m^\dagger - Z_m^\mu a_m) + c_\mu$ , where  $b_\mu$  are the new annihilation operators and  $c_\mu$  is a (complex) constant that is allowed in a Bogoliubov transformation for bosons [RS80].  $b_\mu^\dagger$  is defined correspondingly. It may be that at this point the consistency condition between the second gRPA approximation and the quasi-boson approximation which will be discussed further in sec. 3.3.6, i.e.  $\frac{\delta \langle H \rangle}{\delta \pi} = \frac{\delta \langle H \rangle}{\delta \phi} = 0$ , appears naturally as determining equations for the coefficients of the Bogoliubov transformation. Now one could build up  $Q_\nu^\dagger$  in terms of  $b_{\mu_1} b_{\mu_2}$  and  $b_{\mu_1}^\dagger b_{\mu_2}^\dagger$ . We do not follow this path (and have not investigated its feasibility), since our main goals, i.e. the proof of equivalence of the operator approach to the gRPA to the approach based on the time-dependent variational principle and the discussion of conservation laws, seems simpler in the one-step treatment based on eq. (3.56).

### Properties of A

$A_{minj}$  is *symmetric* in all four indices:

$$A_{minj} = \langle [a_m^\dagger a_i^\dagger, [H, a_n^\dagger a_j^\dagger]] \rangle = \langle [a_n^\dagger a_j^\dagger, [H, a_m^\dagger a_i^\dagger]] \rangle = A_{njmi}. \quad (3.58)$$

It's trivial to show that e.g.  $A_{minj} = A_{imnj}$  etc.

### Properties of B

Consider the *complex conjugate* of  $B_{minj}$ :

$$\begin{aligned} B_{njmi}^* &= \langle [a_n^\dagger a_j^\dagger, [H, a_m a_i]] \rangle^* \\ &= \langle [a_n a_j, [H, a_m^\dagger a_i^\dagger]] \rangle \\ &= -\langle [H, [a_m^\dagger a_i^\dagger, a_n a_j]] \rangle + \langle [a_m^\dagger a_i^\dagger, [H, a_n a_j]] \rangle \\ &= -\langle [H, [a_m^\dagger a_i^\dagger, a_n a_j]] \rangle + B_{minj}. \end{aligned} \quad (3.59)$$

The first term will vanish, as one can see as follows: we compute the commutator

$$[a_m^\dagger a_i^\dagger, a_n a_j] = -\left( \delta_{jm} \delta_{ni} + \delta_{ji} \delta_{nm} + \delta_{jm} a_i^\dagger a_n + \delta_{nm} a_i^\dagger a_j + \delta_{ji} a_m^\dagger a_n + \delta_{ni} a_m^\dagger a_j \right). \quad (3.60)$$

It consists of two different structures:  $\delta\delta$  and  $\delta a^\dagger a$ . We can insert this into the above commutator: obviously  $[H, \delta\delta] = 0$ ; the other contributions vanish upon taking expectation values with the mean-field vacuum (cf. eq. (3.55)). Thus we have shown that

$$B_{njmi}^* = B_{minj} \quad (3.61)$$

or if we introduce a 'super-boson index' that combines  $(mi)$  and  $(nj)$  into one index each, thus making  $B$  a matrix in the usual sense,

$$\boxed{B = B^\dagger}. \quad (3.62)$$

### Properties of E

$E_{nm}$  is a symmetric matrix

$$E_{nm} = \langle [a_n^\dagger, [H, a_m^\dagger]] \rangle = -\langle [a_m^\dagger, [a_n^\dagger, H]] \rangle = E_{mn}. \quad (3.63)$$

### Properties of F

$F$ , in contrast, is *hermitian*:

$$F_{nm}^* = \langle [a_n^\dagger, [H, a_m]] \rangle^* = F_{mn}, \quad (3.64)$$

or, in matrix notation:

$$\boxed{F = F^\dagger}. \quad (3.65)$$

### Other Commutators

Apart from one matrix, all other matrices that arise from inserting the different  $\delta Q$ s into the LHS of eq. (3.47) are trivially related to the matrices  $A, \dots, F$  introduced above; this one non-trivial matrix is

$$\langle [a_n^\dagger, [H, a_m a_i]] \rangle. \quad (3.66)$$

It is related to the matrix D via

$$\langle [a_n^\dagger, [H, a_m a_i]] \rangle = \langle [H, \underbrace{[a_n^\dagger, a_m a_i]}_{-\delta_{in} a_m - \delta_{nm} a_i}] \rangle - \langle [a_m a_i, [a_n^\dagger, H]] \rangle \quad (3.67)$$

$$= \delta_{in} \underbrace{\langle [H, a_m] \rangle}_{\Lambda_m} + \delta_{nm} \underbrace{\langle [H, a_i] \rangle}_{\Lambda_i} + \langle [a_m a_i, [H, a_n^\dagger]] \rangle \quad (3.68)$$

$$= \delta_{in} \Lambda_m + \delta_{nm} \Lambda_i + D_{min}^*. \quad (3.69)$$

Later on, in sec. 3.3.6, the second gRPA approximation will be replaced by the so-called *quasi-boson approximation*. In that formulation, it will be obvious that we have to neglect the terms  $\Lambda$ . When we compute explicitly the expectation values in a later section, we will see that, at the stationary mean-field point<sup>23</sup>,  $\Lambda$  is indeed zero. We note two points:

- the gRPA matrix (essentially the LHS of eq. (3.47)) is hermitian iff  $\Lambda = 0$
- the second gRPA approximation and the quasi-boson approximation introduced below are compatible iff  $\Lambda = 0$ ; such a constraint does not appear in nuclear physics, as is easily comprehensible in two different ways: first, the matrix under consideration (as well as the matrices  $C, D$ ) are non-zero only if the Hamiltonian contains terms with in total three creation/annihilation operators, i.e. terms that violate particle-number conservation. Such terms are not allowed in the usual nuclear physics framework, and thus there is no possibility for the above consistency condition to arise<sup>24</sup>. Second, if we replace (as we will do in sec. 3.3.6) the operators containing two ordinary boson creation operators by a new boson operator, we have in the case of bosonic theories the original boson still left, in contrast to nuclear physics, where it is not necessary to retain the original fermions once one has the formulation in terms of bosonic operators at hand;

This whole discussion allows us now to write down a first form of the gRPA equations:

$$\left( \begin{array}{cccc} \frac{1}{2} B_{ij;kl}^* & -\frac{1}{2} A_{ij;kl}^* & D_{ij;k}^* & -C_{ij;k}^* \\ -\frac{1}{2} A_{ij;kl} & B_{ij;kl} & -C_{ij;k} & D_{ij;k} \\ \frac{1}{2} D_{kl;i} & -\frac{1}{2} C_{kl;i}^* & F_{ik}^* & -E_{ik}^* \\ -\frac{1}{2} C_{kl;i} & \frac{1}{2} D_{kl;i}^* & -E_{ik} & F_{ik} \end{array} \right) \left( \begin{array}{c} \frac{1}{2} X_{\{kl\}}^\nu \\ \frac{1}{2} Y_{\{kl\}}^\nu \\ \tilde{Z}_k^\nu \\ Z_k^\nu \end{array} \right) = \Omega_\nu \left( \begin{array}{ccc} 1 & & \\ & -1 & \\ & & 1 \\ & & & -1 \end{array} \right) \left( \begin{array}{c} \frac{1}{2} X_{\{ij\}}^\nu \\ \frac{1}{2} Y_{\{ij\}}^\nu \\ \tilde{Z}_i^\nu \\ Z_i^\nu \end{array} \right) \quad (3.70)$$

with  $\Omega_\nu = E_\nu - E_0$ . The factors  $\frac{1}{2}$  associated with some of the matrices  $C, D$  shouldn't lead one to conclude that the gRPA matrix on the LHS is not hermitian. In fact, as we will see later on, we can write the gRPA equations in a very compact form resulting from a hermitian Hamiltonian (at the stationary point of the mean-field equations  $\frac{\delta}{\delta \phi_i} \langle H \rangle \stackrel{!}{=} 0$ , and  $\frac{\delta}{\delta \pi_i} \langle H \rangle \stackrel{!}{=} 0$ ).

<sup>23</sup>i.e., that point in parameter space where the energy expectation value is stationary with respect to variations of  $\bar{\phi}, \bar{\pi}, G, \Sigma$ ; for  $\Lambda$  to be zero it is necessary that  $\frac{\delta}{\delta \phi_i} \langle H \rangle = 0$ , and  $\frac{\delta}{\delta \pi_i} \langle H \rangle = 0$ .

<sup>24</sup>In the bosonic theories under consideration here, these terms with three creation/annihilation operators appear in the Hamiltonian usually due to a condensate.

### 3.3.5 Explicit Expressions for $A, \dots, F$

In this paragraph, we want to give explicit expressions that are valid for the theories that have a Hamiltonian of the form eq. (3.32). As we have mentioned above, terms in the Hamiltonian that contain more than four  $c/a$  operators do not contribute to any of the matrix elements due to the second gRPA approximation<sup>25</sup>. Then the computation is straightforward: we simply insert eq. (3.43) into eq. (3.57), and compute the double commutators. The computation is simplified by the observation that only those terms of  $H$  contribute to the matrices where the number of creation operators together with the number of annihilation operators in the definition of the matrix elements match the respective number of annihilation operators. This is the reason for the matrices  $A, C, D, E$  having contributions from one term of  $H$  only.  $B$  obtains contributions from two terms of  $H$  as is to be expected, whereas  $F$  obtains only one. Individually, the matrices read:

#### Matrix A

$$A_{minj} = -24H_{04}^{\{minj\}} \quad (3.71)$$

#### Matrix B

$$B_{minj} = B_{minj}^{11} + B_{minj}^{22} \quad (3.72)$$

with

$$B_{minj}^{11} = (H_{11}^{ji}\delta_{nm} + H_{11}^{ni}\delta_{jm} + H_{11}^{jm}\delta_{ni} + H_{11}^{nm}\delta_{ji}) \quad ; \quad B_{minj}^{22} = 4H_{22}^{\{nj\}\{mi\}} \quad (3.73)$$

#### Matrix C

$$C_{jmi} = -6H_{03}^{\{jmi\}} \quad (3.74)$$

#### Matrix D

$$D_{jmi} = 2H_{12}^{i\{jm\}} \quad (3.75)$$

#### Matrix E

$$E_{mi} = -2H_{02}^{\{mi\}} \quad (3.76)$$

#### Matrix F

$$F_{mi} = H_{11}^{im}, \quad (3.77)$$

where  $\{ij\}$  means: symmetrize in the indices  $i, j$  (i.e. add all permutations and divide by the number of permutations) and  $H_{\ddot{a}b}$  means 'that factor in the Hamiltonian that multiplies  $a$  creation

<sup>25</sup>One can use Wick's theorem to compute the double commutators that appear in the definition of the matrices  $A, \dots, F$ . Then one realizes that if there are terms in the Hamiltonian with more than four  $c/a$  operators, every term appearing in the evaluation of the double commutator contains at least one  $c/a$  operator, and the vacuum expectation value in the second gRPA approximation sets these terms to zero.

and  $b$  annihilation operators'. We see that at the stationary point they simplify considerably:

$$\begin{aligned}
A_{minj} &= -4U_{mm_1}U_{ii_1}U_{nn_1}U_{jj_1}\frac{\delta^2}{\delta G_{m_1i_1}\delta G_{n_1j_1}}\langle V \rangle \\
B_{minj} &= 4U_{mm_1}U_{ii_1}U_{nn_1}U_{jj_1}\frac{\delta^2}{\delta G_{m_1i_1}\delta G_{n_1j_1}}\langle V \rangle + (F_{mn}\delta_{ij} + F_{mj}\delta_{in} + F_{in}\delta_{mj} + F_{ij}\delta_{mn}) \\
C_{jmi} &= -2U_{jj_1}U_{mm_1}U_{ii_1}\frac{\delta^2}{\delta \bar{\phi}_{j_1}\delta G_{m_1i_1}}\langle H \rangle \\
D_{jmi} &= -C_{jmi} \\
E_{mi} &= 0 \\
F_{mi} &= \frac{1}{2}G_{mi}^{-1}.
\end{aligned}$$

(3.78)

### 3.3.6 The Quasi-Boson Approximation

Sometimes, it is useful to have the second gRPA approximation at hand without having to take expectation values. This can be done with the help of the *quasi-boson approximation*. The name has its roots in nuclear physics [MW69], [RS80], where two fermions were combined into one boson. This works only approximately<sup>26</sup>, so that the result was christened a *quasi-boson*. Interestingly enough, we can do the same in a bosonic system: we replace a two boson operator (like  $aa$  or  $a^\dagger a^\dagger$ ) by a new operator that again has bosonic commutation relations. We construct the new boson-pair operators  $B, B^\dagger$  s.t. the commutation relations are identical to the mean-field expectation values of commutators containing still the pair of original boson operators<sup>27</sup>:

$$\begin{aligned}
[a_m a_i, a_j] &= 0 && \rightarrow [B_{mi}, a_j] = 0 \\
[a_m a_i, a_j^\dagger] &= \delta_{ij} a_m + \delta_{mj} a_i && \rightarrow \langle [a_m a_i, a_j^\dagger] \rangle = 0 \rightarrow [B_{mi}, a_j^\dagger] = 0 \\
[a_m^\dagger a_i^\dagger, a_j] &= -\delta_{ij} a_m^\dagger - \delta_{mj} a_i^\dagger && \rightarrow \langle [a_m^\dagger a_i^\dagger, a_j] \rangle = 0 \rightarrow [B_{mi}^\dagger, a_j] = 0.
\end{aligned}$$

The only non-vanishing commutators involving  $B, B^\dagger$  originates from  $[a_m a_i, a_n^\dagger a_j^\dagger]$ :

$$\begin{aligned}
[a_m a_i, a_n^\dagger a_j^\dagger] &= \delta_{in} \delta_{mj} + \delta_{ij} \delta_{mn} + \delta_{in} a_j^\dagger a_m + \delta_{mn} a_j^\dagger a_i + \delta_{ij} a_n^\dagger a_m + \delta_{mj} a_n^\dagger a_i \\
\rightarrow \langle [a_m a_i, a_n^\dagger a_j^\dagger] \rangle &= \delta_{in} \delta_{mj} + \delta_{ij} \delta_{mn} \\
\rightarrow [B_{mi}, B_{nj}^\dagger] &= \delta_{in} \delta_{mj} + \delta_{ij} \delta_{mn}.
\end{aligned}$$

<sup>26</sup>i.e. the ordinary bosonic commutation relations are only fulfilled if we take the mean-field expectation value of the commutator of the boson pairs, and thus in some sense employ the second gRPA approximation, by using the mean-field instead of the exact vacuum state.

<sup>27</sup>Here it seems appropriate to comment once again on the fact that  $a^\dagger a$  does not appear in our excitation operator: the excitation operator is linear in all the different boson creation/annihilation operators that we construct as one can see in eq.(3.83). Thus, we have the question whether we can construct a boson operator from  $a^\dagger a$  similar to how we construct one from  $a^\dagger a^\dagger$ . The problem is immediately apparent: if we consider  $C_{mi} = a_m^\dagger a_i$ , then its adjoint has the same structure as  $C_{mi}$ , since  $C_{mi}^\dagger = a_i^\dagger a_m = C_{im}$ ; if we compute the commutator  $[C_{ij}, C_{kl}^\dagger] = \delta_{jk} a_i^\dagger a_l - \delta_{li} a_k^\dagger a_j$  we see that its mean-field expectation value is zero. Therefore we cannot construct Boson operators with the correct commutation relations from  $a^\dagger a$  in the same way as we did for  $a^\dagger a^\dagger$ , and thus they don't appear in the excitation operators  $Q_\nu^\dagger$ . In nuclear physics this is well-known. There one can see that the quasi-boson operators correspond to a creation of a particle-hole pair (or its annihilation), whereas the operator that creates and annihilates a particle is translated into an operator that creates and annihilates a quasi-boson [MW69].

This last relation implies that the  $B$  operators should be normalized differently, and implies therefore that not  $a_m a_i$  should be replaced by  $B_{mi}$ , but rather one should replace

$$\boxed{\begin{array}{l} \frac{1}{\sqrt{2}}(a_m a_i) \leftrightarrow B_{mi} \\ \frac{1}{\sqrt{2}}(a_m^\dagger a_i^\dagger) \leftrightarrow B_{mi}^\dagger \end{array}} \quad (3.79)$$

They have the following commutation relations

$$[a_j, B_{mi}] = [a_j, B_{mi}^\dagger] = [a_j^\dagger, B_{mi}] = [a_j^\dagger, B_{mi}^\dagger] = [B_{mi}, B_{nj}] = [B_{mi}^\dagger, B_{nj}^\dagger] = 0 \quad (3.80)$$

$$\text{and} \quad [B_{mi}, B_{nj}^\dagger] = \frac{1}{2}(\delta_{in}\delta_{mj} + \delta_{ij}\delta_{mn}). \quad (3.81)$$

With these new operators, the excitation operators

$$Q_\nu^\dagger = \frac{1}{2} \sum_{mi} \left( X_{mi}^\nu a_m^\dagger a_i^\dagger - Y_{mi}^\nu a_m a_i \right) + \sum_m \left( \tilde{Z}_m^\nu a_m^\dagger - Z_m^\nu a_m \right) \quad (3.82)$$

become:

$$\boxed{Q_\nu^\dagger = \frac{1}{\sqrt{2}} \sum_{mi} \left( X_{mi}^\nu B_{mi}^\dagger - Y_{mi}^\nu B_{mi} \right) + \sum_m \left( \tilde{Z}_m^\nu a_m^\dagger - Z_m^\nu a_m \right)}. \quad (3.83)$$

At this point a short comment on how one constructs quasi-boson approximations is in order<sup>28</sup>. Usually we will have to consider only one- and two-body operators, but the procedure should work for higher-body operators as well:

- (i) first, one writes down the operator  $\mathcal{O}$  under consideration as a polynomial of  $a, a^\dagger$  operators. Then one tries to extract the coefficients of the different powers in analogy to eqs. (3.54,3.57) via (a) taking multiple commutators of  $\mathcal{O}$  with up to two  $a, a^\dagger$  operators, and then (b) taking vacuum expectation values of these multiple commutators employing the second gRPA approximation.
- (ii) The quasi-boson approximation  $\mathcal{O}_B$  of this operator  $\mathcal{O}$  is then given as a polynomial of  $B, B^\dagger, a, a^\dagger$  operators. The coefficients of the different powers are extracted by taking multiple commutators of  $\mathcal{O}_B$  with  $a, a^\dagger, B, B^\dagger$  *without* taking expectation values. One then requires that the coefficients of  $\mathcal{O}_B$  determined in this way are identical to those of  $\mathcal{O}$  determined in (i) if one replaces in the multiple commutators of (i)  $\mathcal{O}$  by  $\mathcal{O}_B$  and terms of the structure  $aa$  by  $\sqrt{2}B$  and  $a^\dagger a^\dagger$  by  $\sqrt{2}B^\dagger$  as indicated in eq. (3.79) .

This is precisely the procedure that led to eq. (3.83), and will also be used to obtain the Hamiltonian in quasi-boson approximation. The coefficients mentioned are nothing but the matrices  $A, \dots, F$ . We therefore have the requirements

$$\begin{aligned} A_{njmi} &= \langle [a_n^\dagger a_j^\dagger, [H, a_m^\dagger a_i^\dagger]] \rangle \stackrel{!}{=} [\sqrt{2}B_{nj}^\dagger, [H_B, \sqrt{2}B_{mi}^\dagger]], \\ B_{njmi} &= \langle [a_n^\dagger a_j^\dagger, [H, a_m a_i]] \rangle \stackrel{!}{=} [\sqrt{2}B_{nj}^\dagger, [H_B, \sqrt{2}B_{mi}]], \\ C_{njm} &= \langle [a_n^\dagger a_j^\dagger, [H, a_m^\dagger]] \rangle \stackrel{!}{=} [\sqrt{2}B_{nj}^\dagger, [H_B, a_m^\dagger]], \\ D_{njm} &= \langle [a_n^\dagger a_j^\dagger, [H, a_m]] \rangle \stackrel{!}{=} [\sqrt{2}B_{nj}^\dagger, [H_B, a_m]], \\ E_{nm} &= \langle [a_n^\dagger, [H, a_m^\dagger]] \rangle \stackrel{!}{=} [a_n^\dagger, [H_B, a_m^\dagger]], \\ F_{nm} &= \langle [a_n^\dagger, [H, a_m]] \rangle \stackrel{!}{=} [a_n^\dagger, [H_B, a_m]], \end{aligned} \quad (3.84)$$

<sup>28</sup>A general formula for the quasi-boson approximation of a one-body operator is given in eq. (3.142).

where  $H_B$  denotes the Hamiltonian in quasi-boson approximation. At this point it seems in order to discuss a question that turned up in connection with eq. (3.66): there we saw that one of the double commutators was not directly connected to one of the matrices  $A, \dots, F$  but that some extra terms appeared, the ' $\Lambda$ -terms'. If we consider the same double commutator in the quasi-boson approximation, we obtain

$$\langle [H, [a_n^\dagger, a_m a_i]] \rangle \rightarrow \langle [H, \underbrace{[a_n^\dagger, \sqrt{2} B_{mi}]}_{=0}] \rangle = 0. \quad (3.85)$$

Thus the quasi-boson approximation implies the *vanishing of  $\Lambda$* . An explicit expression can be given for  $\Lambda$  as well

$$\Lambda_i = \langle [H, a_i^\dagger] \rangle = \left( \frac{\delta}{\delta \bar{\phi}_k} \langle \hat{H} \rangle \right) U_{ki} + \left( \frac{\delta}{\delta \bar{\pi}_k} \langle H \rangle \right) \left( \frac{1}{2i} U_{ki}^{-1} + 2 \Sigma_{kl} U_{li} \right), \quad (3.86)$$

which vanishes if we choose the parameters of the reference state s.t. the energy is stationary under their variation (at least w.r.t.  $\bar{\phi}, \bar{\pi}$ ). We obtain a consistency condition between the second gRPA approximation and the quasi-boson approximation: the latter is equivalent to the former *only at the stationary point*<sup>29</sup> of  $\langle H \rangle$ . Thus, in the following we will always assume that the state (which we often call the *mean-field vacuum*) relative to which our creation/annihilation operators are defined has its parameters chosen s.t. it satisfies the Rayleigh-Ritz principle. With this qualification, we can give the (now hermitian) Hamiltonian in quasi-boson approximation:

$$\begin{aligned} H_B = E & - \frac{1}{4} \left( A_{n_1 j_1 n_2 j_2} B_{n_1 j_1} B_{n_2 j_2} + A_{n_1 j_1 n_2 j_2}^* B_{n_1 j_1}^\dagger B_{n_2 j_2}^\dagger \right) + \frac{1}{2} B_{n_2 j_2 n_1 j_1} B_{n_1 j_1}^\dagger B_{n_2 j_2} \\ & - \frac{1}{\sqrt{2}} \left( C_{n_1 j_1 n_2} B_{n_1 j_1} a_{n_2} + C_{n_1 j_1 n_2}^* B_{n_1 j_1}^\dagger a_{n_2}^\dagger \right) \\ & + \frac{1}{\sqrt{2}} \left( D_{n_1 j_1 n_2} B_{n_1 j_1} a_{n_2}^\dagger + D_{n_1 j_1 n_2}^* B_{n_1 j_1}^\dagger a_{n_2} \right) \\ & - \frac{1}{2} \left( E_{n_1 n_2} a_{n_1} a_{n_2} + E_{n_1 n_2}^* a_{n_1}^\dagger a_{n_2}^\dagger \right) + F_{n_2 n_1} a_{n_1}^\dagger a_{n_2}. \end{aligned} \quad (3.87)$$

We have achieved writing the approximated Hamiltonian as a quadratic form, which always can be diagonalized<sup>30</sup>. Using this Hamiltonian  $H_B$ , one can see that the gRPA equations eq. (3.70) can be written in the transparent form<sup>31</sup>

$$[H_B, Q_\nu^\dagger] = \Omega_\nu Q_\nu^\dagger. \quad (3.88)$$

This form of the gRPA equations demonstrates that we have performed the approximation to the dynamics (Hamiltonian) and to the excitation operators consistently, since the form of the equations is identical to the form of the Schrödinger equation eq. (3.45) with the *exact* Hamiltonian and the *exact* excitation operators.

### 3.3.7 Commutation Relations

In this section we want to consider the question 'what are the conditions under which the eigenmodes  $Q_\nu^\dagger$  can be treated as harmonic oscillators?' We start with the observation that eq. (3.88)

<sup>29</sup>At least w.r.t the condensates  $\bar{\phi}, \bar{\pi}$ .

<sup>30</sup>To quote from [MW69]: '*The achievement of a quadratic form in the bosons, which is always diagonalizable has, of course, been the aim of the game.*'

<sup>31</sup>One inserts eq. (3.87) and eq. (3.83) into eq. (3.88) and compares the coefficients of the different operators  $a, a^\dagger, B, B^\dagger$ . This then reproduces eq. (3.70).

implies by hermitian conjugation

$$[H_B, Q_\nu] = -\Omega_\nu Q_\nu. \quad (3.89)$$

Thus, to every eigenfrequency, the negative eigenfrequency also belongs to the spectrum. Thus, without loss of generality<sup>32</sup> in the following we will assume that

$$\Omega_\nu \geq 0, \quad (3.90)$$

otherwise we just exchange the respective  $Q_\nu, Q_\nu^\dagger$ . The next point is that all the commutators

$$[Q_\nu^\dagger, Q_\mu^\dagger] \quad [Q_\nu, Q_\mu^\dagger] \quad [Q_\nu, Q_\mu] \quad (3.91)$$

are pure numbers. This is due to the fact that all operators considered in this context are by construction linear in  $B, B^\dagger, a, a^\dagger$ . We denote these numbers as

$$[Q_\mu^\dagger, Q_\nu^\dagger] = M_{\mu\nu}; \quad [Q_\mu, Q_\nu^\dagger] = N_{\mu\nu}; \quad [Q_\mu, Q_\nu] = O_{\mu\nu}. \quad (3.92)$$

Up to now these numbers are arbitrary; one can, however, put the equations of motion to some good use. Consider

$$\Omega_\nu [Q_\mu, Q_\nu^\dagger] \stackrel{\text{eq. (3.88)}}{=} [Q_\mu, [H_B, Q_\nu^\dagger]] \quad (3.93)$$

$$\stackrel{\text{Jacobi id.}}{=} -[H_B, [Q_\nu^\dagger, Q_\mu]] - [Q_\nu^\dagger, [Q_\nu, H_B]] \quad (3.94)$$

$$= \underbrace{[H_B, N_{\mu\nu}]}_{=0} + [Q_\nu^\dagger, \underbrace{[H_B, Q_\mu]}_{=-\Omega_\mu Q_\mu}] \quad (3.95)$$

$$= \Omega_\mu [Q_\mu, Q_\nu^\dagger]. \quad (3.96)$$

In other words:

$$(\Omega_\nu - \Omega_\mu) N_{\mu\nu} = 0 \quad (\text{no sum over } \mu, \nu). \quad (3.97)$$

If all eigenvalues are distinct and non-zero then eq. (3.97) implies that  $N_{\mu\nu}$  is diagonal. Since the gRPA equations are homogeneous equations, we may now normalize the amplitudes in such a way that<sup>33,34</sup>

$$N_{\mu\nu} = \delta_{\mu\nu}. \quad (3.98)$$

<sup>32</sup>We will see later on in sec. 3.3.10 that the *assumption* that the eigenenergies of the modes are *real* already implies that we are dealing with a stable mean-field solution.

<sup>33</sup>In [RS80] it is stated that one can show that  $N_{\mu\nu}$  is positive if one is considering a positive definite Hessian at the stationary point of the mean-field problem; a possible proof of this statement works as follows: only if the Hessian is a positive matrix it is guaranteed that all eigenvalues  $\Omega^2$  are positive. This has been assumed so far (e.g. how we concluded that for every positive frequency there is also a negative one etc.); thus we know that the system is stable. Knowing this, we can argue as follows: we know that  $[H, Q_\nu^\dagger] = \Omega_\nu Q_\nu^\dagger$ ,  $[H, Q_\nu] = -\Omega_\nu Q_\nu$  and  $[Q_\nu, Q_\nu^\dagger] = \mathcal{N}_\nu \delta_{\nu\nu}$ . From this we conclude that the Hamiltonian has to look like  $H = \sum_\nu (\Omega_\nu / \mathcal{N}_\nu) Q_\nu^\dagger Q_\nu$ . Now we can study two different scenarios, namely  $\mathcal{N}_\nu$  can be positive (we call the set of  $\nu$  for which this is true  $\nu_+$ ) or negative (correspondingly  $\nu_-$ ). In order to have the usual creation/annihilation commutation relations we have - for  $\nu \in \nu_-$  - to interchange 'creation' and 'annihilation' operators; for clarity, we introduce new letters for them, i.e. for  $\nu \in \nu_-$ ,  $Q_\nu \rightarrow P_\nu^\dagger$ ,  $Q_\nu^\dagger \rightarrow P_\nu$ . Now we normalize  $Q$ s and  $P$ s s.t. for  $\nu \in \nu_+$ ,  $\mathcal{N}_\nu = 1$  and for  $\nu \in \nu_-$ ,  $\mathcal{N}_\nu = -1$ . The Hamiltonian then reads  $H = \sum_{\nu \in \nu_+} \Omega_\nu Q_\nu^\dagger Q_\nu + \sum_{\nu \in \nu_-} (-\Omega_\nu) P_\nu^\dagger P_\nu + \text{const}$ . But here we see that we are dealing with a rather unstable system: the more modes are generated by  $P^\dagger$ , the lower the energy becomes. This cannot be true, however, since we know that we started from a stable system (with all frequencies real)! Thus  $\nu_-$  has to be empty.

<sup>34</sup>This relation has also as its consequence that the states generated by  $Q_\mu^\dagger, Q_\nu^\dagger$  from the gRPA vacuum (cf. footnote 18) are indeed orthogonal:  $\langle \text{RPA} | Q_\mu Q_\nu^\dagger | \text{RPA} \rangle = \langle \text{RPA} | [Q_\mu, Q_\nu^\dagger] | \text{RPA} \rangle = \langle [Q_\mu, Q_\nu^\dagger] \rangle = \delta_{\mu\nu}$  where we have used the second gRPA approximation in the next to last step [RS80].



The same procedure can be carried out for  $M_{\mu\nu}, O_{\mu\nu}$ . We derive in analogy to eq. (3.97):

$$(\Omega_\nu + \Omega_\mu)M_{\mu\nu} = 0, \quad (\Omega_\nu + \Omega_\mu)O_{\mu\nu} = 0, \quad (3.99)$$

where again no sum over double indices is performed. From this we conclude, again if there are no zero modes, that

$$M_{\mu\nu} = 0 \quad O_{\mu\nu} = 0. \quad (3.100)$$

Thus, under the aforementioned conditions, the *normal modes satisfy ordinary c/a commutation relations*. To arrive at this, we have indeed used both gRPA approximations, since the basic ingredient was that  $Q^\dagger$  is a one-particle operator (first gRPA approximation) and that all the commutators of  $a, a^\dagger, \mathbf{B}, \mathbf{B}^\dagger$  are pure numbers (quasi-boson approximation).

Using the fact that the normal modes satisfy ordinary Bose commutation relations, we can automatically write

$$H_B = E_{RPA} + \sum_\nu \Omega_\nu Q_\nu^\dagger Q_\nu. \quad (3.101)$$

The sum over  $\nu$  extends over all positive semi-definite  $\Omega_\nu$ . The constant  $E_{RPA}$  can be determined as usual, cf. [RS80], namely by requiring

$$\langle H_B \rangle = E_{MF}. \quad (3.102)$$

Using

$$\langle Q_\nu^\dagger Q_\nu \rangle = \frac{1}{2} \sum_{mi} |Y_{\{mi\}}^\nu|^2 + \sum_i |Z_i^\nu|^2, \quad (3.103)$$

with  $Y_{\{mi\}}^\nu = Y_{mi}^\nu + Y_{im}^\nu$  this gives

$$E_{RPA} = E_{MF} - \sum_\nu \Omega_\nu \left( \frac{1}{2} \sum_{mi} |Y_{\{mi\}}^\nu|^2 + \sum_i |Z_i^\nu|^2 \right). \quad (3.104)$$

A similar expression can be obtained in nuclear physics [RS80] but without the appearance of  $|Z_i^\nu|^2$ .

### 3.3.8 Zero Modes - Preliminary Discussion

We are now in the following position: we have a mean-field vacuum that breaks a certain symmetry. Our class of gRPA excitation operators is s.t. the generator of that symmetry (or at least its quasi-boson approximation) falls into this class. If we can show (and this will be done below in sec. 3.4), that the quasi-boson approximation of the symmetry generator  $\Gamma_B$  commutes with the quasi-boson approximation of the Hamiltonian  $H_B$ , i.e.

$$[H_B, \Gamma_B] = 0 \quad (3.105)$$

we have approximated the *symmetry* and the *dynamics* in a *consistent manner*: the *approximated* symmetry is an *exact* symmetry of the *approximated* dynamics<sup>35</sup>. One should note, however, that eq. (3.105) can also be read in a different way if one compares it to eq. (3.88): the symmetry generator is a *zero-mode* solution of the gRPA equations<sup>36</sup>. This is clear as soon as eq. (3.105) is satisfied.

<sup>35</sup>One should note that the symmetry generated by  $\Gamma_B$  need not be the same as the symmetry that is generated by  $\Gamma$  as we will discuss in sec. 3.4.

<sup>36</sup>It is the main advantage of this approach over the approach via the time-dependent variational principle that this connection is so explicit.

### 3.3.9 Further Discussion of Zero Modes

In the nuclear physics literature it is well-known [MW69] that the appearance of zero-modes, despite being welcome in our case, leads to all sorts of problems, especially that the solutions of the gRPA equations no longer form a complete set<sup>37</sup>. Marshallek *et al.* [MW69] however pointed out that the problems one has are actually an artifact of the creation/annihilation operator formalism. We want to give a very primitive illustration of their point: one can write down a quantum mechanical oscillator in two equivalent forms (we have set the mass equal to one for simplicity):

$$H = \frac{p^2}{2} + \frac{\omega^2}{2}x^2 \quad (3.106)$$

$$= \omega(a^\dagger a + \frac{1}{2}), \quad (3.107)$$

where  $\omega$  denotes the frequency of the harmonic oscillator. If we now send the frequency to zero, something seemingly strange happens:

$$\frac{p^2}{2} + \frac{\omega^2}{2}x^2 \stackrel{\omega \rightarrow 0}{=} \frac{p^2}{2} \quad (3.108)$$

$$\frac{\omega}{2}(a^\dagger a + 1) \stackrel{\omega \rightarrow 0}{=} 0. \quad (3.109)$$

If one now looks at the transformation from canonical to c/a operators, one begins to see more clearly:

$$a = \sqrt{\frac{\omega}{2}}x + \frac{i}{\sqrt{2\omega}}p \stackrel{\omega \rightarrow 0}{=} \frac{i}{\sqrt{2\omega}}p \quad (3.110)$$

$$a^\dagger = \sqrt{\frac{\omega}{2}}x - \frac{i}{\sqrt{2\omega}}p \stackrel{\omega \rightarrow 0}{=} -\frac{i}{\sqrt{2\omega}}p \quad (3.111)$$

$$(3.112)$$

and if we take this small- $\omega$  behaviour into account, there is actually no paradox<sup>38</sup>, since

$$\frac{\omega}{2}a^\dagger a \stackrel{\omega \rightarrow 0}{=} \frac{\omega}{2}\left(\frac{1}{\sqrt{\omega}}\right)^2 p^2 = \frac{p^2}{2}. \quad (3.113)$$

This is actually the solution of the problems involving zero modes: one puts the system into an external field, s.t. there are no zero modes any more, since the external field<sup>39</sup> breaks all

<sup>37</sup>In nuclear physics this is a problem since one there cannot prove that the Hamiltonian can be written as a sum of  $Q_\nu^\dagger Q_\nu$ . Completeness is lost in the following way: we have seen that from every solution of the gRPA equations we can form another solution by considering the adjoint operator, therefore the solutions to the gRPA equations always come in pairs. In the case of zero modes, this is not necessarily true any more, since now the 'excitation operators' that we find may be hermitian; thus, by considering the adjoint, we do not get a new solution. In fact this situation is the usual case for zero modes, since in sec. 3.4 we will see that the excitation operators for the zero modes are just the symmetry generators, which are hermitian. In our previous discussion in sec. 3.3.7, we hit upon the problem from a different direction; we saw that only if there are no zero modes in the spectrum we can show that the excitation operators can be considered as independent oscillators.

<sup>38</sup>One should note that, in this limit  $\omega \rightarrow 0$ , no new information can be obtained by considering the adjoint of  $a^\dagger$ .

<sup>39</sup>The external field can in fact be engineered just to do that, and this works as follows: we solve the gRPA equations and determine all modes available. The operator belonging to the zero mode will be known beforehand

symmetries. One diagonalizes the Hamiltonian into a set of harmonic oscillators using canonical coordinates, and at the end sends the external field to zero. Then the would-be zero modes indeed become zero modes with the correct operator representation, namely  $p^2$ , and the non-zero modes can be rewritten using creation and annihilation operators. As a last comment on this topic, one should keep in mind the following: since we already have some prejudice about the zero mode operators (as the symmetry generators), we cannot just choose their mass to be one as we did in the example. We will rather have to allow for a mass tensor, and this will be dealt with in section 3.5.

*“Now, Watson, confess yourself utterly taken aback,”*  
*said he. “I am.” “I ought to make you sign a paper*  
*to that effect.” “Why?” “Because in five minutes you*  
*will say that it is all so absurdly simple.”*  
 Sherlock Holmes, The Dancing Men

### 3.3.10 p-q Formulation of gRPA

We have seen that at least three formulations of the generalized Random Phase Approximation of bosonic systems are available. In this paragraph we want to add one more, since it simplifies the treatment of those Hamiltonians we set out to consider, cf. eq. (3.32). Since we start from the gRPA formulation using quasi-Boson operators, the whole treatment is only valid for the mean-field vacuum representing a solution of the Rayleigh-Ritz variational principle (at least w.r.t. variations of  $\bar{\phi}$  and  $\bar{\pi}$ ). In this section we assume that the mean-field vacuum is a solution of the Rayleigh-Ritz variational principle w.r.t. all parameters  $\bar{\phi}, \bar{\pi}, \Sigma, G$ . We consider linear combinations of  $a, a^\dagger$  and  $B, B^\dagger$ , s.t.

$$\begin{aligned} q_m &= \frac{1}{\sqrt{2}}(a_m^\dagger + a_m) & p_m &= \frac{i}{\sqrt{2}}(a_m^\dagger - a_m) \\ Q_{mi} &= \frac{1}{\sqrt{2}}(B_{mi}^\dagger + B_{mi}) & P_{mi} &= \frac{i}{\sqrt{2}}(B_{mi}^\dagger - B_{mi}). \end{aligned} \quad (3.114)$$

They fulfil the usual canonical commutation relations:

$$[q_m, p_n] = i\delta_{nm} ; [Q_{mi}, P_{nj}] = \frac{i}{2}(\delta_{mn}\delta_{ij} + \delta_{mj}\delta_{ni}) \quad (3.115)$$

$$\text{and } [q_m, q_n] = [p_m, p_n] = [Q_{mi}, Q_{nj}] = [P_{mi}, P_{nj}] = 0. \quad (3.116)$$

---

- it is just the quasi-boson approximation of the (known) symmetry generator, which is usually a hermitian operator, and so will be the operator associated with the zero mode. One then constructs a canonically conjugate variable, s.t.  $[q, p] = i$  and  $q$  commutes with all other creation/annihilation operators, and adds a term  $\omega^2 q^2$  to the Hamiltonian; this will lift the zero mode to a finite frequency. By this construction, only the zero mode will be lifted and nothing strange will happen to the other modes. Two points should be mentioned: first, the construction of a canonically conjugate coordinate to a such a generator is only possible in the gRPA context, since we will see in sec. 3.4 that the symmetry we have in mind will be reduced to an Abelian symmetry; if we would still have the non-Abelian symmetry this would not be possible (the problems with the construction of 'angle operators' in nuclear physics are well-known, cf. e.g. [TI98]). As a second point, one should mention that in a quantum field theory there might be problems with breaking gauge symmetries in intermediate steps. Since we have indicated here only a formal construction, it is not easy to see where these kinds of problems might surface.

If we now rewrite the Hamiltonian  $H_B$  in terms of these new operators, we obtain a complicated expression where the real and imaginary parts of the matrices  $A, \dots, F$  are separated. We can now put to use that we have computed the matrices  $A, \dots, F$  above; we have found that

1.  $A, C, D$  are always real
2.  $C = -D$
3.  $B, E, F$  may be imaginary; however, as this imaginary part is due to  $\Sigma$ , and in the theories under consideration<sup>40</sup> at the stationary point  $\Sigma = 0$ , the imaginary parts of  $B, E, F$  vanish.
4. As a matter of fact,  $E$  vanishes altogether at the stationary point.
5. A last simplification is that one may decompose  $B = B^{11} + B^{22}$  and, using this notation, we have  $A = -B^{22}$ .

Using this information, the Hamiltonian simplifies considerably:

$$\begin{aligned}
 H_B = E' &+ Q_{n_1 j_1} Q_{n_2 j_2} \frac{1}{4} (B_{n_1 j_1 n_2 j_2} - A_{n_1 j_1 n_2 j_2}) + P_{n_1 j_1} P_{n_2 j_2} \frac{1}{4} (B_{n_1 j_1 n_2 j_2} + A_{n_1 j_1 n_2 j_2}) \\
 &+ \sqrt{2} Q_{n_1 j_1} q_{n_2} D_{n_1 j_1 n_2} + \frac{1}{2} F_{n_2 n_1} (q_{n_2} q_{n_1} + p_{n_2} p_{n_1})
 \end{aligned}
 \tag{3.117}$$

and can even be written in a nice matrix form:

$$\begin{aligned}
 H = E' &+ \frac{1}{2} (P_{n_1 j_1} \quad p_{n_1}) \begin{pmatrix} \frac{1}{2} (B_{n_1 j_1 n_2 j_2} + A_{n_1 j_1 n_2 j_2}) & 0 \\ 0 & F_{n_2 n_1} \end{pmatrix} \begin{pmatrix} P_{n_2 j_2} \\ p_{n_2} \end{pmatrix} \\
 &+ \frac{1}{2} (Q_{n_1 j_1} \quad q_{n_1}) \begin{pmatrix} \frac{1}{2} (B_{n_1 j_1 n_2 j_2} - A_{n_1 j_1 n_2 j_2}) & \sqrt{2} D_{n_1 j_1 n_2} \\ \sqrt{2} D_{n_2 j_2 n_1} & F_{n_2 n_1} \end{pmatrix} \begin{pmatrix} Q_{n_2 j_2} \\ q_{n_2} \end{pmatrix},
 \end{aligned}
 \tag{3.118}$$

where  $E'$  is a constant that has to be chosen s.t.  $\langle H_B \rangle = E_{MF}$ . This is a viable starting point for proving the equivalence between the two gRPA formulations<sup>41</sup>. We will rewrite eq. (3.118) into a Hamiltonian that leads to the same eigenvalue equations as does the Hamiltonian of the small-fluctuation approach given in eq. (3.29). From this we will conclude - since we have both times the same matrix to diagonalize - that the spectra of the Hamiltonians of the two approaches are identical, and we will see a correspondence in the eigenvectors. For this purpose we note the following:

1. We start with the term quadratic in  $p, P$ ; there we have

$$\begin{aligned}
 (B + A)_{n_1 j_1 n_2 j_2} &= (B^{11} + B^{22} - B^{22})_{n_1 j_1 n_2 j_2} \\
 &= \frac{1}{4} (G_{n_1 n_2}^{-1} \delta_{j_1 j_2} + G_{n_1 j_2}^{-1} \delta_{j_1 n_2} + G_{j_1 n_2}^{-1} \delta_{n_1 j_2} + G_{j_1 j_2}^{-1} \delta_{n_1 n_2}) \\
 &= \left( \frac{1}{2} U_{n_1 m_1}^{-1} U_{j_1 i_1}^{-1} \right) \left( \frac{1}{2} U_{n_2 m_2}^{-1} U_{j_2 i_2}^{-1} \right) (G \mathbb{1})_{m_1 i_1 m_2 i_2}
 \end{aligned}
 \tag{3.119}$$

and

$$F_{n_2 n_1} = \left( \frac{1}{\sqrt{2}} U_{n_2 m_2}^{-1} \right) \left( \frac{1}{\sqrt{2}} U_{n_1 m_1}^{-1} \right) \delta_{m_2 m_1}
 \tag{3.120}$$

<sup>40</sup>This excludes the cranking Hamiltonian as it was defined in eq. (2.155) ( $H_{cr} = H - \int d^3 x \omega^a(\mathbf{x}) \Gamma^a(\mathbf{x})$  where  $H$  is the Yang-Mills Hamiltonian) here, since it is not of the form given in eq. (3.32).

<sup>41</sup>Here the formulation using the quasi-Boson operators and the formulation originating from the time-dependent variational principle are meant.

This suggests that one should introduce new momentum operators

$$\mathbf{P}_{m_1 i_1} = \frac{1}{2} U_{n_1 m_1}^{-1} U_{j_1 i_1}^{-1} P_{n_1 j_1} \quad (3.121)$$

$$\mathbf{p}_{m_1} = \frac{1}{\sqrt{2}} U_{n_1 m_1}^{-1} p_{n_1}. \quad (3.122)$$

2. Now we consider the term quadratic in  $q, Q$ ; there the observation

$$\begin{aligned} B_{minj}^{11} &= U_{mk_1} U_{ik_2} U_{nk_3} U_{jk_4} \frac{\delta}{\delta G_{k_1 k_2}} \frac{\delta}{\delta G_{k_3 k_4}} \text{tr}(G^{-1}) \\ &= 8 U_{mk_1} U_{ik_2} U_{nk_3} U_{jk_4} \frac{\delta}{\delta G_{k_1 k_2}} \frac{\delta}{\delta G_{k_3 k_4}} \langle T \rangle \end{aligned} \quad (3.123)$$

(where  $T$  denotes the kinetic energy  $\frac{1}{2}\pi_i^2$ ) is useful. Then one can rewrite

$$\begin{aligned} (B - A)_{minj} &= (B^{11} + B^{22} - (-B^{22}))_{minj} \\ &= B_{minj}^{11} + 2 * 4 U_{mk_1} U_{ik_2} U_{nk_3} U_{jk_4} \frac{\delta}{\delta G_{k_1 k_2}} \frac{\delta}{\delta G_{k_3 k_4}} \langle V \rangle \\ &= 8 U_{mk_1} U_{ik_2} U_{nk_3} U_{jk_4} \frac{\delta}{\delta G_{k_1 k_2}} \frac{\delta}{\delta G_{k_3 k_4}} \langle H \rangle. \end{aligned} \quad (3.124)$$

Next, one can put to use both the stationarity condition, the identity eq.(D.19) from appendix D and the fact that the kinetic energy  $\langle \frac{1}{2}\pi_i^2 \rangle$  is independent of  $\bar{\phi}$ :

$$\begin{aligned} F_{n_2 n_1} &= \frac{1}{2} G_{n_2 n_1}^{-1} = -\frac{1}{2} \left( \frac{\delta}{\delta G_{k_1 k_2}} \text{tr}(G^{-1}) \right) U_{k_1 n_1} U_{k_2 n_2} \\ &= -4 \left( \frac{\delta}{\delta G_{k_1 k_2}} \langle T \rangle \right) U_{k_1 n_1} U_{k_2 n_2} = -4 \left( \frac{\delta}{\delta G_{k_1 k_2}} \langle H - V \rangle \right) U_{k_1 n_1} U_{k_2 n_2} \\ &\stackrel{s.p.}{=} 4 \left( \frac{\delta}{\delta G_{k_1 k_2}} \langle V \rangle \right) U_{k_1 n_1} U_{k_2 n_2} = 2 \left( \frac{\delta^2}{\delta \bar{\phi}_{k_1} \delta \bar{\phi}_{k_2}} \langle V \rangle \right) U_{k_1 n_1} U_{k_2 n_2} \\ &= 2 \left( \frac{\delta^2}{\delta \bar{\phi}_{k_1} \delta \bar{\phi}_{k_2}} \langle H \rangle \right) U_{k_1 n_1} U_{k_2 n_2} \end{aligned} \quad (3.125)$$

where we have used that the mean-field vacuum is a stationary point (s.p.) and thus  $\delta \langle H \rangle / \delta G = 0$ . This now suggests introducing new coordinates as well:

$$\mathbf{Q}_{m_1 i_1} = 2 U_{n_1 m_1} U_{j_1 i_1} Q_{n_1 j_1} \quad (3.126)$$

$$\mathbf{q}_{m_1} = \sqrt{2} U_{n_1 m_1} q_{n_1}. \quad (3.127)$$

3. One should note that the newly defined coordinates and momenta still fulfil the canonical commutation relations eq.(3.116); thus, the new definitions amount to a canonical transformation that leaves the dynamics unchanged.

We therefore end up with a Hamiltonian where the matrices in the quadratic forms are identical to those appearing in the Hamiltonian of the small-fluctuation approach

$$H = E' + \frac{1}{2} \begin{pmatrix} \mathbf{P} & \mathbf{P} \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ 0 & (G\mathbb{1}) \end{pmatrix} \begin{pmatrix} \mathbf{P} \\ \mathbf{P} \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \mathbf{q} & \mathbf{Q} \end{pmatrix} \begin{pmatrix} \frac{\delta^2 \mathcal{H}}{\delta \phi \delta \phi} & \frac{\delta^2 \mathcal{H}}{\delta \phi \delta G} \\ \frac{\delta^2 \mathcal{H}}{\delta G \delta \phi} & \frac{\delta^2 \mathcal{H}}{\delta G \delta G} \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{Q} \end{pmatrix}, \quad (3.128)$$

since  $\mathcal{H} = \langle H \rangle$  as defined in eqs. (3.8, 3.15). As a last point, we want to show that the eigenvalue equations that result from the Hamiltonian given in eq. (3.128) are identical to eqs. (3.27, 3.28). This is in fact quite simple; since the excitation operator  $Q_\nu^\dagger$  is a linear combination of  $\mathbf{B}, \mathbf{B}^\dagger, a, a^\dagger$  one can write it just as well as a linear combination of  $q, Q, p, P$  or  $\mathbf{q}, \mathbf{Q}, \mathbf{p}, \mathbf{P}$ . Thus, we may write

$$Q_\nu^\dagger = \sum_{mi} (\tilde{Q}_{mi}^\nu \mathbf{Q}_{mi} + \tilde{P}_{mi}^\nu \mathbf{P}_{mi}) + \sum_m (\tilde{q}_m^\nu \mathbf{q}_m + \tilde{p}_m^\nu \mathbf{p}_m). \quad (3.129)$$

We can now use the gRPA equations eq. (3.88) to derive the eigenvalue equations: we insert eq. (3.129) and eq. (3.128) into  $[H_B, Q_\nu^\dagger] = \Omega_\nu Q_\nu^\dagger$  and compare the coefficients of the various operators  $\mathbf{q}, \mathbf{p}, \mathbf{Q}, \mathbf{P}$ . The resulting equations are then easily expressed as

$$\begin{pmatrix} \frac{\delta^2 \mathcal{H}}{\delta \phi_m \delta \phi_{m_2}} & \frac{\delta^2 \mathcal{H}}{\delta \phi_m \delta G_{m_1 i_1}} (G\mathbb{1})_{m_1 i_1; m_2 i_2} \\ \frac{\delta^2 \mathcal{H}}{\delta G_{m_i} \delta \phi_{m_2}} & \frac{\delta^2 \mathcal{H}}{\delta G_{m_i} \delta G_{m_1 i_1}} (G\mathbb{1})_{m_1 i_1; m_2 i_2} \end{pmatrix} \begin{pmatrix} \tilde{q}_{m_2}^\nu \\ \frac{1}{2} \tilde{Q}_{\{m_2 i_2\}}^\nu \end{pmatrix} = \Omega_\nu^2 \begin{pmatrix} \tilde{q}_m^\nu \\ \frac{1}{2} \tilde{Q}_{\{mi\}}^\nu \end{pmatrix} \quad (3.130)$$

and

$$\begin{pmatrix} & \frac{\delta^2 \mathcal{H}}{\delta \phi_m \delta \phi_{m_2}} \\ (G\mathbb{1})_{mi; m_1 i_1} \frac{\delta^2 \mathcal{H}}{\delta G_{m_1 i_1} \delta \phi_{m_2}} & \frac{\delta^2 \mathcal{H}}{\delta \phi_m \delta G_{m_2 i_2}} \end{pmatrix} \begin{pmatrix} \tilde{p}_{m_2}^\nu \\ \frac{1}{2} \tilde{P}_{\{m_2 i_2\}}^\nu \end{pmatrix} = \Omega_\nu^2 \begin{pmatrix} \tilde{p}_m^\nu \\ \frac{1}{2} \tilde{P}_{\{mi\}}^\nu \end{pmatrix}. \quad (3.131)$$

These equations are now *identical* to eqs. (3.27, 3.28), only the components of the vectors have acquired *new names*:

$$\delta \bar{\phi} \rightarrow \tilde{p}_m^\nu ; \quad \delta G \rightarrow \frac{1}{2} \tilde{P}_{\{mi\}}^\nu \quad \text{and} \quad \delta \bar{\pi} \rightarrow \tilde{q}_m^\nu ; \quad \delta \Sigma \rightarrow \frac{1}{2} \tilde{Q}_{\{mi\}}^\nu. \quad (3.132)$$

Thus, we have proven that the two different approaches to the generalized RPA, namely the small-fluctuation approach from the time-dependent variational principle, and the operator approach, give in fact the same spectrum of possible excitations. Now the comments made at the end of sec. 3.2 carry over to the operator formulation of gRPA: if the stability matrix of the mean-field problem is positive, all 'eigenvalues'  $\Omega_\nu^2$  are larger than zero, and thus all  $\Omega_\nu$ s are real; if we are not at a minimum of the energy with our choice of the mean-field vacuum, the stability matrix will also have negative eigenvalues, and thus we will obtain complex conjugate pairs  $\pm i|\Omega_\nu|$ . As long as we have real 'eigenvalues'  $\Omega_\nu$  in the gRPA problem, the minimum under consideration will be stable at least w.r.t. small fluctuations. One should note that this relation was of some importance in footnote 33.

### 3.4 Conservation Laws in the Generalized Random Phase Approximation

In this section we want to demonstrate how conservation laws of the full theory are translated into the generalized RPA approximation of that theory. We only study conservation laws that are based on symmetries generated by one-body operators. The important point is that the commutator of the quasi-boson approximation of a general one-body operator with the quasi-boson approximation of the Hamiltonian is related to the mean-field expectation value of the commutator of the full operators.

In this section, we want to show how conservation laws (expressed as  $[H, \mathcal{O}] = 0$ ) translate into the gRPA formalism where the operators  $H, \mathcal{O}$  are replaced by their quasi-boson approximations.

For this purpose, we start by considering the commutator of the quasi-boson approximation  $\Gamma_B$  of a general one-body operator  $\Gamma$  with the Hamiltonian in quasi-boson approximation. It will be possible to relate this commutator to the commutator of the unapproximated operators as could also be done in nuclear physics<sup>42</sup> [MW69]. For a general one-body operator  $\Gamma$

$$\Gamma = \Gamma_0 + \Gamma_{n_1}^{10} a_{n_1}^\dagger + \Gamma_{n_1}^{01} a_{n_1} + \Gamma_{n_1 n_2}^{20} a_{n_1}^\dagger a_{n_2}^\dagger + \Gamma_{n_1 n_2}^{02} a_{n_1} a_{n_2} + \Gamma_{n_1 n_2}^{11} a_{n_1}^\dagger a_{n_2} \quad (3.133)$$

we write down the quasi-boson approximation  $\Gamma_B$

$$\Gamma_B = \Gamma_0 + \left( \Gamma_{n_1}^{10} a_{n_1}^\dagger + \Gamma_{n_1}^{01} a_{n_1} \right) + \sqrt{2} \left( \Gamma_{n_1 n_2}^{20} \mathbf{B}_{n_1 n_2}^\dagger + \Gamma_{n_1 n_2}^{02} \mathbf{B}_{n_1 n_2} \right), \quad (3.134)$$

and take the quasi-boson approximation for the Hamiltonian given in eq. (3.87). We obtain for the commutator

$$\begin{aligned} [H_B, \Gamma_B] = & -\frac{1}{\sqrt{2}} \mathbf{B}_{n_1 j_1} \left( C_{n_1 j_1 m_1} \Gamma_{m_1}^{10} + D_{n_1 j_1 m_1} \Gamma_{m_1}^{01} + A_{n_1 j_1 m_1 m_2} \Gamma_{m_1 m_2}^{20} + B_{n_1 j_1 m_1 m_2} \Gamma_{m_1 m_2}^{02} \right) \\ & + \frac{1}{\sqrt{2}} \mathbf{B}_{n_1 j_1}^\dagger \left( C_{n_1 j_1 m_1}^* \Gamma_{m_1}^{01} + D_{n_1 j_1 m_1}^* \Gamma_{m_1}^{10} + A_{n_1 j_1 m_1 m_2}^* \Gamma_{m_1 m_2}^{02} + B_{n_1 j_1 m_1 m_2}^* \Gamma_{m_1 m_2}^{20} \right) \\ & - a_{n_1} \left( E_{n_1 m_1} \Gamma_{m_1}^{10} + F_{n_1 m_1} \Gamma_{m_1}^{01} + \Gamma_{m_1 m_2}^{20} C_{m_1 m_2 n_1} + \Gamma_{m_1 m_2}^{02} D_{m_1 m_2 n_1}^* \right) \\ & + a_{n_1}^\dagger \left( E_{n_1 m_1}^* \Gamma_{m_1}^{01} + F_{n_1 m_1}^* \Gamma_{m_1}^{10} + \Gamma_{m_1 m_2}^{02} C_{m_1 m_2 n_1}^* + \Gamma_{m_1 m_2}^{20} D_{m_1 m_2 n_1} \right). \end{aligned} \quad (3.135)$$

By formulating the generalized RPA in terms of the quasi-boson approximation, we restrict ourselves to reference states that satisfy the Rayleigh-Ritz variational principle<sup>43</sup>. We now insert the definitions of the matrices  $A, \dots, F$  as expectation values of double commutators of the *exact* Hamiltonian with the creation/annihilation operators, and note that upon usage of the Jacobi identity

$$\langle [a_{m_1}^\dagger a_{m_2}^\dagger, [H, a_{n_1}^\dagger]] \rangle = \langle [a_{n_1}^\dagger, [H, a_{m_1}^\dagger a_{m_2}^\dagger]] \rangle, \quad (3.136)$$

$$\langle [a_{m_1} a_{m_2}, [H, a_{n_1}^\dagger]] \rangle = \langle [a_{n_1}^\dagger, [H, a_{m_1} a_{m_2}]] \rangle + \delta_{n_1 m_1} \langle [H, a_{m_2}] \rangle + \delta_{n_1 m_2} \langle [H, a_{m_1}] \rangle, \quad (3.137)$$

where again at the stationary point we can drop the last two terms. In order to see how one proceeds, take the first line of eq. (3.135)

$$\mathbf{B}_{n_1 j_1} \left( C_{n_1 j_1 m_1} \Gamma_{m_1}^{10} + D_{n_1 j_1 m_1} \Gamma_{m_1}^{01} + A_{n_1 j_1 m_1 m_2} \Gamma_{m_1 m_2}^{20} + B_{n_1 j_1 m_1 m_2} \Gamma_{m_1 m_2}^{02} \right). \quad (3.138)$$

It is now written as

$$\begin{aligned} & \mathbf{B}_{n_1 j_1} \left( \langle [a_{n_1}^\dagger a_{j_1}^\dagger, [H, a_{m_1}^\dagger]] \rangle \Gamma_{m_1}^{10} + \langle [a_{n_1}^\dagger a_{j_1}^\dagger, [H, a_{m_1}]] \rangle \Gamma_{m_1}^{01} + \langle [a_{n_1}^\dagger a_{j_1}^\dagger, [H, a_{m_1}^\dagger a_{m_2}^\dagger]] \rangle \Gamma_{m_1 m_2}^{20} \right. \\ & \quad \left. + \langle [a_{n_1}^\dagger a_{j_1}^\dagger, [H, a_{m_1} a_{m_2}]] \rangle \Gamma_{m_1 m_2}^{02} \right) \\ = & \mathbf{B}_{n_1 j_1} \langle [a_{n_1}^\dagger a_{j_1}^\dagger, [H, \Gamma_{m_1}^{10} a_{m_1}^\dagger + \Gamma_{m_1}^{01} a_{m_1} + \Gamma_{m_1 m_2}^{20} a_{m_1}^\dagger a_{m_2}^\dagger + \Gamma_{m_1 m_2}^{02} a_{m_1} a_{m_2}]] \rangle \\ = & \mathbf{B}_{n_1 j_1} \langle [a_{n_1}^\dagger a_{j_1}^\dagger, [H, \Gamma - \Gamma_0 - \Gamma_{m_1 m_2}^{11} a_{m_1}^\dagger a_{m_2}]] \rangle \\ = & \mathbf{B}_{n_1 j_1} \left( \langle [a_{n_1}^\dagger a_{j_1}^\dagger, [H, \Gamma]] \rangle - \Gamma_{m_1 m_2}^{11} \underbrace{\langle [a_{n_1}^\dagger a_{j_1}^\dagger, [H, a_{m_1}^\dagger a_{m_2}]] \rangle}_{(*)} \right). \end{aligned} \quad (3.139)$$

<sup>42</sup>Further interesting developments can also be found in [Mar77].

<sup>43</sup>For the equivalence of the second gRPA approximation and the quasi-boson approximation it is only necessary that  $\langle H \rangle$  be stationary w.r.t. variations of  $\bar{\pi}$  and  $\bar{\phi}$ . However, we need the stationarity condition w.r.t.  $G, \Sigma$  later on anyway, so we just assume here that our mean-field vacuum satisfies the Rayleigh-Ritz variational principle.

Now consider (\*):

$$\langle [a_{n_1}^\dagger a_{j_1}^\dagger, [H, a_{m_1}^\dagger a_{m_2}]] \rangle = - (H_{n_1 m_1}^{02} \delta_{j_1 m_2} + H_{j_1 m_1}^{02} \delta_{n_1 m_2} + H_{m_1 n_1}^{02} \delta_{j_1 m_2} + H_{m_1 j_1}^{02} \delta_{n_1 m_2}). \quad (3.140)$$

However, it can be seen by explicit computation that at the stationary point  $H^{02} = H^{20} = 0$ , since  $H^{20}$  can be written in terms of derivatives of  $\langle H \rangle$  w.r.t.  $G$  and  $\Sigma$ , cf. eq. (3.43). The other three lines in eq. (3.135) can be treated identically. A slight difference in the treatment will be necessary for the terms multiplying  $a_n, a_n^\dagger$  in eq. (3.135), since there the term additional to the desired commutator is not  $\langle [a_{n_1}^\dagger a_{j_1}^\dagger, [H, a_{m_1}^\dagger a_{m_2}]] \rangle$  but  $\langle [a_{n_1}^\dagger, [H, a_{m_1}^\dagger a_{m_2}]] \rangle$ . However, by a simple computation one sees that it is related to  $H^{10}$ , and will therefore also vanish at the stationary point. Thus, we can conclude

$$\begin{aligned} [H_B, \Gamma_B] &= -\frac{1}{\sqrt{2}} \langle [a_{n_1}^\dagger a_{j_1}^\dagger, [H, \Gamma]] \rangle \mathbf{B}_{n_1 j_1} + \frac{1}{\sqrt{2}} \langle [a_{n_1} a_{j_1}, [H, \Gamma]] \rangle \mathbf{B}_{n_1 j_1}^\dagger \\ &\quad - \langle [a_{n_1}^\dagger, [H, \Gamma]] \rangle a_{n_1} + \langle [a_{n_1}, [H, \Gamma]] \rangle a_{n_1}^\dagger \\ &\quad + \text{terms that vanish at the stationary point.} \end{aligned} \quad (3.141)$$

One should note that

- the treatment has been general in the sense that  $\Gamma$  is an arbitrary one-body operator. If in the full theory  $[H, \Gamma] = 0$ , this obviously implies at the stationary point  $[H_B, \Gamma_B] = 0$ , i.e. a conservation law in the full theory (where the symmetry is generated by a one-body operator) translates into a symmetry of the theory in *quasi-boson approximation*.
- the stationarity condition has been used several times; if we are not at the stationary point, some of the terms neglected above do not vanish, i.e.  $[H, \Gamma] = 0$  *does not imply*  $[H_B, \Gamma_B] = 0$  away from the stationary point.
- in sec. 3.3.6 we have given our construction principle for the quasi-boson approximation of a general one-body operator. One can give also a closed formula for this. If  $\mathcal{O}$  is a general one-body operator, its quasi-boson approximation reads

$$\mathcal{O}_B = \langle \mathcal{O} \rangle - \frac{1}{\sqrt{2}} \langle [a_i^\dagger a_j^\dagger, \mathcal{O}] \rangle \mathbf{B}_{ij} + \frac{1}{\sqrt{2}} \langle [a_i a_j, \mathcal{O}] \rangle \mathbf{B}_{ij}^\dagger - \langle [a_i^\dagger, \mathcal{O}] \rangle a_i + \langle [a_i, \mathcal{O}] \rangle a_i^\dagger. \quad (3.142)$$

Thus, if  $[H, \Gamma]$  is a one-body operator,  $[H_B, \Gamma_B]$  is the quasi-boson approximation of that operator<sup>44</sup> as can be seen by comparing eq. (3.141) to eq. (3.142).

- from eq. (3.142) it is clear that if both  $\mathcal{O}$  and  $\mathcal{O}^\dagger$  annihilate the mean-field vacuum, the quasi-boson approximation of  $\mathcal{O}$  will be *zero*! Thus, in order to have a non-trivial zero mode solution of the gRPA equations the mean-field vacuum has to be *deformed*.

We conclude that our main point of interest, namely the restoration of symmetries, is satisfied only if the reference state that we use to define the creation/annihilation operators is a stationary point of the time-independent variational principle.

Another word of caution is appropriate here. We have seen in this section that generators of symmetries of the Hamiltonian stay (upon quasi-boson approximation) generators of symmetries

<sup>44</sup>Apart from a possible constant part  $\langle [H, \Gamma] \rangle$ .



of the quasi-boson approximated Hamiltonian. Thus, *symmetries stay symmetries*, but the symmetries themselves may change. This can be seen by computing the commutator of two general quasi-boson approximated one-body operators. One can use eq. (3.142) to determine

$$[\mathcal{O}_B, \mathcal{P}_B] = \langle [\mathcal{O}, \mathcal{P}] \rangle. \quad (3.143)$$

In the case of Yang-Mills theories, we would obtain for the commutator of the Gauss law operators

$$[\Gamma_B^a, \Gamma_B^b] = \langle [\Gamma^a, \Gamma^b] \rangle = if^{abc} \langle \Gamma^c \rangle. \quad (3.144)$$

At the stationary point, however, we have<sup>45</sup>  $\bar{\mathbf{e}} = \Sigma = 0$  as was discussed in sec. 2.3.4, thus

$$[\Gamma_B^a, \Gamma_B^b] = 0. \quad (3.145)$$

In other words, the quasi-boson approximation has reduced the non-Abelian  $SU(N)$  symmetry to an Abelian  $U(1)^{N^2-1}$  symmetry. This is a phenomenon also well known from perturbation theory.

## 3.5 Moment of Inertia

In this section, we want to show how one can compute the contribution of the operators generating zero modes to the Hamiltonian in quasi-boson approximation. In order to be able to do this, we need a quantity called 'moment of inertia'. We will be able to give a rather explicit expression in the case of Yang-Mills theory in the perturbative limit.

### 3.5.1 General Discussion

From the discussion in sec. 3.3.9 we saw that we can in general write the Hamiltonian in quasi-boson approximation as

$$H_B = \sum_{\nu \in \nu_+} \Omega_\nu Q_\nu^\dagger Q_\nu + \sum_{\nu \in \nu_0} \frac{1}{2} P_\nu^2, \quad (3.146)$$

where  $\{\nu_+\}$  denotes the set of modes with positive  $\Omega_\nu$  and  $\{\nu_0\}$  denotes the set of zero modes. However, quite often an alternative expression to eq. (3.146) in terms of symmetry generators is useful. For this we have to recall that if our reference state is a solution of the Rayleigh-Ritz equations, and if the symmetry generators under consideration are one-body operators, then the quasi-boson approximations  $\Gamma_B^a$  of the symmetry generators commute with the quasi-boson approximation of the Hamiltonian. This implies that they are zero mode solutions of the gRPA equations. If we now assume that there are no 'accidental zero modes', i.e. the whole space of zero modes is spanned by the  $\Gamma_B^a$ s, then we can write the  $P_\nu$ s,  $\nu \in \{\nu_0\}$ , as linear combinations of the  $\Gamma_B^a$ s, and  $\sum_{\nu \in \{\nu_0\}} P_\nu^2$  becomes a quadratic form in terms of the  $\Gamma_B^a$ s. The advantage of this alternative expression is two-fold: first, in general the quasi-boson approximations of the symmetry operators are known. Second, the expression one obtains is (physically) more transparent, and can be more easily compared to other frameworks like e.g. the Kamlah expansion. The general dependence of  $H_B$  on the generators  $\Gamma_B^a$  will then be<sup>46</sup>

$$H_{B,zm} = \frac{1}{2} \Gamma_B^a (\mathcal{M}^{-1})^{ab} \Gamma_B^b, \quad (3.147)$$

<sup>45</sup>In Yang-Mills theory, we usually use  $\bar{\mathbf{e}}$  instead of  $\bar{\pi}$  to denote the expectation value of the canonical momentum.

<sup>46</sup> $H_{B,zm}$  means 'that part of the Hamiltonian in quasi-boson approximation that only contains the zero mode operators'.

where  $\mathcal{M}$  is the *moment-of-inertia* tensor, and Einstein's summation convention is also used for the indices  $a, b$  which are employed to label the different symmetry generators  $\Gamma_B^a$ . We cannot (as we have done in preceding discussions where masses were set to 1) 'normalize'  $\mathcal{M}$  'away', since the normalization of  $\Gamma_B^a$  is fixed by its very nature of a known operator<sup>47</sup>. Thus, in this section, we will see how one can actually compute the moment-of-inertia tensor, cf. [RS80]. We have seen in sec. 3.3.9 that in cases of appearances of zero modes one has to pass to a description of the oscillators in terms of canonical coordinates<sup>48</sup> and momenta (which we have done above). This actually allows to determine the moment-of-inertia tensor. We assume that we can construct a set of coordinates  $\Theta_B^a$ , s.t.

$$[\Theta_B^a, \Gamma_B^b] = i\delta^{ab}, \quad (3.148)$$

and which commute with all other normal modes. Since we already know the form of the part of  $H_B$  that is not supposed to commute with  $\Theta_B$ , we also require<sup>49</sup>

$$[\Theta_B^a, H_B] = i\mathcal{M}^{ab}\Gamma_B^b. \quad (3.149)$$

As a matter of fact, the usage of the equations is opposite to their motivation. This has its reason in the number of equations that are actually provided: we start by making an *ansatz* of  $\Theta_B^a$  as a generalized one-body operator in quasi-boson approximation<sup>50</sup>:

$$\Theta_B^a = \Theta_{Q;mi}^a Q_{mi} + \Theta_{P;mi}^a P_{mi} + \Theta_{q;m}^a q_m + \Theta_{p;m}^a p_m \quad (3.150)$$

whereas in general  $\Gamma_B$  reads

$$\Gamma_B^a = \Gamma_{Q;mi}^a Q_{mi} + \Gamma_{P;mi}^a P_{mi} + \Gamma_{q;m}^a q_m + \Gamma_{p;m}^a p_m. \quad (3.151)$$

In the latter case the coefficients are obviously known. We now insert eqs. (3.150, 3.151) into eq. (3.149), and compare coefficients. This gives in general four equations, and allows to determine  $\Theta_{Q;mi}^a, \Theta_{P;mi}^a, \Theta_{q;m}^a, \Theta_{p;m}^a$  in terms of  $\mathcal{M}^{-1}$  and the coefficients of  $\Gamma_B$ . If we now insert the thus determined coefficients of  $\Theta_B$  into the one equation that results from eq. (3.148) we obtain an equation of the type

$$(\mathcal{M}^{-1})^{ac}\mathcal{N}^{cb} = i\delta^{ab}, \quad (3.152)$$

where  $\mathcal{N}$  is a matrix given entirely in terms of the matrices  $A, \dots, F$  and the coefficients of  $\Gamma_B$ . Thus, one has to invert the matrix  $\mathcal{N}$  in order to obtain the correct kinetic term for the zero modes. One should note that the logic is just the other way around from what one would expect, namely that  $\Theta_B$  is defined via its commutator with  $\Gamma_B$ . However, for a proper definition of  $\Theta_B$  we also need the fact that it commutes with all the other normal modes. These general considerations find their application to the specific case of Yang-Mills theory in the next section.

<sup>47</sup>If the original symmetry generators (before the quasi-boson approximation) were generators of a non-Abelian symmetry, their normalization is fixed by the commutation relations.

<sup>48</sup>Let us once again mention that the reduction of the non-Abelian to an Abelian symmetry (in the Yang-Mills case) in the quasi-boson approximation seems to be essential since otherwise one cannot construct canonically conjugate 'angle' operators fulfilling the canonical commutation relations [TI98].

<sup>49</sup>We assume here that the moment of inertia tensor is symmetric, which is at least true for the case of Yang-Mills theories, since there  $[\Gamma_B^a, \Gamma_B^b] = 0$ .

<sup>50</sup>The usage of the p-q formulation as in section 3.3.10 will be useful in this context.

### 3.5.2 Yang-Mills Theory

We have repeatedly emphasized that the quasi-boson formulation works properly only if the reference state fulfils the mean-field equations (the parameters are such that 'the energy functional is at its stationary point'). In Yang-Mills theory without a cranking term this leads automatically to<sup>51</sup>

$$\bar{\mathbf{e}} = 0 \quad \text{and} \quad \Sigma = 0. \quad (3.153)$$

This simplifies the expression for the Gauss law operator considerably, since, when we insert these results into the expression given in Appendix C.4.2, we obtain<sup>52</sup>

$$\Gamma_B^a = \Gamma_{P,mi}^a P_{mi} + \Gamma_{p,m}^a p_m = (\Gamma_P^a(\mathbf{x}))_{ij}^{bc}(\mathbf{x}_1, \mathbf{x}_2) P_{ij}^{bc}(\mathbf{x}_1, \mathbf{x}_2) + (\Gamma_p^a(\mathbf{x}))_i^b(\mathbf{x}_1) p_i^b(\mathbf{x}_1) \quad (3.154)$$

with

$$(\Gamma_P^a(\mathbf{x}))_{n_1 n_2}^{b_1 b_2}(\mathbf{z}_1, \mathbf{z}_2) = \frac{1}{2} \left( \frac{\delta}{\delta \Sigma_{\mathbf{x}_1 \mathbf{x}_2}^{a_1 a_2, l_1 l_2}} \langle \hat{\mathbf{D}}_{\mathbf{x}, i}^{ab} \hat{\mathbf{\Pi}}_{i\mathbf{x}}^b \rangle \right) (U^{-1})_{\mathbf{x}_1 \mathbf{z}_1}^{a_1 b_1, l_1 n_1} (U^{-1})_{\mathbf{x}_2 \mathbf{z}_2}^{a_2 b_2, l_2 n_2} \quad (3.155)$$

$$(\Gamma_p^a(\mathbf{x}))_{n_1}^{b_1}(\mathbf{z}_1) = \frac{1}{\sqrt{2}} \left( \frac{\delta}{\delta \mathbf{e}_{l_1 \mathbf{y}_1}^{a_1}} \langle \hat{\mathbf{D}}_{\mathbf{x}, i}^{ab} \hat{\mathbf{\Pi}}_{i\mathbf{x}}^b \rangle \right) (U^{-1})_{\mathbf{y}_1 \mathbf{z}_1}^{a_1 b_1, l_1 n_1}, \quad (3.156)$$

where we don't integrate over  $\mathbf{x}$ . Further remarks on notation can be found in footnote 52. One should note that all double indices are summed over *except for*  $\mathbf{x}$ ! Inserting eq. (3.150) into eq. (3.149), with the Hamiltonian given in eq. (3.117), we obtain (apart from  $\Theta_P = \Theta_p = 0$ )

$$\begin{aligned} \Theta_{q,m}^a F_{mi} &= (\mathcal{M}^{-1})^{ab} \Gamma_{p,i}^b, \\ \Theta_{Q,mi}^a B_{minj}^{11} &= (\mathcal{M}^{-1})^{ab} \Gamma_{P,nj}^b, \end{aligned} \quad (3.157)$$

where we have used the properties of the stationary point, i.e. the matrices  $A, \dots, F$  are all real, etc. (cf. sec. 3.3.10). We invert the second line in a way that will be discussed below in some detail. Let us only mention at this point that  $(B^{11})^{-1}$  is defined by

$$((B^{11})^{-1})_{i_1 m_1 j_1 n_1} (B^{11})_{j_1 n_1 i_2 m_2} = \frac{1}{2} (\delta_{i_1 i_2} \delta_{m_1 m_2} + \delta_{i_1 m_2} \delta_{m_1 i_2}). \quad (3.158)$$

We insert the result into the normalization eq. (3.148) and obtain

$$\boxed{(\mathcal{M}^{-1})^{ac} \left( \Gamma_{p,m}^c (F^{-1})_{mi} \Gamma_{p,i}^b + 2 \Gamma_{P,mi}^c ((B^{11})^{-1})_{minj} \Gamma_{P,nj}^b \right) = \delta^{ab}}, \quad (3.159)$$

which bears some resemblance to the expression obtained in nuclear physics [RS80], especially if one notes that  $(B^{11})_{minj} \propto (A + B)_{minj}$  and  $F_{ij} \propto (E + F)_{ij}$  at the stationary point. Unfortunately, we cannot read off an explicit expression for  $(\mathcal{M}^{-1})^{ab}$  from this in general. However,

<sup>51</sup>We use the standard Yang-Mills notation for parameters of the wave functional etc. as they are also used in Appendix C. At some places there will therefore be deviations from the 'generic field' notation of the rest of this chapter.

<sup>52</sup>In this section we have to give up the super-index notation used until now in some places; instead of one super-index, the operators  $p$  will carry three (colour, spatial, and position index), i.e.  $p_m \rightarrow p_i^b(\mathbf{x})$  where  $b$  is the colour,  $i$  the spatial, and  $\mathbf{x}$  the position index, and correspondingly for  $P_{mi}$ . In this context, also the index  $a$  carried by  $\Gamma_B^a$  has to be re-examined; in fact it is also a super-index, consisting of a colour index  $a$ , and a position index  $\mathbf{x}$ :  $\Gamma_B^a \rightarrow \Gamma_B^a(\mathbf{x})$ ; the same applies to the super-indices that are carried by the moment-of-inertia tensor:  $\mathcal{M}^{ab} \rightarrow \mathcal{M}^{ab}(\mathbf{x}, \mathbf{y})$ . Having clarified this, in the more formal parts of this section, we will still stick to the super-index notation, since otherwise the formulas will become unreadable.

we can go back to perturbation theory to make an evaluation. We note<sup>53</sup> that  $\Gamma_P^a$  is, in the perturbative scaling scheme given in appendix A.5, of higher order in  $g$  than<sup>54</sup>  $\Gamma_P^a$ . Thus, we just compute the leading order piece of the moment of inertia:

$$(\mathcal{M}^{-1})^{ac}(\mathbf{x}, \mathbf{y}) \left( (\Gamma_P^c(\mathbf{y}))_{n_1}^{b_1}(\mathbf{z}_1) (F^{-1})_{n_1 n_2}^{b_1 b_2}(\mathbf{z}_1, \mathbf{z}_2) (\Gamma_P^b(\mathbf{z}))_{n_2}^{b_2}(\mathbf{z}_2) \right) = -(\hat{\mathbf{D}}\hat{\mathbf{D}})^{bc}(\mathbf{z})(\mathcal{M}^{-1})^{ca}(\mathbf{z}, \mathbf{x}) \stackrel{!}{=} \delta^{ba} \delta_{\mathbf{xz}}. \quad (3.160)$$

From this we conclude that the leading order piece of the moment of inertia in a perturbative expansion is just the Green's function of the covariant Laplacian in the background field  $\bar{\mathbf{A}}$ :

$$\boxed{(\mathcal{M}^{-1})_{\mathbf{xy}}^{ab} = -G_{\Delta}^{ab}(\mathbf{x}, \mathbf{y}) + \mathcal{O}(g^2)} \quad (3.161)$$

with

$$\hat{\mathbf{D}}_{\mathbf{x},l}^{ad} \hat{\mathbf{D}}_{\mathbf{x},l}^{db} G_{\Delta}^{bc}(\mathbf{x}, \mathbf{y}) = \delta^{ac} \delta_{\mathbf{xy}}. \quad (3.162)$$

Obviously, in the case of a vanishing background field, we obtain Coulomb's law:

$$(\mathcal{M}^{-1})_{\mathbf{xy}}^{ab} = \frac{\delta^{ab}}{4\pi |\mathbf{x} - \mathbf{y}|}. \quad (3.163)$$

We have now to discuss one point that was passed over before, namely the existence of  $(B^{11})^{-1}$  in the sense defined in eq. (3.158). One can combine the indices  $m, i$  and  $n, j$  into a super-index each, and calculate the determinant of  $B^{11}$ ; it turns out to be zero. This is, however, only a problem at first sight, since it turns out that with the same prescription for the indices the RHS of eq. (3.158) has also a zero determinant. In the following, we call the RHS of eq. (3.158)  $W_{i_1 i_2 m_1 m_2}$ . Writing suggestively

$$\begin{aligned} B_{i_1 i_2 m_1 m_2}^{11} &= F_{i_1 m_1} \delta_{i_2 m_2} + F_{i_1 m_2} \delta_{i_2 m_1} + F_{i_2 m_1} \delta_{i_1 m_2} + F_{i_2 m_2} \delta_{i_1 m_1} \\ W_{i_1 i_2 m_1 m_2} &= \frac{1}{4} \delta_{i_1 m_1} \delta_{i_2 m_2} + \frac{1}{4} \delta_{i_1 m_2} \delta_{i_2 m_1} + \frac{1}{4} \delta_{i_2 m_1} \delta_{i_1 m_2} + \frac{1}{4} \delta_{i_2 m_2} \delta_{i_1 m_1}, \end{aligned} \quad (3.164)$$

we see that  $W$  has the same structure as  $B^{11}$ , in fact it is just a special case with  $F_{ij} = \frac{1}{4} \delta_{ij}$ . This motivates the idea that both  $B^{11}$  and  $W$  could have the same kernel. Since we know that  $F$  is symmetric, and has positive definite eigenvalues<sup>55</sup>,  $F$  itself has an empty kernel; the kernel will consist of objects carrying two indices (not yet combined into one super-index). These objects come in two types

$$L^{ab} = -L^{ba} \text{ (antisymmetric)} \quad L^{ab} = L^{ba} \text{ (symmetric)}. \quad (3.165)$$

The first span the kernel of both  $W$

$$W_{i_1 i_2 m_1 m_2} L^{m_1 m_2} = L^{i_1 i_2} + L^{i_2 i_1} = 0 \quad (3.166)$$

and  $B^{11}$ :

$$B_{i_1 i_2 m_1 m_2}^{11} L^{m_1 m_2} = F_{i_1 m} (L^{m i_2} + L^{i_2 m}) + F_{i_2 m} (L^{m i_1} + L^{i_1 m}) = 0. \quad (3.167)$$

We see also that for symmetric  $L$  no new zeros are produced: the entire kernel is spanned by objects antisymmetric in the two indices, and therefore one can give an inverse of  $B^{11}$  in the subspace of symmetric objects<sup>56</sup>. One can define a basis for this subspace, and obtain a new  $B^{11}$

<sup>53</sup>This can be read off the expressions eqs. (3.155, 3.156) together with mean-field expectation value of  $\Gamma^a(\mathbf{x})$  given in eq. (2.123).

<sup>54</sup>For the purpose of counting powers of  $g$ , we take  $\bar{\mathbf{A}}$  to be of  $\mathcal{O}(g^{-1})$ , s.t.  $\hat{\mathbf{D}}$  is completely of  $\mathcal{O}(g^0)$ .

<sup>55</sup>This is so, since  $F$  is directly connected to the kernel  $G^{-1}$  in the Gaussian wave functional, cf. eq. (3.78).

<sup>56</sup>In this context one should note that both  $\Theta_{Q,mi}^a$  and  $\Gamma_{P,mi}^a$  are symmetric, thus considering the subspace of symmetric objects is sufficient.

defined solely in this subspace, but we refrain from commenting on the procedure further since we would need it only if we wanted to calculate  $\mathcal{M}^{-1}$  to higher order in  $g$ .

### 3.5.3 Energy Contributions of the Zero Modes

We have discussed in some detail that zero modes cannot be treated via the ordinary creation/annihilation operator formalism; they have to be treated with the help of canonical coordinates and momenta. This changes their contribution to the gRPA vacuum energy. The gRPA energy in eq. (3.101) was fixed s.t.

$$\langle H_B \rangle = E_{MF}. \quad (3.168)$$

Since now  $H_B$  no longer only contains oscillator modes but looks like

$$H_B = E_{\text{RPA}} + \frac{1}{2} \Gamma_B^a (\mathcal{M}^{-1})^{ab} \Gamma_B^b + \sum_{\nu \in \{\nu_+\}} \Omega_\nu Q_\nu^\dagger Q_\nu, \quad (3.169)$$

where  $\{\nu_+\}$  denotes the set of modes with positive  $\Omega_\nu$ , eq. (3.104) becomes in this context

$$E_{\text{RPA}} = E_{\text{MF}} - \frac{1}{2} \langle \Gamma_B^a (\mathcal{M}^{-1})^{ab} \Gamma_B^b \rangle - \sum_{\nu \in \{\nu_+\}} \Omega_\nu \left( \frac{1}{2} \sum_{mi} |Y_{\{mi\}}^\nu|^2 + \sum_i |Z_i^\nu|^2 \right), \quad (3.170)$$

which is again similar to the result obtained in nuclear physics [RS80]. We obtain an energy correction to the mean-field energy due to the zero modes that is very similar in structure to what we obtained in the second order Kamlah expansion<sup>57,58</sup>, cf. eq. (2.303), but also with an important difference: the energy contribution which is due to the zero modes (and thus ultimately due to the deformation) is subtracted off *after variation* of the mean-field vacuum wave functional, and not before, as in the case of the Kamlah expansion<sup>59</sup>; therefore, the determination of the parameters of the mean-field vacuum is not influenced by the correction.

*'Have you anything positive to tell him?' - 'I think so.'* - *'You have formed a conclusion?' - 'Yes, my dear Watson, I have solved the mystery.'*

Sherlock Holmes, The Three Students

## 3.6 Summary and Conclusion

Let us shortly summarize what has been achieved in this chapter, and which problems remain to be solved. We started by considering the formulation of the Random Phase Approximation that has been the usual one to date in field theory, namely the one which is derived from the time-dependent variational principle. We then turned to the operator formulation that is common in nuclear physics. We demonstrated that this approach can also be implemented in a bosonic field

<sup>57</sup>If we integrate partially twice in eq. (2.303), we see that the energy correction in the second-order Kamlah expansion (to the order in  $g$  considered) is given as  $-\frac{1}{2} \int d^3x_1 d^3x_2 (-G_\Delta^{ba}(\mathbf{x}_2, \mathbf{x}_1)) \langle \Gamma^a(\mathbf{x}_1) \Gamma^b(\mathbf{x}_2) \rangle$ .

<sup>58</sup>It is also very similar in structure to the so-called 'Thouless-Valatin term' proposed in [HMVI98], [HIMV00].

<sup>59</sup>Also in the Thouless-Valatin method, the Thouless-Valatin term is subtracted before variation [HMVI98], [HIMV00].

theory, but that the class of excitation operators to be considered has to be larger than in nuclear physics; namely, one has to also allow for terms linear in creation/annihilation operators of the fundamental boson fields. It turned out to be possible (at least for a certain class of Hamiltonians with standard kinetic term) to prove the equivalence of the operator formulation to the formulation starting from the time-dependent variational principle. Then we demonstrated that, in the absence of zero modes, the gRPA Hamiltonian is just a collection of harmonic oscillators. The zero modes required special attention, but the problems could be solved along lines paralleling nuclear physics. We then considered the question of how conservation laws of the full theory translate into conservation laws of the theory in generalized Random Phase Approximation, and saw that, at least in the case of symmetries generated by one-body operators, existence of symmetries in the full theory implies existence of symmetries in the gRPA-approximated theory, although these symmetries need not be the same; in Yang-Mills theory, the generalized RPA only carries an Abelian symmetry. As a last point we investigated the difference between the mean-field energy and the energy of the gRPA ground state with special emphasis on the energy contribution of the zero modes. For this purpose we had to calculate the moment-of-inertia tensor which (at least to lowest order in perturbation theory) turned out to be the Green's function of the covariant Laplacian in the background field at the stationary point.

To put the method into perspective, let us summarize the main positive and negative aspects: on the positive side, we first have to mention that in the generalized RPA only energy differences w.r.t. the ground state are computed. This simplifies matters, since that part of renormalization that is usually done by normal-ordering is automatically taken care of. This brings us directly to the second point: energies of excited states can be computed. This is usually very difficult if one relies upon e.g. the Rayleigh-Ritz principle. The most important point, however, is the effective implementation of the Gauss law constraint. Even though the gauge symmetry is broken in the mean-field treatment, the unphysical excitations generated by the (gRPA approximated) Gauss law operator (in the sense of footnote 17) are orthogonal to all the other physical excited states, which is almost as good as if they didn't even exist. But there are also a number of drawbacks of the method presented. The first has to do with the ground state energy: Whereas one does obtain a lowering of the ground state energy w.r.t. the mean-field energy due to deformation, in a manner which is even formally quite similar to the lowering obtained in the second order Kamlah expansion (at least to the order in perturbation theory considered), the point of the calculation at which the energy correction due to the deformation is considered is fundamentally different. In the Kamlah expansion, the corrections are subtracted *before* the variation is carried out, whereas in the generalized RPA they are subtracted only *after* the variation. Therefore the energy correction does not have any influence on the parameters of the mean-field. This brings us directly to the next problematic point: of course the mean-field vacuum is not the gRPA ground state. In nuclear physics, one was able, however, to construct the gRPA ground state from the mean-field ground state; but, in the presence of zero modes, this state has a divergent norm. This is due to the fact that the gRPA is a 'small angle' approximation [MW69], or in other words, the compact nature of the non-Abelian symmetry is lost. We have seen explicitly that in the case of Yang-Mills theory, the compact  $SU(N)$  symmetry is replaced by the non-compact  $U(1)^{N^2-1}$  symmetry. In nuclear physics, at least in the case of two-dimensional rotations, the fact that RPA is only a small-angle approximation was not so much of a problem, since the global dependence on the angle is generally known and therefore one can extract enough information from the small-angle approximation to determine the whole wave function [MW69]. In Yang-Mills theory, we have no comparable knowledge that could be put to use practically and therefore, we cannot compute the ground-state wave functional. Lacking this knowledge, however, one needs

other methods to evaluate matrix elements of operators, which up to now we haven't developed. Therefore, the only quantities we currently can calculate are the energies of the excited states. As a last point, we have to mention that just like in the mean-field calculations of Chapter 2, we have not dealt with the problems of renormalization. However, it should be possible to deal with them, since (at least in the case of  $\phi^4$  theory) this problem has been faced already by Kerman *et al* [KL95], [KL98] in the context of the generalized RPA derived from the time-dependent variational principle.

## Chapter 4

# Conclusions

*"The division seems rather unfair," I remarked. "You have done all the work in this business. I get a wife out of it, Jones gets the credit, pray what remains for you?" "For me," said Sherlock Holmes, "there still remains the cocaine-bottle." And he stretched his long white hand up for it.*

Sherlock Holmes, The Sign of the Four

In this thesis, we have studied Yang-Mills theory in the Weyl gauge employing the Schrödinger picture. The motivation for this investigation was drawn from the fact that the formulation in the Schrödinger picture had previously allowed for a successful treatment of topological and kinematic questions, but only to a lesser extent dynamical calculations, at least in Yang-Mills theories. We took from quantum mechanics the variational principles due to Dirac and to Rayleigh and Ritz that have proved to be successful in many-body theory, especially in nuclear physics. We then considered the problem of gauge invariance of the wave functionals, which is a necessary property if one wants to have the same equations of motion in the Hamiltonian framework as in the Lagrangian formalism. First, we considered a variety of methods that have been proposed in the literature starting from construction of gauge invariant variables, over gauge fixing all the way to models inspired by nuclear physics, where one deals with the system in a colour-rotating, intrinsic frame.

However, there exist still further techniques inspired by nuclear physics, to which we then turned. A common problem in nuclear physics is that the simple wave functions one wants to use for calculations cannot contain interesting correlations, if they have to respect all the symmetries of the Hamiltonian. Therefore, one starts with a simple wave function and projects it onto a state that carries good quantum numbers. We follow the same approach, only our motivation is a bit different: we are not able to write down a non-trivial wave function at all that is gauge invariant to begin with. Therefore, we take as trial state a state that is close to the Slater determinant in nuclear physics, since it shares its most important property - the factorizability of all expectation values of arbitrary  $\mathbf{A}$ -dependent operators (they have to be expandable in a power series in  $\mathbf{A}$ , though) into expectation values of one or two  $\mathbf{A}$  operators. This is the class of Gaussian states. Then we project it, and deal with the projection in an approximate fashion. Unfortunately, the evaluation of these approximations, be it within the cranking approach or the Kamlah expansion, was limited to a combination with perturbation theory, and restricted to low orders. In addition, at least the Kamlah expansion makes - for the purpose of explicit computations - quite heavy



use of the factorization properties. However, since the usage of Gaussian states has tied us to the Hartree-Fock approximation (which in a certain sense is a two-loop approximation) anyway, it is indeed questionable whether we ever have to go to higher order than  $g^2$  in the evaluation of the Kamlah expansion, since the energy isn't more accurate anyway. We ended Chapter 2 with an evaluation of the Savvidy vacuum which reproduced the well-known results.

The third chapter was devoted to the generalized Random Phase Approximation which is also known from nuclear physics. Here we have a different example of how Gauss' law may be realized in an approximation scheme: if the mean-field ground state is not annihilated by the Gauss law operator, the excitations associated with the Gauss law operator are orthogonal to all physical excitations, and thus effectively decouple from the physical part of the Hilbert space. We were also able to prove the equivalence of the operator approach used here for the generalized Random Phase Approximation to the formulation found in the literature which is based on the time-dependent variational principle for a certain class of Hamiltonians. The approach presented here has the advantage that conservation laws can (under certain conditions) be transcribed from the full theory to the theory in generalized RPA treatment, and the fact that one can see explicitly the connection between the generators of symmetries and excitation operators that are zero mode solutions of the gRPA equations.

In this entire thesis, we have refrained from discussing renormalization. This nevertheless is an important point, since many of the expressions presented here are only formal, as they contain products of operators at the same point in space-time. Before this point is clarified, detailed calculations of e.g. the glueball spectrum, which could be carried out in the generalized Random Phase Approximation, remain ambiguous. However, the fact that the renormalization of  $\phi^4$  theory was carried out successfully by Kerman *et al* within the generalized Random Phase Approximation (albeit starting from the time-dependent variational principle) gives rise to the hope that this can also be done in Yang-Mills theory.

# Appendix A

## Units and Conventions

*Those are the facts of the case, Doctor, and if they are of any use to your collection, I am sure that they are very heartily at your service.*

Sherlock Holmes, The “Gloria Scott”

### A.1 Units

Throughout this thesis we work in *natural units*

$$\hbar = c = 1. \tag{A.1}$$

In these units, time and length have dimension of inverse energies. Especially, we have

$$1 \text{ fm} = 10^{-15} \text{ m} = (197.327 \text{ MeV})^{-1}. \tag{A.2}$$

### A.2 Indices and Summation Conventions

In this thesis, four different kinds of indices appear: colour indices, spatial indices, position indices and super-indices, combining several of the former three kinds as will be explicitly stated wherever they are introduced. To each kind of index a certain range of letters is attached: colour indices:  $a, b, c, \dots$ , spatial indices:  $i, j, k, \dots$ , position indices:  $\mathbf{x}, \mathbf{y} \dots$ , super-indices:  $i, j, k, \dots$ . Unless explicitly stated, Einstein’s summation convention will be used throughout. Discrete indices will be summed over, continuous indices will be integrated over. We will also use a uniform notation for  $\delta$  functions, regardless of the nature of indices (discrete or continuous); thus,  $\delta_{\mathbf{x}\mathbf{y}}$  in this thesis corresponds to  $\delta^{(3)}(\mathbf{x} - \mathbf{y})$  in the usual notation for Dirac’s  $\delta$ , whereas e.g.  $\delta^{ab}$  is simply Kronecker’s  $\delta$ .

On some occasions it is useful to indicate only those indices explicitly that shall not be summed (integrated) over by Einstein’s summation convention, e.g. we use  $\text{tr}(\Sigma G \Sigma)_{\mathbf{x}\mathbf{x}}$  as an abbreviation of  $(\sum_{\mathbf{x}\mathbf{x}_1}^{ab_1, ik_1} G_{\mathbf{x}_1 \mathbf{x}_2}^{b_1 b_2, k_1 k_2} \sum_{\mathbf{x}_2 \mathbf{x}}^{b_2 a, k_2 i})$  where all double indices are summed or integrated over (as appropriate) *except for*  $\mathbf{x}$ .

### A.3 Minkowski Space

We use as metric for the Minkowski space

$$g_{\mu\nu} = \text{diag}(1, -1, -1, -1), \tag{A.3}$$

and thus have as four-vectors  $a^\mu$  and  $a_\mu = g_{\mu\nu}a^\nu$

$$a^\mu = (a_0, \mathbf{a}) \ , \ a_\mu = (a_0, -\mathbf{a}) \tag{A.4}$$

with the scalar product

$$a \cdot b = a_\mu b^\mu = a_0 b_0 - \mathbf{a} \cdot \mathbf{b}. \tag{A.5}$$

Only for the four-derivative, signs are distributed differently:

$$\partial^\mu = (\partial_0, -\nabla) \ , \ \partial_\mu = (\partial_0, \nabla) \tag{A.6}$$

with  $\nabla_i = \frac{\partial}{\partial x_i}$ . Sometimes we need a gradient w.r.t. another variable. This we denote by attaching the variable name to  $\nabla$ , e.g.  $\nabla_i^y = \frac{\partial}{\partial y_i}$ .

## A.4 Group Theory Conventions

We will be very brief here, since we only need very few conventions. We will concentrate on SU(N) groups. Group elements  $U$  of SU(N) can be written as

$$U = e^{i\lambda^a \Theta^a}, \tag{A.7}$$

where  $\Theta^a$  are the parameters of the group element, and  $\lambda$  denote the generators, defined in the Lie algebra. The representation of the algebra has to be chosen according to which representation the  $U$ s are to be considered in (fundamental, adjoint, etc), and they satisfy the commutation relations

$$[\lambda^a, \lambda^b] = i f^{abc} \lambda^c. \tag{A.8}$$

We therefore take the generators to be hermitian. The generators in the fundamental representation(s) are normalized to (1/2):

$$\text{tr} \left( \lambda_{fund}^a \lambda_{fund}^b \right) = \frac{1}{2} \delta^{ab} \tag{A.9}$$

and we have used a special notation for the generators of the adjoint representation *times minus i*:

$$(\hat{T}^a)^{bc} = f^{bac}. \tag{A.10}$$

The structure constants satisfy the *Jacobi identity*

$$f_{abr} f_{cdr} + f_{acr} f_{dbr} + f_{adr} f_{bcr} = 0 \tag{A.11}$$

and are normalized as

$$f_{abc} f_{dbc} = -\text{tr}(\hat{T}^a \hat{T}^d) = N \delta^{ad}. \tag{A.12}$$

Further useful formulas can be found in [Ten00].

## A.5 Factors of $g$

In Yang-Mills theory one has basically two options concerning where one wants to put the coupling constant, either in front of the action<sup>1</sup>, or in front of the commutator term in the field strength<sup>2</sup>. In this appendix we give a short list concerning which convention leads to which placing of factors of  $g$  in other quantities of interest:

	non-perturbative scaling	perturbative scaling
covariant derivative	$D_\mu = \partial_\mu - iA_\mu$	$D_\mu = \partial_\mu - igA_\mu$
field strength	$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu - i[A_\mu, A_\nu]$ $= i[D_\mu, D_\nu]$	$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu - ig[A_\mu, A_\nu]$ $= \frac{i}{g}[D_\mu, D_\nu]$
action	$S = -\frac{1}{4g^2} \int d^4x F_{\mu\nu}^a(x) F^{a\mu\nu}(x)$	$S = -\frac{1}{4} \int d^4x F_{\mu\nu}^a(x) F^{a\mu\nu}(x)$
electrical field	$\mathbf{E}_i^a = F_{0i}^a$	$\mathbf{E}_i^a = F_{0i}^a$
magnetic field	$\mathbf{B}_i^a = -\frac{1}{2}\epsilon_{ijk}F^{ajk}$ $= (\nabla \times \mathbf{A})_i^a - \frac{1}{2}f^{abc}(\mathbf{A}^b \times \mathbf{A}^c)_i$	$\mathbf{B}_i^a = -\frac{1}{2}\epsilon_{ijk}F^{ajk}$ $= (\nabla \times \mathbf{A})_i^a - \frac{g}{2}f^{abc}(\mathbf{A}^b \times \mathbf{A}^c)_i$
momenta $\Pi_i^a = \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{A}}_i^a}$	$\Pi_i^a = \frac{1}{g^2}F_{i0}^a = -\frac{1}{g^2}\mathbf{E}_i^a$	$\Pi_i^a = F_{i0}^a = -\mathbf{E}_i^a$
Hamiltonian	$H = \frac{g^2}{2}\Pi_i^a\Pi_i^a + \frac{1}{2g^2}\mathbf{B}_i^a\mathbf{B}_i^a$ $= \frac{1}{2g^2}(\mathbf{E}_i^a\mathbf{E}_i^a + \mathbf{B}_i^a\mathbf{B}_i^a)$	$H = \frac{1}{2}\Pi_i^a\Pi_i^a + \frac{1}{2}\mathbf{B}_i^a\mathbf{B}_i^a$ $= \frac{1}{2}(\mathbf{E}_i^a\mathbf{E}_i^a + \mathbf{B}_i^a\mathbf{B}_i^a)$
wave functional of 'free' theory	$\psi[\mathbf{A}] \sim e^{-\frac{1}{g^2}\mathbf{A}G^{-1}\mathbf{A}}$	$\psi[\mathbf{A}] \sim e^{-\mathbf{A}G^{-1}\mathbf{A}}$
gauge transformations	$U = e^{i\phi^a\lambda^a}$	$U = e^{ig\phi^a\lambda^a}$
generators	$[(-\Gamma_{\mathbf{x}}^a), (-\Gamma_{\mathbf{y}}^b)] = i\delta_{\mathbf{x}\mathbf{y}}f^{abc}(-\Gamma_{\mathbf{x}}^c)$	$[\frac{1}{g}(-\Gamma_{\mathbf{x}}^a), \frac{1}{g}(-\Gamma_{\mathbf{y}}^b)] = \frac{g}{g}\delta_{\mathbf{x}\mathbf{y}}f^{abc}\frac{1}{g}(-\Gamma_{\mathbf{x}}^c)$
finite gauge trafos	$\mathcal{G} = e^{i\int \phi^a\Gamma^a}$	$\mathcal{G} = e^{i\int g\phi^a\frac{1}{g}\Gamma^a}$

## A.6 Generalized Projectors

In this appendix we want to give some notions on the generalized projectors as they are used in sec. 2.6. First let us note that the projection operators are thought of as bilocal objects, i.e. they depend on two spatial coordinates. Consider e.g. the (generalized) longitudinal projector ( $\Pi_L$ ):

$$(\Pi_L)_{ij}^{ab}(\mathbf{x}, \mathbf{y}). \quad (\text{A.13})$$

<sup>1</sup>in the following, this will be called 'non-perturbative scaling'

<sup>2</sup>in the following, this will be called 'perturbative scaling'

As is to be expected for a projector,  $(\Pi_L)$  is idempotent (if we include an integration over the double continuous index as well):

$$(\Pi_L)_{ij}^{ab}(\mathbf{x}, \mathbf{y}) = \int d^3z (\Pi_L)_{ik}^{ac}(\mathbf{x}, \mathbf{z})(\Pi_L)_{kj}^{cb}(\mathbf{z}, \mathbf{y}). \quad (\text{A.14})$$

The (generalized) longitudinal projector  $(\Pi_L)$  is a symmetric operator in the sense that<sup>3</sup>

$$\int d^3x d^3y f_i^a(\mathbf{x})(\Pi_L)_{ij}^{ab}(\mathbf{x}, \mathbf{y})g_j^b(\mathbf{y}) = \int d^3x d^3y g_i^a(\mathbf{x})(\Pi_L)_{ij}^{ab}(\mathbf{x}, \mathbf{y})f_j^b(\mathbf{y}). \quad (\text{A.15})$$

The latter property implies that it can be diagonalized, and from eq. (A.14) one can conclude that its eigenvalues are 0, 1. The generalized longitudinal projector can be given in different forms; for this it might be useful to recall that the ordinary longitudinal projector  $P^L$  also can be given in different forms that are under the usual circumstances (i.e. all functions of  $\mathbf{y}$  are found to the right<sup>4</sup> of  $(P^L)_{ij}(\mathbf{x}, \mathbf{y})$ )

$$(P^L)_{ij}(\mathbf{x}, \mathbf{y}) = \left( \nabla_i^x G_\Delta(\mathbf{x}, \mathbf{y}) \right) \nabla_j^y \quad (\text{A.16})$$

$$= - \left( \nabla_j^y \nabla_i^x G_\Delta(\mathbf{x}, \mathbf{y}) \right) \quad (\text{A.17})$$

$$= \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})} \frac{\mathbf{k}_i \mathbf{k}_j}{\mathbf{k}^2}, \quad (\text{A.18})$$

where  $G_\Delta(\mathbf{x}, \mathbf{y})$  denotes the Green's function of the Laplace operator. Under the given circumstances all three definitions are equivalent; however, only the first one really has to 'act to the right' in order to make sense. The (ordinary) transversal projector can also easily be defined as

$$(P^T)_{ij}(\mathbf{x}, \mathbf{y}) = \delta_{ij} \delta_{\mathbf{x}\mathbf{y}} - (P^L)_{ij}(\mathbf{x}, \mathbf{y}). \quad (\text{A.19})$$

For the generalized longitudinal projectors we can now give corresponding definitions:

$$(\Pi_L)_{ij}^{ab}(\mathbf{x}, \mathbf{y}) = \left( \hat{\mathbf{D}}_i^{aa_1}(\mathbf{x}) G_\Delta^{a_1 b_1}(\mathbf{x}, \mathbf{y}) \right) \hat{\mathbf{D}}_j^{b_1 b}(\mathbf{y}) \quad (\text{A.20})$$

$$= - \left( \hat{\mathbf{D}}_j^{bb_1}(\mathbf{y}) \hat{\mathbf{D}}_i^{aa_1}(\mathbf{x}) G_\Delta^{a_1 b_1}(\mathbf{x}, \mathbf{y}) \right) \quad (\text{A.21})$$

$$= \sum_n (\xi_n^*)_i^a(\mathbf{x}) (\xi_n)_j^b(\mathbf{y}) \quad (\text{A.22})$$

where  $G_\Delta^{a_1 b_1}(\mathbf{x}, \mathbf{y})$  is the Green's function of the covariant Laplacian<sup>5</sup>  $(\hat{\mathbf{D}}\hat{\mathbf{D}})^{c_1 b_1}(\mathbf{x})$ ,  $(\xi_n)_i^a(\mathbf{x})$  are the normalized eigenfunctions of  $(\Pi_L)_{ij}^{ab}(\mathbf{x}, \mathbf{y})$  with eigenvalue 1, and we do not integrate over  $\mathbf{x}, \mathbf{y}$ . Here the corresponding generalized transversal projectors are given by

$$(\Pi_T)_{ij}^{ab}(\mathbf{x}, \mathbf{y}) = \delta_{ij} \delta^{ab} \delta_{\mathbf{x}\mathbf{y}} - (\Pi_L)_{ij}^{ab}(\mathbf{x}, \mathbf{y}). \quad (\text{A.23})$$

<sup>3</sup>Here we have dropped boundary terms from two partial integrations.

<sup>4</sup>In other words, for expressions of the type  $f_i(\mathbf{x})(P^L)_{ij}(\mathbf{x}, \mathbf{y})g_j(\mathbf{y})$  (with a sum or integral over all double indices) all these definitions are equivalent, otherwise they will usually be not.

<sup>5</sup>For simplicity, we assume that the covariant Laplacian has no eigenvalues zero.

## Appendix B

# Perturbation Theory in Weyl Gauge

In this appendix we want to present a number of tools that are used in sec.2.2, and some explicit expressions for propagators and interaction parts of the action, cf. also [TR80a], [TR80b], [LMR84].

### B.1 Adjoint Representation and Integral

Assume that we have a  $SU(N)$  group element  $U_h$

$$U_h = \exp(igh_a \lambda^a). \quad (\text{B.1})$$

An ingredient that is used frequently in diverse computations to follow is

$$\int_0^1 dt 2 \operatorname{tr}(\lambda^a U_{th}^\dagger \lambda^b U_{th}) = \int_0^1 dt \sigma_{ab}(th). \quad (\text{B.2})$$

We first start out by deriving a useful representation for  $\sigma$  by considering the differential equation it satisfies,

$$\sigma_{ab}(0) = \delta_{ab} \quad (\text{B.3})$$

$$\frac{d}{dt} \sigma_{ab}(th) = \sigma_{ad}(th) \gamma_{db} = \gamma_{ad} \sigma_{db}(th) \text{ with } \gamma_{ab} = ig f^{cab} h_c. \quad (\text{B.4})$$

Thus we can write  $\sigma$  as

$$\sigma_{ab}(th) = (e^{it\gamma})_{ab}. \quad (\text{B.5})$$

With this we can now perform the integration and obtain

$$\boxed{\int_0^1 dt \sigma_{ab}(th) = (i\gamma)_{ac}^{-1} (e^{i\gamma} - 1)_{cb}.} \quad (\text{B.6})$$

### B.2 Pure Gauge Potentials

The first instance where the above formula can be applied is in deriving a form of a pure gauge potential in terms of  $h$  that can be easily expanded in terms of  $g$ :

$$\mathbf{A}^{U_h} = -\frac{i}{g} U_h^\dagger \nabla U_h \rightarrow (\mathbf{A}^{U_h})^a = (\nabla h^b) \int_0^1 dt \sigma_{ab}(th) = (\delta_{ab} + F_{ab})(\nabla h^b) \quad (\text{B.7})$$

with  $F = (i\gamma)^{-1}(e^{i\gamma} - i\gamma - 1)$ . The advantage of  $F$  is that - upon expansion of the exponential in powers of  $g$  - it is of  $\mathcal{O}(g)$ . In the main text we will need the expansion of  $F$  up to second order in  $g$ :

$$F_{ab} = -\frac{1}{2}gh^c f^{cab} + \frac{g^2}{6}h^{c_1}h^{c_2} f^{c_1ac} f^{c_2cb} + \mathcal{O}(g^3). \quad (\text{B.8})$$

### B.3 Haar Measure, General

In this section, we want to construct the Haar measure from its property that it is left-invariant, following [Cor84]. We start by considering a group element  $U_a$  that is parametrized by the parameters  $a_1, \dots, a_n$ . The Haar measure  $d\mu[U_a]$  can be written as a 'measure function'  $\rho(a_1, \dots, a_n)$  times a flat integration measure  $da_1 \dots da_n$ . Thus, we try to compute  $\rho$ . If we consider a fixed group element  $U_b$ , the left-invariance of the Haar measure implies that  $d\mu[U_a] = d\mu[U_b U_a]$ ; we call the group element obtained by that left-multiplication  $U_c = U_b U_a$ . This is almost enough to determine the Haar measure:

$$\begin{aligned} d\mu[U_a] &= \rho(a_1, \dots, a_n) da_1 \dots da_n \\ &= d\mu[\underbrace{U_b U_a}_{=: U_c}] = \rho(c_1, \dots, c_n) dc_1 \dots dc_n \\ &= \rho(c_1, \dots, c_n) \left| \det \frac{\partial c}{\partial a} \right| da_1 \dots da_n. \end{aligned} \quad (\text{B.9})$$

Thus  $\rho(a_1, \dots, a_n) = \left| \det \frac{\partial c}{\partial a} \right| \rho(c_1, \dots, c_n)$ . Now consider  $U_a = \mathbb{1}$ , i.e.  $a_1 = \dots = a_n = 0$ , then  $U_c = U_b$ , and we obtain

$$\boxed{\rho(b_1, \dots, b_n) = \frac{\rho(0)}{\left| \det \frac{\partial c}{\partial a} \right|_{a=0}}}. \quad (\text{B.10})$$

In order to calculate the determinant, we use the identity  $U_c = U_b U_a$ ; then

$$\frac{\partial}{\partial a^k} U_c \Big|_{a=0} = \frac{\partial U_c}{\partial c^e} \frac{\partial c^e}{\partial a^k} \Big|_{a=0} = U_b \frac{\partial}{\partial a^k} U_a \Big|_{a=0} = U_b (ig\lambda^k) = U_c|_{a=0} (ig\lambda^k). \quad (\text{B.11})$$

Thus

$$ig\delta^{kn} = 2ig \operatorname{tr}(\lambda^n \lambda^k) = 2 \operatorname{tr}(\lambda^n U_c^\dagger \frac{\partial U_c}{\partial c^e}) \Big|_{a=0} \frac{\partial c^e}{\partial a^k} \Big|_{a=0} = ig \int_0^1 ds \sigma_{ne}(sc) \frac{\partial c^e}{\partial a^k} \Big|_{a=0}. \quad (\text{B.12})$$

This implies that (using a matrix notation)

$$\mathbb{1} = \left( (i\gamma)^{-1} (e^{i\gamma} - 1) \right) \left( \frac{\partial c}{\partial a} \right) \quad (\text{B.13})$$

and for the determinant we get

$$\frac{1}{\det \frac{\partial c}{\partial a}} = \det \left( (i\gamma)^{-1} (e^{i\gamma} - 1) \right) = \det (1 + F), \quad (\text{B.14})$$

where  $F$  was defined above. Thus we end up with the Haar measure of the  $SU(N)$  group

$$\rho(b_1, \dots, b_n) = \rho(0) \det (1 + F). \quad (\text{B.15})$$

## B.4 Functional Haar Measure

In the following we neglect<sup>1</sup>  $\rho(0)$ , i.e. we set it equal to 1, since it is just a constant that will cancel out in the end. In order to define the functional Haar measure, we “just” take a product of Haar measures at every point in space<sup>2</sup>, cf. also [LNT94]:

$$\begin{aligned}
\mathcal{D}\mu &= \left( \prod_{\mathbf{x}} \rho(h(\mathbf{x})) \right) \mathcal{D}h = \exp \left( \sum_{\mathbf{x}} \log \rho \right) \mathcal{D}h \\
&= \exp \left( \frac{1}{a^3} a^3 \sum_{\mathbf{x}} \log \rho \right) \mathcal{D}h = \exp \left( \frac{1}{a^3} \int d^3x \log \rho \right) \mathcal{D}h \\
&= \exp \left( \delta^3(0) \int d^3x \operatorname{tr} \left( \log (1 + F) \right) \right) \mathcal{D}h.
\end{aligned} \tag{B.16}$$

## B.5 Explicit Expressions Used in the Computations of Sec. 2.2

Please note that we have put in this section in a number of places the position indices that are usually put in brackets behind the objects to which they belong in a real index position, e.g.  $h^a(\mathbf{x})$  has been replaced by  $h_{\mathbf{x}}^a$ , since otherwise the formulas would become too complex.

### B.5.1 Propagators

We have three different types of propagators, one for the projector field eq. (B.17), one for the spatial components of the vector potential eq. (B.19), and a mixed propagator eq. (B.18).

$$\langle h_{\mathbf{x}}^a h_{\mathbf{y}}^b \rangle = \frac{T \delta^{ab}}{4\pi |\mathbf{x} - \mathbf{y}|} \tag{B.17}$$

$$\langle h_{\mathbf{x}}^a \mathbf{A}_{j,\mathbf{y}}^b(t) \rangle = \delta^{ab} \left( t + \frac{1}{2} T (1 + 2\rho) \right) \nabla_j^y \frac{1}{4\pi |\mathbf{x} - \mathbf{y}|} \tag{B.18}$$

$$\begin{aligned}
\langle \mathbf{A}_{i,\mathbf{x}}^a(t) \mathbf{A}_{j,\mathbf{y}}^b(t') \rangle &= \delta^{ab} \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} \left\{ \mathbf{P}_{ij}^T \left( -\frac{1}{|\mathbf{p}| \sinh |\mathbf{p}| T} \right. \right. \\
&\quad \times \left[ \Theta(t - t') \sinh \left( |\mathbf{p}| \left( t - \frac{T}{2} \right) \right) \sinh \left( |\mathbf{p}| \left( t' + \frac{T}{2} \right) \right) \right. \\
&\quad \left. \left. + \Theta(t' - t) \sinh \left( |\mathbf{p}| \left( t' - \frac{T}{2} \right) \right) \sinh \left( |\mathbf{p}| \left( t + \frac{T}{2} \right) \right) \right] \right) \\
&\quad \left. + \mathbf{P}_{ij}^L \left( -\frac{1}{2} |t - t'| + \frac{1}{2} (t + t') (1 + 2\rho) + \frac{1}{2} T (1 + 2\rho + 2\rho^2) \right) \right\}.
\end{aligned} \tag{B.19}$$

### B.5.2 Contributions to the Action

There are three contributions to the interacting part of the action. The first, eq. (B.20), contains the three- and four-gluon vertex of the original action (albeit only the spatial components of

<sup>1</sup>In principle it could be computed from the property that the integral over the Haar measure is normalized to one:  $\int d\mu = 1$ .

<sup>2</sup> $1 = a^3 \frac{1}{a^3} = \delta^{(3)}(0) d^3x \rightarrow 1/a^3 \stackrel{a \rightarrow 0}{=} \delta^3(0)$ .



the vector potential are contained), the second one, eq. (B.21) contains the contribution from the measure of the projector integral, and thus corresponds to the Faddeev-Popov determinant of the Polyakov gauge, and the third contribution, eq. (B.22), describes the interaction of the projector field with the spatial components of the vector potential.

$$S_I[-\frac{\delta}{\delta \mathbf{J}}] = -\frac{g}{2} f^{abc} \int d^3x dt \left\{ \left( \nabla_i \frac{\delta}{\delta \mathbf{J}_j^a(\mathbf{x}, t)} \right) - \left( \nabla_j \frac{\delta}{\delta \mathbf{J}_i^a(\mathbf{x}, t)} \right) \right\} \frac{\delta}{\delta \mathbf{J}_i^b(\mathbf{x}, t)} \frac{\delta}{\delta \mathbf{J}_j^c(\mathbf{x}, t)} \quad (\text{B.20})$$

$$-\frac{g^2}{4} f^{abc} f^{ade} \int d^3x dt \left\{ \frac{\delta}{\delta \mathbf{J}_i^b(\mathbf{x}, t)} \frac{\delta}{\delta \mathbf{J}_j^c(\mathbf{x}, t)} \frac{\delta}{\delta \mathbf{J}_i^d(\mathbf{x}, t)} \frac{\delta}{\delta \mathbf{J}_j^e(\mathbf{x}, t)} \right\}$$

$$S_m[-\frac{\delta}{\delta f}] = \delta^3(0) \int d^3x \text{Tr} \left( \log \left[ 1 + F \left( -\frac{\delta}{\delta f} \right) \right] \right) \quad (\text{B.21})$$

$$S'_I[\mathbf{J}, -\frac{\delta}{\delta f}] = \int d^3x d^3y \left\{ \int dt \left[ F_{ab} \left( -\rho \frac{\delta}{\delta f} \right) \left( -\rho \nabla_i^x \frac{\delta}{\delta f_x^b} \right) G_{ij}(\mathbf{x}, -\frac{T}{2}; \mathbf{y}, t) \mathbf{J}_j^a(\mathbf{y}, t) \right] \right. \quad (\text{B.22})$$

$$+ \frac{1}{2} F_{ab} \left( -\rho \frac{\delta}{\delta f} \right) \left( \rho \nabla_i^x \frac{\delta}{\delta f_x^b} \right) \chi_1^{ij}(\mathbf{x}, \mathbf{y}) F_{ac} \left( -\rho \frac{\delta}{\delta f} \right) \left( \rho \nabla_j^y \frac{\delta}{\delta f_y^c} \right)$$

$$- \int dt \left[ F_{ab} \left( -(1+\rho) \frac{\delta}{\delta f} \right) \left( -(1+\rho) \nabla_i^x \frac{\delta}{\delta f_x^b} \right) G_{ij}(\mathbf{x}, +\frac{T}{2}; \mathbf{y}, t) \mathbf{J}_j^a(\mathbf{y}, t) \right]$$

$$+ \frac{1}{2} F_{ab} \left( -(1+\rho) \frac{\delta}{\delta f} \right) \left( (1+\rho) \nabla_i^x \frac{\delta}{\delta f_x^b} \right) \chi_1^{ij}(\mathbf{x}, \mathbf{y})$$

$$\times F_{ac} \left( -(1+\rho) \frac{\delta}{\delta f} \right) \left( (1+\rho) \nabla_j^y \frac{\delta}{\delta f_y^c} \right)$$

$$+ F_{ab} \left( -\rho \frac{\delta}{\delta f} \right) \left( \rho \nabla_i^x \frac{\delta}{\delta f_x^b} \right) \chi_2^{ij}(\mathbf{x}, \mathbf{y})$$

$$\times F_{ac} \left( -(1+\rho) \frac{\delta}{\delta f} \right) \left( (1+\rho) \nabla_j^y \frac{\delta}{\delta f_y^c} \right) \left. \right\}$$

$$+ \int d^3x \frac{1}{T} \left[ \rho \left( \nabla_i^x \frac{\delta}{\delta f_x^a} \right) F_{ab} \left( -\rho \frac{\delta}{\delta f} \right) \left( \nabla_i^x \frac{\delta}{\delta f_x^b} \right) - \right.$$

$$\left. + (1+\rho) \left( \nabla_i^x \frac{\delta}{\delta f_x^a} \right) F_{ab} \left( -(1+\rho) \frac{\delta}{\delta f} \right) \left( \nabla_i^x \frac{\delta}{\delta f_x^b} \right) \right].$$

### B.5.3 Condensed Notation

As a last point in this appendix we want to explain briefly the very condensed notation used from eq. (2.75) onwards. As an example we take the term

$$\mathbb{G}_1^{abc} \left( \frac{\delta}{\delta \mathbf{J}^a} \right) \left( \frac{\delta}{\delta \mathbf{J}^b} \right) \left( \frac{\delta}{\delta \mathbf{J}^c} \right) \quad (\text{B.23})$$

that is to be identical to

$$-\frac{g}{2} f^{abc} \int d^3x dt \left\{ \left( \nabla_i \frac{\delta}{\delta \mathbf{J}_j^a(\mathbf{x}, t)} \right) - \left( \nabla_j \frac{\delta}{\delta \mathbf{J}_i^a(\mathbf{x}, t)} \right) \right\} \frac{\delta}{\delta \mathbf{J}_i^b(\mathbf{x}, t)} \frac{\delta}{\delta \mathbf{J}_j^c(\mathbf{x}, t)}. \quad (\text{B.24})$$

This can be achieved if we include into the super-indices also a time label, and the summing over double indices has also to include a time integration (this is not necessary for super-indices that connect  $\frac{\delta}{\delta f}$  to vertices). Thus, we expand the super-indices as follows:  $a \rightarrow (a, i_a, \mathbf{x}_a, t_a)$  with ' $a$ ' colour index, ' $i_a$ ' spatial index, ' $\mathbf{x}_a$ ' position index, ' $t_a$ ' time index:

$$\begin{aligned}
& \mathbb{G}_1^{abc} \left( \frac{\delta}{\delta \mathbf{J}^a} \right) \left( \frac{\delta}{\delta \mathbf{J}^b} \right) \left( \frac{\delta}{\delta \mathbf{J}^c} \right) \\
&= -\frac{g}{2} f^{a_1 b_1 c_1} \int d^3 x dt \left[ \left( \nabla_i \frac{\delta}{\delta \mathbf{J}_j^{a_1}(\mathbf{x}, t)} \right) - \left( \nabla_j \frac{\delta}{\delta \mathbf{J}_i^{a_1}(\mathbf{x}, t)} \right) \right] \frac{\delta}{\delta \mathbf{J}_i^{b_1}(\mathbf{x}, t)} \frac{\delta}{\delta \mathbf{J}_j^{c_1}(\mathbf{x}, t)} \\
&= -\frac{g}{2} f^{a_1 b_1 c_1} \left\{ \int d^3 x dt \left[ \left( \nabla_i \delta^{a_1 a} \delta_{j i_a} \int dt_a \delta_{t t_a} \int d^3 x_a \delta_{\mathbf{x} \mathbf{x}_a} \frac{\delta}{\delta \mathbf{J}_{i_a}^a(\mathbf{x}_a, t_a)} \right) \right. \right. \\
&\quad \left. \left. - \left( \nabla_j \delta^{a_1 a} \delta_{i i_a} \int dt_a \delta_{t t_a} \int d^3 x_a \delta_{\mathbf{x} \mathbf{x}_a} \frac{\delta}{\delta \mathbf{J}_{i_a}^a(\mathbf{x}_a, t_a)} \right) \right] \times \right. \\
&\quad \left. \delta^{b_1 b} \delta_{i i_b} \int dt_b \delta_{t t_b} \int d^3 x_b \delta_{\mathbf{x} \mathbf{x}_b} \frac{\delta}{\delta \mathbf{J}_{i_b}^b(\mathbf{x}_b, t_b)} \delta^{c_1 c} \delta_{j i_c} \int dt_c \delta_{t t_c} \int d^3 x_c \delta_{\mathbf{x} \mathbf{x}_c} \frac{\delta}{\delta \mathbf{J}_{i_c}^c(\mathbf{x}_c, t_c)} \right\} \\
&= \left\{ \int d^3 x_a d^3 x_b d^3 x_c dt_a dt_b dt_c \right. \\
&\quad \left[ \int d^3 x dt \delta_{t t_a} \delta_{t t_b} \delta_{t t_c} \delta^{a a_1} \delta^{b b_1} \delta^{c c_1} \left[ (\nabla_i \delta_{j i_a} \delta_{\mathbf{x} \mathbf{x}_a}) - (\nabla_j \delta_{i i_a} \delta_{\mathbf{x} \mathbf{x}_a}) \right] \delta_{\mathbf{x} \mathbf{x}_b} \delta_{\mathbf{x} \mathbf{x}_c} \delta_{i i_b} \delta_{j i_c} \right] \\
&\quad \left. \frac{\delta}{\delta \mathbf{J}_{i_a}^a(\mathbf{x}_a, t_a)} \frac{\delta}{\delta \mathbf{J}_{i_b}^b(\mathbf{x}_b, t_b)} \frac{\delta}{\delta \mathbf{J}_{i_c}^c(\mathbf{x}_c, t_c)} \right\}.
\end{aligned}$$

We want to consider the last part of this equation:

- $\int d^3 x_a d^3 x_b d^3 x_c dt_a dt_b dt_c$  denotes the summation over the continuous double indices, position and time;
- the last line  $\frac{\delta}{\delta \mathbf{J}_{i_a}^a(\mathbf{x}_a, t_a)} \frac{\delta}{\delta \mathbf{J}_{i_b}^b(\mathbf{x}_b, t_b)} \frac{\delta}{\delta \mathbf{J}_{i_c}^c(\mathbf{x}_c, t_c)}$  would be abbreviated in the super-index notation as  $\frac{\delta}{\delta \mathbf{J}^a} \frac{\delta}{\delta \mathbf{J}^b} \frac{\delta}{\delta \mathbf{J}^c}$ ;
- the symmetrization of the expression given in the middle-line then gives  $\mathbb{G}_1^{abc}$ .

With the procedure indicated here corresponding expressions for  $\mathbb{G}_2^{abcd}$  and  $\mathbb{H}_1^{a;bc}$  can be derived easily.

# Appendix C

## Explicit Expressions Used in gRPA

### C.1 General Remark

In this appendix there is no integration over  $\mathbf{x}$  unless explicitly stated.

### C.2 Decomposing $\mathbf{B}^2$ into Creation/Annihilation Operators

Here, we want to calculate the magnetic field and its square in the creation/annihilation operator decomposition for further usage in the gRPA calculations.

#### C.2.1 Preliminaries, Definitions

First, a comment on notation: the objects that appear in this appendix carry three different types of indices: colour indices ( $a, b, \dots$ ), spatial indices ( $i, j, \dots$ ), and position indices ( $\mathbf{x}, \mathbf{y}, \dots$ ). Whereas usually position indices are put in brackets *behind* the object to which this index belongs, in this chapter we have to put them as an index to the respective object, since otherwise the formulas in this appendix would have become unbearably complex. In the following, we need three basic definitions and expressions<sup>1</sup>:

$$\mathbf{B}_{i\mathbf{x}}^a = \epsilon_{ijk} \nabla_j \mathbf{A}_{k\mathbf{x}}^a - \frac{g}{2} f^{abc} \epsilon_{ijk} \mathbf{A}_{j\mathbf{x}}^b \mathbf{A}_{k\mathbf{x}}^c. \quad (\text{C.1})$$

$$\mathbf{A}_{i,\mathbf{x}}^a = \bar{\mathbf{A}}_{i,\mathbf{x}}^a + U_{\mathbf{xy}}^{ab,ij} (a_{\mathbf{y}}^{\dagger bj} + a_{\mathbf{y}}^{bj}) \quad (\text{C.2})$$

$$[a_{\mathbf{x}}^{ai}, a_{\mathbf{y}}^{\dagger bj}] = \delta^{ab} \delta^{ij} \delta_{\mathbf{xy}}. \quad (\text{C.3})$$

Note that in the following, every double index is summed over *except for*  $\mathbf{x}$ , which is only summed over if explicitly indicated.  $\text{tr}(\dots)$  denotes the trace over colour and spatial indices only. We will also use the following notation:

$$\bar{\mathbf{B}}_{i\mathbf{x}}^a = \epsilon_{ijk} \nabla_j \bar{\mathbf{A}}_{k\mathbf{x}}^a - \frac{g}{2} f^{abc} \epsilon_{ijk} \bar{\mathbf{A}}_{j\mathbf{x}}^b \bar{\mathbf{A}}_{k\mathbf{x}}^c \quad (\text{C.4})$$

for the *classical* magnetic field. Often, the adjoint representations of the colour group and  $\text{SU}(2)$  come into our formulas, we use thus

$$f^{bac} = (\hat{T}^a)^{bc} \quad (\text{C.5})$$

$$\epsilon_{jik} = (S_i)_{jk} \quad (\text{C.6})$$

---

<sup>1</sup>In this appendix we use 'perturbative scaling' as defined in Appendix A. In contrast to chapter 2 we do *not* rescale  $\bar{\mathbf{A}}$  to  $\frac{1}{g}\bar{\mathbf{A}}$ .

to make their appearance explicit (though the generators of the adjoint representation of the respective groups are in fact  $i$  times the LHS of eqs. (C.5,C.6)).

### C.2.2 Calculating $B_{ix}^a$

One simply inserts eq. (C.2) into eq. (C.1) and uses eq. (C.3) to bring everything into normal order. Then one obtains

$$\begin{aligned} \mathbf{B}_{ix}^a &= \bar{\mathbf{B}}_{ix}^a - \frac{g}{2} \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}}) + \epsilon_{ijk} (\nabla_j^{\mathbf{x}} \delta^{ac} - g f^{abc} \bar{\mathbf{A}}_{j\mathbf{x}}^b) U_{\mathbf{xz}}^{cd,kl} (a_{\mathbf{z}}^{\dagger dl} + a_{\mathbf{z}}^{dl}) \\ &\quad - \frac{g}{2} f^{abc} \epsilon_{ijk} U_{\mathbf{xy}}^{bd,jl} U_{\mathbf{xz}}^{ce,km} (a_{\mathbf{y}}^{\dagger dl} a_{\mathbf{z}}^{\dagger em} + a_{\mathbf{y}}^{dl} a_{\mathbf{z}}^{em} + 2a_{\mathbf{y}}^{\dagger dl} a_{\mathbf{z}}^{em}), \end{aligned} \quad (\text{C.7})$$

where we have introduced  $\nabla_j^{\mathbf{x}}$  to indicate a gradient w.r.t.  $\mathbf{x}$ . However, one can rewrite this into a more interesting form if one realizes that

$$\frac{\delta \bar{\mathbf{B}}_{ix}^a}{\delta \bar{\mathbf{A}}_{ly}^b} = \epsilon_{ijl} (\delta^{ab} \nabla_j^{\mathbf{x}} - g f^{acb} \bar{\mathbf{A}}_{j\mathbf{x}}^c) \delta_{\mathbf{xy}} = \epsilon_{ijl} \hat{\mathbf{D}}_{\mathbf{x},j}^{ab} \delta_{\mathbf{xy}}, \quad (\text{C.8})$$

$$\frac{\delta^2 \bar{\mathbf{B}}_{ix}^a}{\delta \bar{\mathbf{A}}_{ly}^b \delta \bar{\mathbf{A}}_{mz}^c} = -g \epsilon_{ilm} f^{abc} \delta_{\mathbf{xz}} \delta_{\mathbf{xy}} = -g (S_i)_{lm} (\hat{T}^a)^{bc} \delta_{\mathbf{xz}} \delta_{\mathbf{xy}}, \quad (\text{C.9})$$

where we have introduced the covariant derivative in the background field  $\bar{\mathbf{A}}$  as

$$\hat{\mathbf{D}}_{\mathbf{x},j}^{ab} = \delta^{ab} \nabla_j^{\mathbf{x}} - g f^{acb} \bar{\mathbf{A}}_{j\mathbf{x}}^c. \quad (\text{C.10})$$

Note that the vacuum expectation value of the magnetic field is not only given by the classical term, but one gets an additional term from normal ordering:

$$\langle \mathbf{B}_{ix}^a \rangle = \bar{\mathbf{B}}_{ix}^a - \frac{g}{2} \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}}) \quad (\text{C.11})$$

and via the relation

$$\frac{\delta}{\delta G_{\mathbf{yz}}^{bc,lm}} g \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}}) = g \delta_{\mathbf{xy}} \delta_{\mathbf{xz}} (S_i)_{lm} (\hat{T}^a)^{bc} = -\frac{\delta^2 \bar{\mathbf{B}}_{ix}^a}{\delta \bar{\mathbf{A}}_{ly}^b \delta \bar{\mathbf{A}}_{mz}^c} \quad (\text{C.12})$$

this allows for an interesting identity<sup>2</sup>:

$$\frac{\delta}{\delta G_{\mathbf{yz}}^{bc,lm}} \langle \mathbf{B}_{ix}^a \rangle = -\frac{1}{2} \frac{\delta}{\delta G_{\mathbf{yz}}^{bc,lm}} g \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}}) = -\frac{1}{2} \left( -\frac{\delta^2 \bar{\mathbf{B}}_{ix}^a}{\delta \bar{\mathbf{A}}_{ly}^b \delta \bar{\mathbf{A}}_{mz}^c} \right) = \frac{1}{2} \frac{\delta^2 \langle \mathbf{B}_{ix}^a \rangle}{\delta \bar{\mathbf{A}}_{ly}^b \delta \bar{\mathbf{A}}_{mz}^c}. \quad (\text{C.13})$$

One can therefore trade a second derivative w.r.t.  $\bar{\mathbf{A}}$  for a first derivative in  $G$ .

$$\mathbf{B}_{ix}^a = \bar{\mathbf{B}}_{ix}^a - \frac{g}{2} \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}}) + \frac{\delta \bar{\mathbf{B}}_{ix}^a}{\delta \bar{\mathbf{A}}_{ly}^b} U_{\mathbf{yz}_1}^{bb_1, ll_1} (a_{\mathbf{z}_1}^{\dagger b_1 l_1} + a_{\mathbf{z}_1}^{b_1 l_1}) \quad (\text{C.14})$$

$$\begin{aligned} &+ \frac{1}{2} \frac{\delta^2 \bar{\mathbf{B}}_{ix}^a}{\delta \bar{\mathbf{A}}_{ly}^b \delta \bar{\mathbf{A}}_{mz}^c} U_{\mathbf{yz}_1}^{bb_1, ll_1} U_{\mathbf{zz}_2}^{cb_2, ml_2} (a_{\mathbf{z}_1}^{\dagger b_1 l_1} a_{\mathbf{z}_2}^{\dagger b_2 l_2} + a_{\mathbf{z}_1}^{b_1 l_1} a_{\mathbf{z}_2}^{b_2 l_2} + 2a_{\mathbf{z}_1}^{\dagger b_1 l_1} a_{\mathbf{z}_2}^{b_2 l_2}) \\ &= \langle \mathbf{B}_{ix}^a \rangle + \frac{\delta \langle \mathbf{B}_{ix}^a \rangle}{\delta \bar{\mathbf{A}}_{ly}^b} U_{\mathbf{yz}_1}^{bb_1, ll_1} (a_{\mathbf{z}_1}^{\dagger b_1 l_1} + a_{\mathbf{z}_1}^{b_1 l_1}) \end{aligned} \quad (\text{C.15})$$

<sup>2</sup>This is a special example of the general relation eq. (D.19).

$$\begin{aligned}
 & + \frac{1}{2} \frac{\delta^2 \langle \mathbf{B}_{ix}^a \rangle}{\delta \bar{\mathbf{A}}_{ly}^b \delta \bar{\mathbf{A}}_{mz}^c} U_{yz_1}^{bb_1, ll_1} U_{zz_2}^{cb_2, ml_2} (a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{\dagger b_2 l_2} + a_{z_1}^{b_1 l_1} a_{z_2}^{b_2 l_2} + 2a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{b_2 l_2}) \\
 = & \langle \mathbf{B}_{ix}^a \rangle + \frac{\delta \langle \mathbf{B}_{ix}^a \rangle}{\delta \bar{\mathbf{A}}_{ly}^b} U_{yz_1}^{bb_1, ll_1} (a_{z_1}^{\dagger b_1 l_1} + a_{z_1}^{b_1 l_1}) \\
 & + \frac{\delta^2 \langle \mathbf{B}_{ix}^a \rangle}{\delta G_{yz}^{bc, lm}} U_{yz_1}^{bb_1, ll_1} U_{zz_2}^{cb_2, ml_2} (a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{\dagger b_2 l_2} + a_{z_1}^{b_1 l_1} a_{z_2}^{b_2 l_2} + 2a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{b_2 l_2}).
 \end{aligned} \tag{C.16}$$

### C.2.3 Calculating $\mathbf{B}_{ix}^a \mathbf{B}_{ix}^a$

This is a good starting point for the calculation of  $\mathbf{B}_{ix}^a \mathbf{B}_{ix}^a$ : one squares eq. (C.16) and normal orders the expression. The calculation is not really very interesting apart from the fact that one usually obtains by direct calculation an expression where the symmetry under permutation is carried by the operators, and can trade this for an expression where the prefactor multiplying the operators is symmetric in all the indices<sup>3</sup> and the operators have a definite order. Then one obtains

$$\begin{aligned}
 \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a = & \bar{\mathbf{B}}_{ix}^a \bar{\mathbf{B}}_{ix}^a - g \bar{\mathbf{B}}_{ix}^a \text{tr}(S_i \hat{T}^a G_{xx}) + \frac{\delta \bar{\mathbf{B}}_{ix}^a}{\delta \bar{\mathbf{A}}_{ly_1}^b} G_{y_1 y_2}^{bc, lk} \frac{\delta \bar{\mathbf{B}}_{ix}^a}{\delta \bar{\mathbf{A}}_{ky_2}^c} \\
 & + \frac{g^2}{4} \text{tr}(S_i \hat{T}^a G_{xx}) \text{tr}(S_i \hat{T}^a G_{xx}) + \frac{g^2}{2} \text{tr}(S_i \hat{T}^a G_{xx} S_i \hat{T}^a G_{xx}) \\
 & + \left( \frac{\delta}{\delta \bar{\mathbf{A}}_{n_1 x_1}^{a_1}} \langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle \right) U_{x_1 z_1}^{a_1 b_1, n_1 l_1} (a_{z_1}^{\dagger b_1 l_1} + a_{z_1}^{b_1 l_1}) \\
 & + \left( \frac{\delta}{\delta G_{x_1 x_2}^{a_1 a_2, n_1 n_2}} \langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle \right) U_{x_1 z_1}^{a_1 b_1, n_1 l_1} U_{x_2 z_2}^{a_2 b_2, n_2 l_2} (a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{\dagger b_2 l_2} + a_{z_1}^{b_1 l_1} a_{z_2}^{b_2 l_2} + 2a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{b_2 l_2}) \\
 & + \frac{1}{3} \left( \frac{\delta}{\delta \bar{\mathbf{A}}_{n_1 x_1}^{a_1}} \frac{\delta}{\delta G_{x_2 x_3}^{a_2 a_3, n_2 n_3}} \langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle \right) U_{x_1 z_1}^{a_1 b_1, n_1 l_1} U_{x_2 z_2}^{a_2 b_2, n_2 l_2} U_{x_3 z_3}^{a_3 b_3, n_3 l_3} \\
 & \quad (a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{\dagger b_2 l_2} a_{z_3}^{\dagger b_3 l_3} + 3a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{\dagger b_2 l_2} a_{z_3}^{b_3 l_3} + 3a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{b_2 l_2} a_{z_3}^{\dagger b_3 l_3} + a_{z_1}^{b_1 l_1} a_{z_2}^{\dagger b_2 l_2} a_{z_3}^{b_3 l_3}) \\
 & + \frac{1}{6} \left( \frac{\delta}{\delta G_{x_1 x_2}^{a_1 a_2, n_1 n_2}} \frac{\delta}{\delta G_{x_3 x_4}^{a_3 a_4, n_3 n_4}} \langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle \right) U_{x_1 z_1}^{a_1 b_1, n_1 l_1} U_{x_2 z_2}^{a_2 b_2, n_2 l_2} U_{x_3 z_3}^{a_3 b_3, n_3 l_3} U_{x_4 z_4}^{a_4 b_4, n_4 l_4} \\
 & \quad (a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{\dagger b_2 l_2} a_{z_3}^{\dagger b_3 l_3} a_{z_4}^{\dagger b_4 l_4} + 4a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{\dagger b_2 l_2} a_{z_3}^{\dagger b_3 l_3} a_{z_4}^{b_4 l_4} + 6a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{\dagger b_2 l_2} a_{z_3}^{b_3 l_3} a_{z_4}^{\dagger b_4 l_4} \\
 & \quad + 4a_{z_1}^{\dagger b_1 l_1} a_{z_2}^{b_2 l_2} a_{z_3}^{\dagger b_3 l_3} a_{z_4}^{b_4 l_4} + a_{z_1}^{b_1 l_1} a_{z_2}^{\dagger b_2 l_2} a_{z_3}^{b_3 l_3} a_{z_4}^{\dagger b_4 l_4}).
 \end{aligned} \tag{C.17}$$

For further usage, we give the explicit expressions:

1.  $\left( \frac{\delta}{\delta \bar{\mathbf{A}}_{n x_1}^{a_1}} \langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle \right)$   
 $= 2 \left( \bar{\mathbf{B}}_{ix}^a - \frac{g}{2} \text{tr}(S_i \hat{T}^a G_{xx}) \right) (S_j)_{in} (\hat{\mathbf{D}}_{x,j}^{a a_1} \delta_{xx_1})$   
 $- 2g (S_j)_{in_1} (\hat{\mathbf{D}}_{x,j}^{a b_1} \delta_{xy_1}) G_{y_1 y_2}^{b_1 b_2, n_1 n_2} (S_i)_{n_2 n} (\hat{T}^a)^{b_2 a_1} \delta_{xy_2} \delta_{xx_1}$
2.  $\left( \frac{\delta}{\delta G_{x_1 x_2}^{a_1 a_2, n_1 n_2}} \langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle \right)$   
 $= -g \left( \bar{\mathbf{B}}_{ix}^a - \frac{g}{2} \text{tr}(S_i \hat{T}^a G_{xx}) \right) (S_i)_{n_1 n_2} (\hat{T}^a)^{a_1 a_2} \delta_{xx_1} \delta_{xx_2}$

<sup>3</sup>Only these symmetric prefactors can usually be written as derivatives of  $\langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle$ .

$$\begin{aligned}
& +g^2(S_i\hat{T}^a G_{\mathbf{x}\mathbf{x}} S_i\hat{T}^a)_{n_1 n_2}^{a_1 a_2} \delta_{\mathbf{x}\mathbf{x}_1} \delta_{\mathbf{x}\mathbf{x}_2} + \frac{\delta\bar{\mathbf{B}}_{i\mathbf{x}}^a}{\delta\bar{\mathbf{A}}_{n_1\mathbf{x}_1}^{a_1}} \frac{\delta\bar{\mathbf{B}}_{i\mathbf{x}}^a}{\delta\bar{\mathbf{A}}_{n_2\mathbf{x}_2}^{a_2}} \\
3. & \left( \frac{\delta}{\delta\bar{\mathbf{A}}_{n_1\mathbf{x}_1}^{a_1}} \frac{\delta}{\delta G_{\mathbf{x}_2\mathbf{x}_3}^{a_2 a_3, n_2 n_3}} \langle \mathbf{B}_{i\mathbf{x}}^a \mathbf{B}_{i\mathbf{x}}^a \rangle \right) \\
& = g(S_j)_{in_1} (\hat{\mathbf{D}}_{\mathbf{x},j}^{aa_1} \delta_{\mathbf{x}\mathbf{x}_1}) (S_i)_{n_2 n_3} (\hat{T}^a)^{a_2 a_3} \delta_{\mathbf{x}\mathbf{x}_2} \delta_{\mathbf{x}\mathbf{x}_3} + g(S_j)_{in_2} (\hat{\mathbf{D}}_{\mathbf{x},j}^{aa_2} \delta_{\mathbf{x}\mathbf{x}_2}) (S_i)_{n_3 n_1} (\hat{T}^a)^{a_3 a_1} \delta_{\mathbf{x}\mathbf{x}_3} \delta_{\mathbf{x}\mathbf{x}_1} \\
& + g(S_j)_{in_3} (\hat{\mathbf{D}}_{\mathbf{x},j}^{aa_3} \delta_{\mathbf{x}\mathbf{x}_3}) (S_i)_{n_1 n_2} (\hat{T}^a)^{a_1 a_2} \delta_{\mathbf{x}\mathbf{x}_1} \delta_{\mathbf{x}\mathbf{x}_2} \\
4. & \left( \frac{\delta}{\delta G_{\mathbf{x}_1\mathbf{x}_2}^{a_1 a_2, n_1 n_2}} \frac{\delta}{\delta G_{\mathbf{x}_3\mathbf{x}_4}^{a_3 a_4, n_3 n_4}} \langle \mathbf{B}_{i\mathbf{x}}^a \mathbf{B}_{i\mathbf{x}}^a \rangle \right) \\
& = \frac{g^2}{2} \delta_{\mathbf{x}\mathbf{x}_1} \delta_{\mathbf{x}\mathbf{x}_2} \delta_{\mathbf{x}\mathbf{x}_3} \delta_{\mathbf{x}\mathbf{x}_4} \left( (S_i\hat{T}^a)_{n_1 n_2}^{a_1 a_2} (S_i\hat{T}^a)_{n_3 n_4}^{a_3 a_4} + (S_i\hat{T}^a)_{n_1 n_3}^{a_1 a_3} (S_i\hat{T}^a)_{n_2 n_4}^{a_2 a_4} + (S_i\hat{T}^a)_{n_1 n_4}^{a_1 a_4} (S_i\hat{T}^a)_{n_2 n_3}^{a_2 a_3} \right).
\end{aligned}$$

### C.3 Decomposing $\Pi^2$ into Creation/Annihilation Operators

The calculation is a lot simpler than the calculation of the magnetic field in appendix C.2, but the result will be comparably less compact, since  $\Pi$  not only depends on  $\bar{\mathbf{e}}$  and  $G$ , but also on  $\Sigma$ :

$$\mathbf{\Pi}_{i\mathbf{x}}^b = \bar{\mathbf{e}}_{i\mathbf{x}}^b + 2i \left( \left( \frac{1}{4} (G^{-1})_{\mathbf{x}\mathbf{x}_1}^{bb_1, ii_1} - i \Sigma_{\mathbf{x}\mathbf{x}_1}^{bb_1, ii_1} \right) U_{\mathbf{x}_1\mathbf{y}_1}^{b_1 c_1, i_1 j_1} a_{\mathbf{y}_1}^{\dagger c_1 j_1} - \left( \frac{1}{4} (G^{-1})_{\mathbf{x}\mathbf{x}_1}^{bb_1, ii_1} + i \Sigma_{\mathbf{x}\mathbf{x}_1}^{bb_1, ii_1} \right) U_{\mathbf{x}_1\mathbf{y}_1}^{b_1 c_1, i_1 j_1} a_{\mathbf{y}_1}^{c_1 j_1} \right). \quad (\text{C.18})$$

As usual, all double indices will be summed over *except for*  $\mathbf{x}$ . As in the case of the magnetic field, one simply squares eq.(C.18) and normal orders the resulting expression. In order to write the prefactors of most of the terms as total derivatives, one has to note that

$$\frac{\delta}{\delta G_{\mathbf{y}_1\mathbf{y}_2}^{a_1 a_2, j_1 j_2}} (\Sigma_{\mathbf{x}\mathbf{x}_1}^{ab_1, i_1 l_1} G_{\mathbf{x}_1\mathbf{x}_2}^{b_1 b_2, l_1 l_2} \Sigma_{\mathbf{x}_2\mathbf{x}}^{b_2 a, l_2 i}) = \Sigma_{\mathbf{x}\mathbf{y}_2}^{aa_2, ij_2} \Sigma_{\mathbf{x}\mathbf{y}_1}^{aa_1, ij_1} \quad (\text{C.19})$$

$$\frac{\delta}{\delta G_{\mathbf{y}_1\mathbf{y}_2}^{a_1 a_2, j_1 j_2}} (G^{-1})_{\mathbf{x}\mathbf{x}}^{aa, ii} = -(G^{-1})_{\mathbf{x}\mathbf{y}_1}^{aa_1, ij_1} (G^{-1})_{\mathbf{x}\mathbf{y}_2}^{aa_2, ij_2}. \quad (\text{C.20})$$

Then one obtains

$$\begin{aligned}
\mathbf{\Pi}_{i\mathbf{x}}^b \mathbf{\Pi}_{i\mathbf{x}}^b & = \bar{\mathbf{e}}_{i\mathbf{x}}^b \bar{\mathbf{e}}_{i\mathbf{x}}^b + \frac{1}{4} \text{tr}(G_{\mathbf{x}\mathbf{x}}^{-1}) + 4 \text{tr}(\Sigma G \Sigma)_{\mathbf{x}\mathbf{x}} \\
& + 2 \left( \frac{\delta}{\delta \bar{\mathbf{e}}_{i_1\mathbf{x}_1}^{a_1}} \langle \mathbf{\Pi}_{i\mathbf{x}}^b \mathbf{\Pi}_{i\mathbf{x}}^b \rangle \right) \left( \frac{i}{4} (U^{-1})_{\mathbf{x}_1\mathbf{z}_1}^{a_1 b_1, l_1 n_1} (a_{\mathbf{z}_1}^{\dagger b_1 n_1} - a_{\mathbf{z}_1}^{b_1 n_1}) \right. \\
& \quad \left. + \Sigma_{\mathbf{x}_1\mathbf{y}_1}^{a_1 c_1, l_1 k_1} U_{\mathbf{y}_1\mathbf{z}_1}^{c_1 b_1, k_1 n_1} (a_{\mathbf{z}_1}^{\dagger b_1 n_1} + a_{\mathbf{z}_1}^{b_1 n_1}) \right) \\
& + \left( \frac{\delta}{\delta G_{\mathbf{x}_1\mathbf{x}_2}^{a_1 a_2, l_1 l_2}} \langle \mathbf{\Pi}_{i\mathbf{x}}^b \mathbf{\Pi}_{i\mathbf{x}}^b \rangle \right) U_{\mathbf{x}_1\mathbf{z}_1}^{a_1 b_1, l_1 n_1} U_{\mathbf{x}_2\mathbf{z}_2}^{a_2 b_2, l_2 n_2} (a_{\mathbf{z}_1}^{\dagger b_1 n_1} a_{\mathbf{z}_2}^{\dagger b_2 n_2} + a_{\mathbf{z}_1}^{b_1 n_1} a_{\mathbf{z}_2}^{b_2 n_2} + 2 a_{\mathbf{z}_1}^{\dagger b_1 n_1} a_{\mathbf{z}_2}^{b_2 n_2}) \\
& + \left( \frac{\delta}{\delta \Sigma_{\mathbf{x}_1\mathbf{x}_2}^{a_1 a_2, l_1 l_2}} \langle \mathbf{\Pi}_{i\mathbf{x}}^b \mathbf{\Pi}_{i\mathbf{x}}^b \rangle \right) \frac{i}{4} (U^{-1})_{\mathbf{x}_1\mathbf{z}_1}^{a_1 b_1, l_1 n_1} (U^{-1})_{\mathbf{x}_2\mathbf{z}_2}^{a_2 b_2, l_2 n_2} (a_{\mathbf{z}_1}^{\dagger b_1 n_1} a_{\mathbf{z}_2}^{\dagger b_2 n_2} - a_{\mathbf{z}_1}^{b_1 n_1} a_{\mathbf{z}_2}^{b_2 n_2}) \\
& + \left( (U^{-1})_{\mathbf{z}_1\mathbf{x}}^{b_1 b, n_1 i} (U^{-1})_{\mathbf{x}\mathbf{z}_2}^{bb_2, in_2} \right. \\
& \quad \left. + 2i \left( (U^{-1})_{\mathbf{z}_1\mathbf{x}}^{b_1 b, n_1 i} \Sigma_{\mathbf{x}\mathbf{x}_2}^{ba_2, il_2} U_{\mathbf{x}_2\mathbf{z}_2}^{a_2 b_2, l_2 n_2} - U_{\mathbf{z}_1\mathbf{x}_1}^{b_1 a_1, n_1 l_1} \Sigma_{\mathbf{x}_1\mathbf{x}}^{a_1 b, l_1 i} (U^{-1})_{\mathbf{x}\mathbf{z}_2}^{bb_2, in_2} \right) \right) a_{\mathbf{z}_1}^{\dagger b_1 n_1} a_{\mathbf{z}_2}^{b_2 n_2},
\end{aligned} \quad (\text{C.21})$$

where  $\text{tr}$  denotes a trace over spatial and colour indices, and  $\text{tr}(\Sigma G \Sigma)_{\mathbf{x}\mathbf{x}}$  is an abbreviation for  $(\sum_{\mathbf{x}\mathbf{x}_1}^{ab_1, ik_1} G_{\mathbf{x}_1 \mathbf{x}_2}^{b_1 b_2, k_1 k_2} \sum_{\mathbf{x}_2 \mathbf{x}}^{b_2 a, k_2 i})$  where over all double indices are summed or integrated over (as appropriate) *except for*  $\mathbf{x}$ . If one integrates over  $\mathbf{x}$  the next to last line in eq. (C.21) simplifies to  $(G^{-1})_{\mathbf{z}_1 \mathbf{z}_2}^{b_1 b_2, n_1 n_2}$ . One should note that in contrast to  $\mathbf{B}^2$ , at the stationary point terms of the form  $a_{\mathbf{z}_1}^\dagger b_{\mathbf{z}_1}^{n_1} a_{\mathbf{z}_2} b_{\mathbf{z}_2}^{n_2}$  survive. In the language of nuclear physics, one would call this the kinetic energy, whereas the magnetic term provides (apart from the terms involving three creation/annihilation operators) something like a two-particle potential.

## C.4 Decomposing the Gauss Law Operator into Creation/Annihilation Operators

### C.4.1 Preliminaries, Definitions

In this section we want to express the Gauss law operator in terms of creation/annihilation operators. We find that the decomposition has the same structure as the decomposition of the Hamiltonian, i.e. we find the same operator structures (with up to 2 creation/annihilation operators) as in the Hamiltonian, only the prefactors are given as functional derivatives of the mean-field vacuum expectation value of the Gauss law operator, instead of the Hamiltonian. From this we can conclude that - just as the ordinary Yang-Mills Hamiltonian - the cranking Hamiltonian eq. (2.155) also can be written in the form eq. (3.43). Since in the case of the cranking Hamiltonian we look for a stationary point of the cranking Hamiltonian as our mean-field vacuum, the decomposition of the cranking Hamiltonian into creation/annihilation operators will also be free from linear terms just as in the case of the ordinary Yang-Mills Hamiltonian. Schematically

$$\begin{aligned} H &= \langle H \rangle + \frac{\delta \langle H \rangle}{\delta \bar{\mathbf{A}}} (a^\dagger + a) + \frac{\delta \langle H \rangle}{\delta \bar{\mathbf{e}}} i(a^\dagger - a) \\ &\quad + \frac{\delta \langle H \rangle}{\delta G} (a^\dagger a^\dagger + aa + 2a^\dagger a) + \frac{\delta \langle H \rangle}{\delta \Sigma} i(a^\dagger a^\dagger - aa) \\ &\quad + \text{terms containing more than two creation/annihilation operators} \\ &\quad + \text{a non-derivative term } \propto a^\dagger a \end{aligned}$$

$$\begin{aligned} \hat{\mathbf{D}}\Pi &= \langle \hat{\mathbf{D}}\Pi \rangle + \frac{\delta \langle \hat{\mathbf{D}}\Pi \rangle}{\delta \bar{\mathbf{A}}} (a^\dagger + a) + \frac{\delta \langle \hat{\mathbf{D}}\Pi \rangle}{\delta \bar{\mathbf{e}}} i(a^\dagger - a) \\ &\quad + \frac{\delta \langle \hat{\mathbf{D}}\Pi \rangle}{\delta G} (a^\dagger a^\dagger + aa + 2a^\dagger a) + \frac{\delta \langle \hat{\mathbf{D}}\Pi \rangle}{\delta \Sigma} i(a^\dagger a^\dagger - aa) \\ &\quad + \text{a non-derivative term } \propto a^\dagger a. \end{aligned}$$

Thus, we obtain as a cranking Hamiltonian ( $\mu$  is an arbitrary local function):

$$\begin{aligned} H - \mu \hat{\mathbf{D}}\Pi &= \langle H - \mu \hat{\mathbf{D}}\Pi \rangle + \frac{\delta \langle H - \mu \hat{\mathbf{D}}\Pi \rangle}{\delta \bar{\mathbf{A}}} (a^\dagger + a) + \frac{\delta \langle H - \mu \hat{\mathbf{D}}\Pi \rangle}{\delta \bar{\mathbf{e}}} i(a^\dagger - a) \\ &\quad + \frac{\delta \langle H - \mu \hat{\mathbf{D}}\Pi \rangle}{\delta G} (a^\dagger a^\dagger + aa + 2a^\dagger a) + \frac{\delta \langle H - \mu \hat{\mathbf{D}}\Pi \rangle}{\delta \Sigma} i(a^\dagger a^\dagger - aa) \\ &\quad + \text{terms containing more than two creation/annihilation operators} \\ &\quad + \text{non-derivative terms } \propto a^\dagger a. \end{aligned}$$

Thus, we get no additional linear terms in the cranking Hamiltonian if we go to the stationary point of the cranking Hamiltonian. In addition to the definitions and decompositions used before in this appendix we only need

$$\hat{\mathbf{D}}_{\mathbf{x},j}^{ab} = \delta^{ab} \nabla_j^x - g f^{acb} \mathbf{A}_{j\mathbf{x}}^c. \quad (\text{C.22})$$

### C.4.2 Calculating $\Gamma_{\mathbf{x}}^a$

The calculation is again not very interesting: one inserts all the definitions into one another and normal orders the resulting expression. Only one useful trick shall be given:

$$\begin{aligned} \hat{\mathbf{D}}_{\mathbf{x},i}^{ab} (G^{-1})_{\mathbf{xy}_1}^{ii_1,bb_1} &= \hat{\mathbf{D}}_{\mathbf{x},i}^{ab} (\delta_{\mathbf{xy}} \delta_{ij} \delta^{bd}) (G^{-1})_{\mathbf{yy}_1}^{ji_1,db_1} = \hat{\mathbf{D}}_{\mathbf{x},i}^{ab} \left( \frac{\delta \bar{\mathbf{e}}_{i\mathbf{x}}^b}{\delta \bar{\mathbf{e}}_{j\mathbf{y}}^d} \right) (G^{-1})_{\mathbf{yy}_1}^{ji_1,db_1} \\ &= \left( \frac{\delta}{\delta \bar{\mathbf{e}}_{j\mathbf{y}}^d} \langle \hat{\mathbf{D}}_{\mathbf{x},i}^{ab} \hat{\mathbf{\Pi}}_{i\mathbf{x}}^b \rangle \right) (G^{-1})_{\mathbf{yy}_1}^{ji_1,db_1}. \end{aligned} \quad (\text{C.23})$$

After normal ordering, we obtain the result

$$\begin{aligned} \hat{\mathbf{D}}_{\mathbf{x},i}^{ab} \hat{\mathbf{\Pi}}_{i\mathbf{x}}^b &= \hat{\mathbf{D}}_{\mathbf{x},i}^{ab} \bar{\mathbf{e}}_{i\mathbf{x}}^b + 2g \text{tr}(\hat{T}^a \Sigma_{\mathbf{xx}_1} G_{\mathbf{x}_1\mathbf{x}}) \\ &+ \left( \frac{\delta}{\delta \mathbf{A}_{l_1\mathbf{x}_1}^{a_1}} \langle \hat{\mathbf{D}}_{\mathbf{x},i}^{ab} \hat{\mathbf{\Pi}}_{i\mathbf{x}}^b \rangle \right) U_{\mathbf{x}_1\mathbf{z}_1}^{a_1 b_1, l_1 n_1} (a_{\mathbf{z}_1}^{\dagger b_1 n_1} + a_{\mathbf{z}_1}^{b_1 n_1}) \\ &+ 2 \left( \frac{\delta}{\delta \bar{\mathbf{e}}_{l_1\mathbf{x}_1}^{a_1}} \langle \hat{\mathbf{D}}_{\mathbf{x},i}^{ab} \hat{\mathbf{\Pi}}_{i\mathbf{x}}^b \rangle \right) \left( \frac{i}{4} (U^{-1})_{\mathbf{x}_1\mathbf{z}_1}^{a_1 b_1, l_1 n_1} (a_{\mathbf{z}_1}^{\dagger b_1 n_1} - a_{\mathbf{z}_1}^{b_1 n_1}) \right. \\ &\quad \left. + \Sigma_{\mathbf{x}_1\mathbf{y}_1}^{a_1 c_1, l_1 k_1} U_{\mathbf{y}_1\mathbf{z}_1}^{c_1 b_1, k_1 n_1} (a_{\mathbf{z}_1}^{\dagger b_1 n_1} + a_{\mathbf{z}_1}^{b_1 n_1}) \right) \\ &+ \left( \frac{\delta}{\delta G_{\mathbf{x}_1\mathbf{x}_2}^{a_1 a_2, l_1 l_2}} \langle \hat{\mathbf{D}}_{\mathbf{x},i}^{ab} \hat{\mathbf{\Pi}}_{i\mathbf{x}}^b \rangle \right) U_{\mathbf{x}_1\mathbf{z}_1}^{a_1 b_1, l_1 n_1} U_{\mathbf{x}_2\mathbf{z}_2}^{a_2 b_2, l_2 n_2} (a_{\mathbf{z}_1}^{\dagger b_1 n_1} a_{\mathbf{z}_2}^{\dagger b_2 n_2} + a_{\mathbf{z}_1}^{b_1 n_1} a_{\mathbf{z}_2}^{b_2 n_2} + 2a_{\mathbf{z}_1}^{\dagger b_1 n_1} a_{\mathbf{z}_2}^{b_2 n_2}) \\ &+ \left( \frac{\delta}{\delta \Sigma_{\mathbf{x}_1\mathbf{x}_2}^{a_1 a_2, l_1 l_2}} \langle \hat{\mathbf{D}}_{\mathbf{x},i}^{ab} \hat{\mathbf{\Pi}}_{i\mathbf{x}}^b \rangle \right) \frac{i}{4} (U^{-1})_{\mathbf{x}_1\mathbf{z}_1}^{a_1 b_1, l_1 n_1} (U^{-1})_{\mathbf{x}_2\mathbf{z}_2}^{a_2 b_2, l_2 n_2} (a_{\mathbf{z}_1}^{\dagger b_1 n_1} a_{\mathbf{z}_2}^{\dagger b_2 n_2} - a_{\mathbf{z}_1}^{b_1 n_1} a_{\mathbf{z}_2}^{b_2 n_2}) \\ &- g \frac{i}{2} f^{aa_1 a_2} (U_{\mathbf{xx}_1}^{a_1 b_1, l_1 n_1} (U^{-1})_{\mathbf{xz}_2}^{a_2 b_2, l_2 n_2} + (U^{-1})_{\mathbf{xz}_1}^{a_1 b_1, l_1 n_1} U_{\mathbf{xz}_2}^{a_2 b_2, l_2 n_2}) a_{\mathbf{z}_1}^{\dagger b_1 n_1} a_{\mathbf{z}_2}^{b_2 n_2}. \end{aligned} \quad (\text{C.24})$$

## C.5 Gauge Transformations in the Generalized RPA

In this section, we want to consider how various objects that appear in the generalized RPA transform under gauge transformations.

### C.5.1 Preliminaries

In this section we want to study the behaviour of the parameters of the Gaussian reference state and the related creation/annihilation operators under (time-independent) gauge transformations. We take the same conventions for gauge transformations as given in the introduction:

$$A_\mu \xrightarrow{V} A_\mu^V := V A_\mu V^\dagger + iV \partial_\mu V^\dagger \quad (\text{C.25})$$

$$F_{\mu\nu} \xrightarrow{V} F_{\mu\nu}^V := V F_{\mu\nu} V^\dagger \quad (\text{C.26})$$



with

$$A_\mu = A_\mu^a \lambda^a \quad \text{tr}(\lambda^a \lambda^b) = \frac{1}{2} \delta^{ab} \quad (\text{C.27})$$

$$\partial_\mu = \left( \frac{\partial}{\partial t}, \nabla \right) \quad A_\mu = (A^0, -\mathbf{A}). \quad (\text{C.28})$$

In our three-dimensional formalism with the fields  $\mathbf{A}, \mathbf{\Pi}$  we thus have

$$\boxed{\begin{array}{l} \mathbf{A} \xrightarrow{V} \mathbf{A}^V := V \mathbf{A} V^\dagger - i V \nabla V^\dagger \\ \mathbf{\Pi} \xrightarrow{V} \mathbf{\Pi}^V := V \mathbf{\Pi} V^\dagger. \end{array}} \quad (\text{C.29})$$

In the following it is useful to have formulas for the gauge transformations of the components of the gauge fields. They can be easily derived and if one introduces the abbreviations

$$R^{ab}[V] = 2\text{tr}(V^\dagger \lambda^a V \lambda^b) \quad \Omega_i^a[V] = 2\text{tr}(V \nabla_i V^\dagger \lambda^a), \quad (\text{C.30})$$

then the gauge transformation of  $\mathbf{A}$  can be written as

$$\boxed{\mathbf{A}_{i\mathbf{x}}^{Vb} = R^{ba}[V_{\mathbf{x}}] \mathbf{A}_{i\mathbf{x}}^a - i \Omega_i^b[V_{\mathbf{x}}].} \quad (\text{C.31})$$

The  $R$  matrices form an adjoint representation of  $\text{SU}(N)$ , and using the *Fierz identity* ( $\lambda^a$  form a fundamental representation of  $\text{SU}(N)$ )

$$(\lambda^a)_{ij} (\lambda^a)_{kl} = \frac{1}{2} \delta_{il} \delta_{kj} - \frac{1}{2N} \delta_{ij} \delta_{kl} \quad (\text{C.32})$$

one can easily show that

$$R^{ac}[UV] = R^{ab}[U] R^{bc}[V] \quad (\text{C.33})$$

and therefore

$$R^{ab}[U] R^{bc}[U^\dagger] = R^{ac}[UU^\dagger] = \delta^{ac}. \quad (\text{C.34})$$

With the same technique one can rewrite

$$R^{ab}[V_{\mathbf{x}}^\dagger] \Omega_i^b[V_{\mathbf{x}}] = -\Omega_i^a[V_{\mathbf{x}}^\dagger]. \quad (\text{C.35})$$

### C.5.2 Behaviour of the Parameters of the Gaussian Reference State under Gauge Transformations

We start from

$$\psi_{G,\Sigma,\bar{\mathbf{A}},\bar{\mathbf{e}}}[\mathbf{A}] = \mathcal{N} \exp \left\{ - (\mathbf{A} - \bar{\mathbf{A}})_{i\mathbf{x}}^a \left( \frac{1}{4} (G^{-1})_{\mathbf{xy}}^{ab,ij} - i \Sigma_{\mathbf{xy}}^{ab,ij} \right) (\mathbf{A} - \bar{\mathbf{A}})_{j\mathbf{y}}^b + i \bar{\mathbf{e}}_{i\mathbf{x}}^a (\mathbf{A} - \bar{\mathbf{A}})_{i\mathbf{x}}^a \right\}, \quad (\text{C.36})$$

where  $\mathcal{N}$  is a normalization constant. Performing a gauge transformation

$$\mathbf{A} \rightarrow \mathbf{A}^V \rightsquigarrow \psi_{G,\Sigma,\bar{\mathbf{A}},\bar{\mathbf{e}}}[\mathbf{A}] \rightarrow \psi_{G,\Sigma,\bar{\mathbf{A}},\bar{\mathbf{e}}}[\mathbf{A}^V] \quad (\text{C.37})$$

explicitly

$$\begin{aligned}
& \psi_{G,\Sigma,\bar{\mathbf{A}},\bar{\mathbf{e}}}[\mathbf{A}^V] \\
&= \mathcal{N} \exp \left\{ - (\mathbf{A}_{ix}^{Va} - \bar{\mathbf{A}}_{ix}^a) \left( \frac{1}{4}(G^{-1})_{xy}^{ab,ij} - i\Sigma_{xy}^{ab,ij} \right) (\mathbf{A}_{jy}^{Vb} - \bar{\mathbf{A}}_{jy}^b) + i\bar{\mathbf{e}}_{ix}^a (\mathbf{A}_{ix}^{Va} - \bar{\mathbf{A}}_{ix}^a) \right\} \\
&= \mathcal{N} \exp \left\{ - \left( R^{aa_1}[V_x] \mathbf{A}_{ix}^{a_1} - i\Omega_i^a[V_x] - \bar{\mathbf{A}}_{ix}^a \right) \left( \frac{1}{4}(G^{-1})_{xy}^{ab,ij} - i\Sigma_{xy}^{ab,ij} \right) \right. \\
&\quad \left. \times \left( R^{bb_1}[V_y] \mathbf{A}_{jy}^{b_1} - i\Omega_j^b[V_y] - \bar{\mathbf{A}}_{jy}^b \right) \right\} \\
&\quad \times \exp \left\{ i\bar{\mathbf{e}}_{ix}^a \left( R^{aa_1}[V_x] \mathbf{A}_{ix}^{a_1} - i\Omega_i^a[V_x] - \bar{\mathbf{A}}_{ix}^a \right) \right\} \\
&= \mathcal{N} \exp \left\{ - \left[ \mathbf{A}_{ix}^{a_1} - R^{a_1a_2}[V_x^\dagger] \left( \bar{\mathbf{A}}_{ix}^{a_2} + i\Omega_i^{a_2}[V_x] \right) \right] R^{a_1a}[V_x^\dagger] \left( \frac{1}{4}(G^{-1})_{xy}^{ab,ij} - i\Sigma_{xy}^{ab,ij} \right) \right. \\
&\quad \left. \times R^{bb_1}[V_y] \left[ \mathbf{A}_{jy}^{b_1} - R^{b_1b_2}[V_y^\dagger] \left( \bar{\mathbf{A}}_{jy}^{b_2} + i\Omega_j^{b_2}[V_y] \right) \right] \right\} \\
&\quad \times \exp \left\{ iR^{a_1a}[V_x^\dagger] \bar{\mathbf{e}}_{ix}^a \left( \mathbf{A}_{ix}^{a_1} - R^{a_1a_2}[V_x^\dagger] \left( \bar{\mathbf{A}}_{ix}^{a_2} + i\Omega_i^{a_2}[V_x] \right) \right) \right\} \\
&= \psi_{G^V,\Sigma^V,\bar{\mathbf{A}}^V,\bar{\mathbf{e}}^V}[\mathbf{A}] \tag{C.38}
\end{aligned}$$

with

$$\begin{aligned}
(G^V)_{xy}^{a_1b_1,ij} &= R^{a_1a}[V_x^\dagger] G_{xy}^{ab,ij} R^{bb_1}[V_y] \\
(\Sigma^V)_{xy}^{a_1b_1,ij} &= R^{a_1a}[V_x^\dagger] \Sigma_{xy}^{ab,ij} R^{bb_1}[V_y] \\
\bar{\mathbf{e}}_{ix}^{Va_1} &= R^{a_1a}[V_x^\dagger] \bar{\mathbf{e}}_{ix}^{a_1} \\
\bar{\mathbf{A}}_{ix}^{Va_1} &= R^{a_1a}[V_x^\dagger] \bar{\mathbf{A}}_{ix}^{a_1} - i\Omega_i^{a_1}[V_x^\dagger],
\end{aligned} \tag{C.39}$$

i.e. one can write the gauge transformed Gaussian wave functional again as a Gaussian, albeit with different parameters.

### C.5.3 Behaviour of Creation/Annihilation Operators under Gauge Transformations

The same procedure as in the case of the wave functional will be pursued: here we start from the definition of the operators  $a, a^\dagger$ , and gauge transform their operator content (i.e.  $\mathbf{A}, \mathbf{\Pi}$ ). Then we reorder the terms such that the original structure will again become apparent, however with different parameters. In this context we will need an extended notation for the creation/annihilation operators, too, since we have to make their parameter dependence explicit:

$$a_{\mathbf{x},G,\Sigma,\bar{\mathbf{A}},\bar{\mathbf{e}}}^{ai} = 2U_{\mathbf{xx}_1}^{aa_1,ii_1} \left\{ \left( \frac{1}{4}(G^{-1})_{\mathbf{x}_1\mathbf{y}}^{a_1b,i_1j} - i\Sigma_{\mathbf{x}_1\mathbf{y}}^{a_1b,i_1j} \right) (\mathbf{A}_{j\mathbf{y}}^b - \bar{\mathbf{A}}_{j\mathbf{y}}^b) + \frac{i}{2} (\mathbf{\Pi}_{i_1\mathbf{x}_1}^{a_1} - \bar{\mathbf{e}}_{i_1\mathbf{x}_1}^{a_1}) \right\} \tag{C.40}$$

$$a_{\mathbf{x},G,\Sigma,\bar{\mathbf{A}},\bar{\mathbf{e}}}^{\dagger ai} = 2U_{\mathbf{xx}_1}^{aa_1,ii_1} \left\{ \left( \frac{1}{4}(G^{-1})_{\mathbf{x}_1\mathbf{y}}^{a_1b,i_1j} + i\Sigma_{\mathbf{x}_1\mathbf{y}}^{a_1b,i_1j} \right) (\mathbf{A}_{j\mathbf{y}}^b - \bar{\mathbf{A}}_{j\mathbf{y}}^b) - \frac{i}{2} (\mathbf{\Pi}_{i_1\mathbf{x}_1}^{a_1} - \bar{\mathbf{e}}_{i_1\mathbf{x}_1}^{a_1}) \right\}. \tag{C.41}$$

Thus, in the first step

$$\begin{aligned}
 a_{\mathbf{x},G,\Sigma,\bar{\mathbf{A}},\bar{\mathbf{e}}}^{ai} &\xrightarrow{V} a_{\mathbf{x},G,\Sigma,\bar{\mathbf{A}},\bar{\mathbf{e}}}^{Vai} \\
 &= 2U_{\mathbf{xx}\mathbf{x}_1}^{aa_1,ii_1} \left\{ \left( \frac{1}{4}(G^{-1})_{\mathbf{x}_1\mathbf{y}}^{a_1b,i_1j} - i\Sigma_{\mathbf{x}_1\mathbf{y}}^{a_1b,i_1j} \right) \left( R^{bb_1}[V_{\mathbf{y}}]\mathbf{A}_{j\mathbf{y}}^{b_1} - i\Omega_{j\mathbf{y}}^b[V_{\mathbf{y}}] - \bar{\mathbf{A}}_{j\mathbf{y}}^b \right) \right. \\
 &\quad \left. + \frac{i}{2} \left( R^{a_1b_1}[V_{\mathbf{x}_1}]\mathbf{\Pi}_{i_1\mathbf{x}_1}^{b_1} - \bar{\mathbf{e}}_{i_1\mathbf{x}_1}^{a_1} \right) \right\}.
 \end{aligned} \tag{C.42}$$

In the second step, we insert the transformed parameters<sup>4</sup> as given by eq. (C.39), and obtain

$$\boxed{a_{\mathbf{x},G,\Sigma,\bar{\mathbf{A}},\bar{\mathbf{e}}}^{Vai} = R^{ab}[V_{\mathbf{x}}]a_{\mathbf{x},G^V,\Sigma^V,\bar{\mathbf{A}}^V,\bar{\mathbf{e}}^V}^{bi}}, \tag{C.43}$$

i.e. the gauge transformed creation/annihilation operators are of the same form as the original ones with parameters transformed as in the Gaussian reference state and multiplied by the adjoint representation transformation matrix.

#### C.5.4 Behaviour of the Hamiltonian under Gauge Transformations

In the context of this section, 'gauge transformation' means the transformation of the parameters, i.e.  $(G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}}) \rightarrow (G^V, \Sigma^V, \bar{\mathbf{A}}^V, \bar{\mathbf{e}}^V)$ .

We will consider the two contributions to the Hamiltonian, i.e.  $\mathbf{B}_i^a\mathbf{B}_i^a$  and  $\mathbf{\Pi}_i^a\mathbf{\Pi}_i^a$ , separately. Since most of the terms in the Hamiltonian can be written as derivatives of expectation values in the Gaussian reference state ('Gaussian expectation value'), it makes sense to study these expectation values first.

##### Transformation of $\mathbf{B}_i^a\mathbf{B}_i^a$

The Gaussian expectation value is given as

$$\begin{aligned}
 \langle \mathbf{B}_{i\mathbf{x}}^a\mathbf{B}_{i\mathbf{x}}^a \rangle &= \bar{\mathbf{B}}_{i\mathbf{x}}^a\bar{\mathbf{B}}_{i\mathbf{x}}^a - g\bar{\mathbf{B}}_{i\mathbf{x}}^a \text{tr}(S_i\hat{T}^a G_{\mathbf{xx}}) + \frac{\delta\bar{\mathbf{B}}_{i\mathbf{x}}^a}{\delta\bar{\mathbf{A}}_{l,\mathbf{y}_1}^b} G_{\mathbf{y}_1\mathbf{y}_2}^{bc,lk} \frac{\delta\bar{\mathbf{B}}_{i\mathbf{x}}^a}{\delta\bar{\mathbf{A}}_{k,\mathbf{y}_2}^c} \\
 &+ \frac{g^2}{4} \text{tr}(S_i\hat{T}^a G_{\mathbf{xx}}) \text{tr}(S_i\hat{T}^a G_{\mathbf{xx}}) + \frac{g^2}{2} \text{tr}(S_i\hat{T}^a G_{\mathbf{xx}} S_i\hat{T}^a G_{\mathbf{xx}}).
 \end{aligned} \tag{C.44}$$

Consider each term in turn:

- $\bar{\mathbf{B}}_{i\mathbf{x}}^a$  is the classical magnetic field and thus transforms homogeneously under the adjoint representation

$$\bar{\mathbf{B}}_{i\mathbf{x}}^{Va} = R^{aa_1}[V_{\mathbf{x}}^\dagger]\bar{\mathbf{B}}_{i\mathbf{x}}^{a_1}, \tag{C.45}$$

which immediately leads to

$$\bar{\mathbf{B}}_{i\mathbf{x}}^{Va}\bar{\mathbf{B}}_{i\mathbf{x}}^{Va} = R^{aa_1}[V_{\mathbf{x}}^\dagger]\bar{\mathbf{B}}_{i\mathbf{x}}^{a_1} R^{ab_1}[V_{\mathbf{x}}^\dagger]\bar{\mathbf{B}}_{i\mathbf{x}}^{b_1} = \underbrace{R^{a_1a}[V_{\mathbf{x}}]R^{ab_1}[V_{\mathbf{x}}^\dagger]}_{\delta^{a_1b_1}} \bar{\mathbf{B}}_{i\mathbf{x}}^{a_1}\bar{\mathbf{B}}_{i\mathbf{x}}^{b_1} = \bar{\mathbf{B}}_{i\mathbf{x}}^{a_1}\bar{\mathbf{B}}_{i\mathbf{x}}^{a_1}. \tag{C.46}$$

<sup>4</sup>It is trivial to show that U transforms in the same way as G and  $\Sigma$ .

- For the next two terms it is useful to realize that<sup>5</sup>

$$R^{b_1 b} [V_{\mathbf{x}}] (\hat{T}^a)^{bc} R^{cc_1} [V_{\mathbf{x}}^\dagger] = R^{ab} [V_{\mathbf{x}}^\dagger] (\hat{T}^b)^{b_1 c_1} \quad (\text{C.47})$$

which is not really surprising, since  $\hat{T}^a$  are the generators of the adjoint representation (up to an in this context unimportant factor of  $-i$ ).

- Using this relation, one sees that

$$\text{tr}(S_i \hat{T}^a G_{\mathbf{xx}})^V = R^{ab} [V_{\mathbf{x}}^\dagger] \text{tr}(S_i \hat{T}^b G_{\mathbf{xx}}) \quad (\text{C.48})$$

$$\rightsquigarrow \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}})^V \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}})^V = \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}}) \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}}) \quad (\text{C.49})$$

$$\text{tr}(S_i \hat{T}^a G_{\mathbf{xx}} S_i \hat{T}^a G_{\mathbf{xx}})^V = \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}} S_i \hat{T}^a G_{\mathbf{xx}}). \quad (\text{C.50})$$

- Combining eq. (C.45) and eq. (C.48), one obtains

$$\bar{\mathbf{B}}_{i\mathbf{x}}^V \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}})^V = \bar{\mathbf{B}}_{i\mathbf{x}}^a \text{tr}(S_i \hat{T}^a G_{\mathbf{xx}}). \quad (\text{C.51})$$

- For the last term in the Gaussian expectation value of  $\mathbf{B}_i^a \mathbf{B}_i^a$  one has to consider

$$\left( \frac{\delta \bar{\mathbf{B}}_{i\mathbf{x}}^a}{\delta \bar{\mathbf{A}}_{l\mathbf{y}}^b} \right)^V = \epsilon_{ijl} \left( \hat{\mathbf{D}}_{\mathbf{x},j}^{ab} \right)^V \delta_{\mathbf{xy}}. \quad (\text{C.52})$$

Using eq. (C.47) and the fact that

$$R^{aa_1} [V_{\mathbf{x}}^\dagger] \delta^{a_1 b_1} [R^{b_1 b} [V_{\mathbf{x}}], \nabla_j^{\mathbf{x}}] = -i (\hat{T}^c)^{ab} \Omega_j^c [V_{\mathbf{x}}^\dagger], \quad (\text{C.53})$$

one obtains

$$\epsilon_{ijl} \left( \hat{\mathbf{D}}_{\mathbf{x},j}^{ab} \delta_{\mathbf{xy}} \right)^V = \epsilon_{ijl} R^{aa_1} [V_{\mathbf{x}}^\dagger] \left( \hat{\mathbf{D}}_{\mathbf{x},j}^{a_1 b_1} R^{b_1 b} [V_{\mathbf{x}}] \delta_{\mathbf{xy}} \right). \quad (\text{C.54})$$

Thus

$$\begin{aligned} & \left( \frac{\delta \bar{\mathbf{B}}_{i\mathbf{x}}^a}{\delta \bar{\mathbf{A}}_{l\mathbf{y}_1}^b} G_{y_1 y_2}^{bc, lk} \frac{\delta \bar{\mathbf{B}}_{i\mathbf{x}}^a}{\delta \bar{\mathbf{A}}_{k\mathbf{y}_2}^c} \right)^V \\ &= \epsilon_{ij_1 l} \left( \hat{\mathbf{D}}_{\mathbf{x}, j_1}^{ab} \delta_{\mathbf{xy}_1} \right)^V \left( G_{y_1 y_2}^{bc, lk} \right)^V \epsilon_{ij_2 k} \left( \hat{\mathbf{D}}_{\mathbf{x}, j_2}^{ac} \delta_{\mathbf{xy}_2} \right)^V \\ &= \epsilon_{ij_1 l} R^{aa_1} [V_{\mathbf{x}}^\dagger] \left( \hat{\mathbf{D}}_{\mathbf{x}, j_1}^{a_1 b_1} R^{b_1 b} [V_{\mathbf{x}}] \delta_{\mathbf{xy}_1} \right) R^{ba_2} [V_{y_1}^\dagger] G_{y_1 y_2}^{a_2 b_2, lk} R^{b_2 c} [V_{y_2}] \epsilon_{ij_2 k} R^{aa_3} [V_{\mathbf{x}}^\dagger] \left( \hat{\mathbf{D}}_{\mathbf{x}, j_2}^{a_3 b_3} R^{b_3 c} [V_{\mathbf{x}}] \delta_{\mathbf{xy}_2} \right) \\ &= \frac{\delta \bar{\mathbf{B}}_{i\mathbf{x}}^a}{\delta \bar{\mathbf{A}}_{l\mathbf{y}_1}^b} G_{y_1 y_2}^{bc, lk} \left( \frac{\delta \bar{\mathbf{B}}_{i\mathbf{x}}^a}{\delta \bar{\mathbf{A}}_{k\mathbf{y}_2}^c} \right). \end{aligned} \quad (\text{C.55})$$

We see that the Gaussian expectation value of  $\mathbf{B}_i^a \mathbf{B}_i^a$  is unchanged under gauge transformations. The next topic is 'derivatives'. We will discuss it for one example, since the rest follows trivially. Consider

$$\left( \frac{\delta}{\delta \bar{\mathbf{A}}_{n_1 \mathbf{x}_1}^{a_1}} \langle \mathbf{B}_{i\mathbf{x}}^a \mathbf{B}_{i\mathbf{x}}^a \rangle \right) U_{\mathbf{x}_1 \mathbf{z}_1}^{a_1 b_1, n_1 l_1}. \quad (\text{C.56})$$

<sup>5</sup>Once again, the Fierz identity is used.

It is important<sup>6</sup> that under a gauge transformation not only  $\langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle$  and  $U_{\mathbf{x}_1 \mathbf{z}_1}^{a_1 b_1, n_1 l_1}$  are transformed but also  $\frac{\delta}{\delta \mathbf{A}_{n_1 \mathbf{x}_1}^{a_1}}$  becomes  $\frac{\delta}{\delta \mathbf{A}_{n_1 \mathbf{x}_1}^{V a_1}}$ . Thus

$$\begin{aligned}
 & \left( \frac{\delta}{\delta \mathbf{A}_{n_1 \mathbf{x}_1}^{a_1}} \langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle \right) U_{\mathbf{x}_1 \mathbf{z}_1}^{a_1 b_1, n_1 l_1} \\
 \xrightarrow{V} & \left( \frac{\delta}{\delta \mathbf{A}_{n_1 \mathbf{x}_1}^{V a_1}} \langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle^V \right) U_{\mathbf{x}_1 \mathbf{z}_1}^{V a_1 b_1, n_1 l_1} \\
 = & \frac{\delta \mathbf{A}_{n_2 \mathbf{x}_2}^{a_2}}{\delta \mathbf{A}_{n_1 \mathbf{x}_1}^{V a_1}} \left( \frac{\delta}{\delta \mathbf{A}_{n_2 \mathbf{x}_2}^{a_2}} \langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle \right) R^{a_1 a_3} [V_{\mathbf{x}_1}^\dagger] U_{\mathbf{x}_1 \mathbf{z}_1}^{a_3 b_3, n_1 l_1} R^{b_3 b_1} [V_{\mathbf{z}_1}] \\
 = & R^{a_2 a_1} [V_{\mathbf{x}_1}] \delta_{n_2 n_1} \delta_{\mathbf{x}_2 \mathbf{x}_1} \left( \frac{\delta}{\delta \mathbf{A}_{n_2 \mathbf{x}_2}^{a_2}} \langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle \right) R^{a_1 a_3} [V_{\mathbf{x}_1}^\dagger] U_{\mathbf{x}_1 \mathbf{z}_1}^{a_3 b_3, n_1 l_1} R^{b_3 b_1} [V_{\mathbf{z}_1}] \\
 = & \left( \frac{\delta}{\delta \mathbf{A}_{n_1 \mathbf{x}_1}^{a_1}} \langle \mathbf{B}_{ix}^a \mathbf{B}_{ix}^a \rangle \right) U_{\mathbf{x}_1 \mathbf{z}_1}^{a_1 b_2, n_1 l_1} R^{b_2 b_1} [V_{\mathbf{z}_1}]. \tag{C.57}
 \end{aligned}$$

This is the general behaviour: every free colour index that is to be multiplied later on by a creation/annihilation operator obtains a corresponding  $R[V]$ , or to put it another way: call the prefactor  $(G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}})^{b_1 b_2 \dots b_2}$ , then

$$(G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}})^{b_1 b_2 \dots b_n} R^{b_1 a_1} [V] R^{b_2 a_2} [V] \dots R^{b_2 a_2} [V] = (G^V, \Sigma^V, \bar{\mathbf{A}}^V, \bar{\mathbf{e}}^V)^{a_1 a_2 \dots a_n}. \tag{C.58}$$

Now we can look at an arbitrary part of the decomposition of the magnetic field<sup>7</sup>:

$$\begin{aligned}
 & (G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}})^{b_1 \dots b_n} a_{G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}}}^{b_1} \dots a_{G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}}}^{b_n} \\
 \xrightarrow{V} & (G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}})^{b_1 \dots b_n} a_{G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}}}^{V b_1} \dots a_{G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}}}^{V b_n} \\
 = & (G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}})^{b_1 \dots b_n} R^{b_1 a_1} [V] a_{G^V, \Sigma^V, \bar{\mathbf{A}}^V, \bar{\mathbf{e}}^V}^{a_1} \dots R^{b_n a_n} [V] a_{G^V, \Sigma^V, \bar{\mathbf{A}}^V, \bar{\mathbf{e}}^V}^{a_n} \\
 = & \left( (G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}})^{b_1 \dots b_n} R^{b_1 a_1} [V] \dots R^{b_n a_n} [V] \right) a_{G^V, \Sigma^V, \bar{\mathbf{A}}^V, \bar{\mathbf{e}}^V}^{a_1} \dots a_{G^V, \Sigma^V, \bar{\mathbf{A}}^V, \bar{\mathbf{e}}^V}^{a_n} \\
 = & (G^V, \Sigma^V, \bar{\mathbf{A}}^V, \bar{\mathbf{e}}^V)^{a_1 \dots a_n} a_{G^V, \Sigma^V, \bar{\mathbf{A}}^V, \bar{\mathbf{e}}^V}^{a_1} \dots a_{G^V, \Sigma^V, \bar{\mathbf{A}}^V, \bar{\mathbf{e}}^V}^{a_n}.
 \end{aligned}$$

In short

$$\boxed{(G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}})^{b_1 \dots b_n} a_{G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}}}^{b_1} \dots a_{G, \Sigma, \bar{\mathbf{A}}, \bar{\mathbf{e}}}^{b_n} \xrightarrow{V} (G^V, \Sigma^V, \bar{\mathbf{A}}^V, \bar{\mathbf{e}}^V)^{a_1 \dots a_n} a_{G^V, \Sigma^V, \bar{\mathbf{A}}^V, \bar{\mathbf{e}}^V}^{a_1} \dots a_{G^V, \Sigma^V, \bar{\mathbf{A}}^V, \bar{\mathbf{e}}^V}^{a_n}} \tag{C.59}$$

### Transformation of $\Pi_i^a \Pi_i^a$

Compared to the magnetic field, the calculation for the electric field is quite trivial. We again start from the Gaussian expectation value

$$\langle \hat{\Pi}_{ix}^b \hat{\Pi}_{ix}^b \rangle = \bar{\mathbf{e}}_{ix}^b \bar{\mathbf{e}}_{ix}^b + \frac{1}{4} \text{tr}(G_{\mathbf{xx}}^{-1}) + 4 \text{tr}(\Sigma G \Sigma)_{\mathbf{xx}} \tag{C.60}$$

and consider the three terms in turn:

<sup>6</sup>However, it seems quite obvious that it should be like this, since the derivative annihilates a term in the expression of which the derivative is taken, which afterwards cannot be transformed any more, e.g.  $\mathbb{1} = \delta \mathbf{A} / \delta \mathbf{A} = (\delta \mathbf{A} / \delta \mathbf{A})^V = \delta \mathbf{A}^V / \delta \mathbf{A}^V \neq \delta \mathbf{A}^V / \delta \mathbf{A}$ .

<sup>7</sup>In the following, 'gauge transformation' recovers its original meaning: *transformation of the operators  $\mathbf{A}, \mathbf{\Pi}$* .

- $\bar{\mathbf{e}}_{i\mathbf{x}}^b \bar{\mathbf{e}}_{i\mathbf{x}}^b$  transforms identically to  $\bar{\mathbf{B}}_i^a \bar{\mathbf{B}}_i^a$ , cf. eq. (C.46).
- $\text{tr}(G_{\mathbf{xx}}^{-1})$  is also trivial.
- Only the last term is remotely worth considering

$$\begin{aligned}
& \text{tr}(\Sigma^V G^V \Sigma^V)_{\mathbf{xx}} \\
&= \left( R^{ab} [V_{\mathbf{x}}^\dagger] \Sigma_{\mathbf{xx}_1}^{bb_1, ii_1} R^{b_1 a_1} [V_{\mathbf{x}_1}] \right) \left( R^{a_1 c_1} [V_{\mathbf{x}_1}^\dagger] G_{\mathbf{x}_1 \mathbf{x}_2}^{c_1 c_2, i_1 i_2} R^{c_2 a_2} [V_{\mathbf{x}_2}] \right) \left( R^{a_2 b_2} [V_{\mathbf{x}_2}^\dagger] \Sigma_{\mathbf{x}_2 \mathbf{x}}^{b_2 b_3, i_2 i} R^{b_3 a} [V_{\mathbf{x}}] \right) \\
&= \text{tr}(\Sigma G \Sigma)_{\mathbf{xx}}.
\end{aligned} \tag{C.61}$$

Thus  $\langle \hat{\mathbf{\Pi}}_{i\mathbf{x}}^b \hat{\mathbf{\Pi}}_{i\mathbf{x}}^b \rangle$  stays invariant under this parameter transformation, and the rest of the argument follows as in the case of the  $\mathbf{B}^2$ . We therefore conclude that the decomposition of the Hamiltonian is form-invariant in the sense that after a gauge transformation of the operators  $\mathbf{A}, \mathbf{\Pi}$  the decomposition of the Hamiltonian into creation/annihilation operators stays the same albeit with changed parameters.

### C.5.5 Behaviour of the Gauss Law Operator under Gauge Transformations

Again, we start from the Gaussian expectation value of the Gauss law operator, which contains the following two parts

- $\hat{\mathbf{D}}_{\mathbf{x},i}^{ab} \bar{\mathbf{e}}_{i\mathbf{x}}^b$ : we use eq. (C.39) and eq. (C.54) to obtain

$$\hat{\mathbf{D}}_{\mathbf{x},i}^{ab} \bar{\mathbf{e}}_{i\mathbf{x}}^b = \left( R^{aa_1} [V_{\mathbf{x}}^\dagger] \hat{\mathbf{D}}_{\mathbf{x},i}^{a_1 b_1} R^{b_1 b} [V_{\mathbf{x}}] \right) \left( R^{bc_1} [V_{\mathbf{x}}^\dagger] \bar{\mathbf{e}}_{i\mathbf{x}}^{c_1} \right) = R^{aa_1} [V_{\mathbf{x}}^\dagger] \hat{\mathbf{D}}_{\mathbf{x},i}^{a_1 b} \bar{\mathbf{e}}_{i\mathbf{x}}^b. \tag{C.62}$$

- $\text{tr}(\hat{T}^a \Sigma_{\mathbf{xx}_1} G_{\mathbf{x}_1 \mathbf{x}})$ : we use eq. (C.39) and eq. (C.47) to obtain

$$\text{tr}(\hat{T}^a \Sigma_{\mathbf{xx}_1}^V G_{\mathbf{x}_1 \mathbf{x}}^V) = R^{ad} [V_{\mathbf{x}}^\dagger] \text{tr}(\hat{T}^d \Sigma_{\mathbf{xx}_1} G_{\mathbf{x}_1 \mathbf{x}}). \tag{C.63}$$

Thus, the Gaussian expectation value of the Gauss law operator transforms under gauge transformations in the adjoint representation as expected. The rest of the argument goes through as in the previous section, so we see that the decomposition of the Gauss law operator is form-invariant, but the whole operator transforms in the adjoint representation (as it should).

## Appendix D

# General Potential

In this appendix we will demonstrate that a potential that is an arbitrary polynomial in the field operators, can - once one decomposes the field operator into creation and annihilation operators - be written in normal ordered form s.t. all the coefficients appearing in front of the normal ordered products of creation/annihilation operators can be written as functional derivatives w.r.t. to  $G$  and  $\bar{\phi}$  of the vacuum expectation value of the potential (the creation/annihilation operators are defined with respect to that vacuum).

For simplicity we take the potential of the form

$$V[\phi] = \mathcal{M}_{x_1 \dots x_n} \phi_{x_1} \cdots \phi_{x_n}, \quad (\text{D.1})$$

where  $x_i$  are super-indices. It is clear that, if the claims hold for this potential, they will hold for an arbitrary polynomial since it will be a sum of terms of type (D.1).

Since the field operators commute, it is sufficient to consider an  $\mathcal{M}_{x_1 \dots x_n}$  that is symmetric in all indices. We have seen in chapter 3 that one can write

$$\phi_x = \bar{\phi}_x + U_{xy}(b_y^\dagger + b_y), \quad (\text{D.2})$$

where  $x, y$  are super-indices,  $U^2 = G$ , and  $[b_x, b_y^\dagger] = \delta_{xy}$ . For our purposes, it will be more useful to define rescaled operators

$$a_x^\dagger = U_{xy} b_y^\dagger \quad ; \quad a_x = U_{xy} b_y \quad \text{with} \quad [a_x, a_y^\dagger] = G_{xy}. \quad (\text{D.3})$$

Sometimes we find it also useful to write

$$\phi_x = \bar{\phi}_x + \varphi_x \quad \text{with} \quad \varphi_x = a_x^\dagger + a_x. \quad (\text{D.4})$$

After all this notational introduction, let's come to the proof. We note that, similar to  $\phi$ , both  $\bar{\phi}$  and  $\varphi$  commute; thus we can write equally<sup>1</sup> instead of eq. (D.1):

$$V[\phi] = \mathcal{M}_{x_1 \dots x_n} \sum_{m=0}^n \binom{n}{m} \bar{\phi}_{x_1} \cdots \bar{\phi}_{x_m} \varphi_{x_{m+1}} \cdots \varphi_{x_n}. \quad (\text{D.5})$$

---

<sup>1</sup>It is understood, obviously, that the index of  $x$  increases from left to right; if it should ever decrease, as in the case  $m = 0$ , the  $\bar{\phi}$ s are to be considered absent.

Now we normal order the terms with a fixed  $m$ :

$$\begin{aligned}
& \varphi_{x_{m+1}} \cdots \varphi_{x_n} \\
= & (a_{x_{m+1}} + a_{x_{m+1}}^\dagger) \cdots (a_{x_n} + a_{x_n}^\dagger) \\
= & a_{x_{m+1}}^\dagger a_{x_{m+2}}^\dagger \cdots a_{x_n}^\dagger \\
& + a_{x_{m+1}} a_{x_{m+2}}^\dagger a_{x_{m+3}}^\dagger \cdots a_{x_n}^\dagger + a_{x_{m+1}}^\dagger a_{x_{m+2}} a_{x_{m+3}}^\dagger \cdots a_{x_n}^\dagger + \cdots + a_{x_{m+1}}^\dagger a_{x_{m+2}}^\dagger a_{x_{m+3}}^\dagger \cdots a_{x_n} \\
& + a_{x_{m+1}} a_{x_{m+2}} a_{x_{m+3}}^\dagger \cdots a_{x_n}^\dagger + a_{x_{m+1}}^\dagger a_{x_{m+2}} a_{x_{m+3}} \cdots a_{x_n}^\dagger + \cdots + a_{x_{m+1}}^\dagger a_{x_{m+2}}^\dagger a_{x_{m+3}}^\dagger \cdots a_{x_n} \\
& \vdots \\
& + a_{x_{m+1}} a_{x_{m+2}} \cdots a_{x_n}.
\end{aligned} \tag{D.6}$$

We see that every row contains a fixed number of creation/annihilation operators and that it contains all possible permutations of types (creation or annihilation) among the possible indices. Especially for every term

$$\cdots a_{x_p}^\dagger \cdots a_{x_q} \cdots \tag{D.7}$$

there also exists a term

$$\cdots a_{x_p} \cdots a_{x_q}^\dagger \cdots \tag{D.8}$$

with all undenoted operators identical. We now use Wick's theorem, cf. e.g. [RS80], [Nol92], to put every line into normal order. It is practical to deal with the whole line for the following reason: if we use Wick's theorem naively we obtain the normal ordered expression plus the normal ordered expression of two less operators times their contraction etc.. However, a lot of these contractions are zero, since (we denote the contraction of two operators by  $\mathcal{C}$ )

$$\mathcal{C}(a_i^\dagger a_j) = 0. \tag{D.9}$$

However, if we deal with the complete line at once, we can use that, since for every arrangement eq. (D.7) there also exists a partner eq. (D.8), we will always obtain contractions

$$\mathcal{C}(a_i^\dagger a_j + a_i a_j^\dagger) = G_{ij}. \tag{D.10}$$

It is clear that for  $k$  contractions present we need  $2^k$  partners to obtain a non-vanishing contribution. The important point is that they exist if we deal with the whole line at once. Remember that the contractions are multiplied by normal ordered terms, and that  $[a, a] = [a^\dagger, a^\dagger] = 0$ . Since in addition  $\mathcal{M}_{x_1 \dots x_n}$  is symmetric in all its indices, all terms with a fixed number of contractions, creation, and annihilation operators, will give an identical contribution. Thus the question appears: assume we start out from the line where every term contains  $p$  creation operators,  $q$  annihilation operators and consider now terms with  $k$  contractions; how many terms will we obtain? The answer is simple,

$$\text{number of terms} = \frac{1}{2^k} \times \frac{(p+q)!}{p!q!} \times \left( \frac{1}{k!} \frac{p!}{(p-k)!} \frac{q!}{(q-k)!} \right), \tag{D.11}$$

and comes about as follows:<sup>2</sup>

1. the line containing  $p$  c's and  $q$  a's contains  $\frac{(p+q)!}{p!q!}$  terms;

<sup>2</sup>In the following, we abbreviate 'creation operators' as c's and 'annihilation operators' as a's.



2. out of the  $p$   $c$ 's and  $q$   $a$ 's we take  $k$  each, and put them together to form contractions: there are obviously  $\frac{p!}{(p-k)!} \frac{q!}{(q-k)!}$  ways to do this.
3. However, it does not matter in which order we perform the contractions since the contractions commute; thus in the step before we have overcounted by a factor of  $k!$ .
4. We now have to take into account what was said above: on the one hand, a lot of contractions are zero. On the other hand we can form pairs - this gives as argued above an additional factor of  $2^{-k}$ .

With this formula at hand, we can at first answer the following important question: assume that we have started from an expression with  $n$  field operators; upon normal ordering we obtain expressions with  $n, n-2, \dots, n-2k$   $c/a$  operators each; the question now is: is the *relative* number of  $P$   $c$ 's and  $Q$   $a$ 's with  $P+Q$  fixed always the same, no matter from which  $n$  one starts and how many contractions one needs<sup>3</sup> (provided  $n - (P+Q)$  is even) ? This question can be answered in the affirmative in the following way: we start out with an expression that contains  $p$   $c$ 's and  $q$   $a$ 's; after  $k$  contractions we will end up with  $P = p - k$   $c$ 's and  $Q = q - k$   $a$ 's. Since in the beginning  $p + q = n$  was fixed, and we end up with  $P + Q = n'$  fixed we need for every term the same number of contractions, namely  $2k = n - n'$ . With this we can rewrite the eq. (D.11) as

$$\frac{n!}{2^k k!} \frac{1}{P!(n'-P)!} = \frac{n!}{2^k k!} \frac{1}{P!Q!}. \quad (\text{D.12})$$

Thus, we have decomposed the number of terms into a factor that depends on  $n, n'$  which is a constant for  $P+Q = n'$  fixed and  $P$  varying, and a factor that depends on the number of creation and annihilation operators. If we go back to eq. (D.5) we see that we have different possibilities to end up with  $P$   $c$ 's and  $Q$   $a$ 's ( $P+Q = n'$ ): either start from  $n$   $\varphi$ s, and perform  $k$  contractions, or start from two  $\bar{\phi}$ s,  $(n-2)\varphi$ s and perform  $k-1$  contractions etc. Thus the contribution to  $\mathcal{M}_{x_1 \dots x_n} \phi_{x_1} \dots \phi_{x_n}$  containing  $n'$   $c$ 's and  $a$ 's can be written as<sup>4</sup>

$$\begin{aligned} & \mathcal{M}_{x_1 \dots x_n} \left[ \sum_{P=0}^{n'} \frac{1}{P!(n'-P)!} a_{x_1}^\dagger \dots a_{x_P}^\dagger a_{x_{P+1}} \dots a_{x_{n'}} \right] \\ & \times \sum_{k=0}^{\lfloor \frac{1}{2}(n-n') \rfloor} \left( \frac{n!}{2^k k! (n-n'-2k)!} G_{x_{n'+1} x_{n'+2}} \dots G_{x_{n'+(2k-1)} x_{n'+2k}} \bar{\phi}_{x_{n'+2k+1}} \dots \bar{\phi}_{x_n} \right), \end{aligned} \quad (\text{D.13})$$

where the latter sum runs to  $\frac{1}{2}(n-n')$  if  $n-n'$  is even, and to  $\frac{1}{2}(n-n'-1)$  if it is odd - we will deal with these details below. This expression allows us to write down the vacuum expectation value (VEV) of  $V[\phi]$  since it corresponds to the case  $n' = 0$ . Distinguish

- $n = 2N$ : the VEV reads

$$\langle V[\phi] \rangle = \mathcal{M}_{x_1 \dots x_{2N}} \sum_{k=0}^N \left( \frac{n!}{2^k k! (n-2k)!} G_{x_1 x_2} \dots G_{x_{(2k-1)} x_{2k}} \bar{\phi}_{x_{2k+1}} \dots \bar{\phi}_{x_{2N}} \right) \quad (\text{D.14})$$

<sup>3</sup>As an example: no matter where one starts - if one can get to the expression with, in total, two  $c$ 's and  $a$ 's, will they always come as  $aa + a^\dagger a^\dagger + 2a^\dagger a$  ?

<sup>4</sup>Note that the factors of the contractions and of the binomial decomposition of eq. (D.5) can be put together in a practical manner:  $\frac{(n'+2k)!}{2^k k!} \binom{n}{n+1-(n'+2k+1)} = \frac{n!}{2^k k! (n-n'-2k)!}$ . Note also that we have arranged here  $\varphi, \bar{\phi}$  opposite to eq. (D.5).

- $n = 2N + 1$ : the VEV reads

$$\langle V[\phi] \rangle = \mathcal{M}_{x_1 \dots x_{2N+1}} \sum_{k=0}^N \left( \frac{n!}{2^k k! (n-2k)!} G_{x_1 x_2} \cdots G_{x_{(2k-1)x_{2k}} \bar{\phi}_{x_{2k+1}} \cdots \bar{\phi}_{x_{2N}}} \right) \bar{\phi}_{x_{2N+1}}. \quad (\text{D.15})$$

For the following treatment, we can treat both cases with the same formula if we realize that  $\mathcal{M}_{x_1 \dots x_{2N+1}} \bar{\phi}_{x_{2N+1}}$  has the same properties as  $\mathcal{M}_{x_1 \dots x_{2N}}$  and that in the sum in eq. (D.15) always at least one  $\bar{\phi}$  survives. Thus we only have to treat the case with  $n = 2N$ . We now consider

$$\begin{aligned} & \frac{\delta}{\delta G_{y_1 y_2}} \langle V[\phi] \rangle \\ &= \frac{\delta}{\delta G_{y_1 y_2}} \mathcal{M}_{x_1 \dots x_{2N}} \sum_{k=0}^N \left( \frac{n!}{2^k k! (n-n'-2k)!} \Big|_{n'=0} G_{x_1 x_2} \cdots G_{x_{(2k-1)x_{2k}} \bar{\phi}_{x_{2k+1}} \cdots \bar{\phi}_{x_{2N}}} \right) \\ &\stackrel{(*)}{=} \mathcal{M}_{y_1 y_2 x_3 \dots x_{2N}} \sum_{k=1}^N \left( \frac{n!}{2^k k! (n-n'-2k)!} \Big|_{n'=0} {}^k G_{x_3 x_4} \cdots G_{x_{(2k-1)x_{2k}} \bar{\phi}_{x_{2k+1}} \cdots \bar{\phi}_{x_{2N}}} \right) \\ &= \frac{1}{2^{N'}} \mathcal{M}_{y_1 y_2 x_{n'+1} \dots x_{2N}} \\ &\quad \times \sum_{k=0}^{N-N'} \left( \frac{n!}{2^k k! (n-n'-2k)!} G_{x_{n'+1} x_{n'+2}} \cdots G_{x_{(2k-1)x_{2k}} \bar{\phi}_{x_{2k+1}} \cdots \bar{\phi}_{x_{2N}}} \Big|_{n'=2=2N'} \right). \end{aligned} \quad (\text{D.16})$$

In (\*) we have used the symmetry of  $\mathcal{M}$ . Obviously, as has been indicated by the suggestive notation, one is not restricted to one functional derivative but one can also perform  $N'$  of them, and then the restriction  $N' = 1$  in the last line is rendered unnecessary. We see clearly that, apart from the factor  $2^{-N'}$  the outcome of  $N'$  derivatives of the vacuum expectation value w.r.t.  $G$  is identical to the prefactor of the addend containing  $P + Q = n' = 2N'$  c's and a's in eq. (D.13). Thus we can rewrite eq. (D.13) as

$$2^{N'} \left[ \sum_{P=0}^{n'} \frac{1}{P!(n'-P)!} a_{y_1}^\dagger \cdots a_{y_P}^\dagger a_{y_{P+1}} \cdots a_{y_{n'}} \right] \frac{\delta}{\delta G_{y_1 y_2}} \cdots \frac{\delta}{\delta G_{y_{n'-1} y_{n'}}} \langle V[\phi] \rangle. \quad (\text{D.17})$$

The treatment we have presented up to here is valid for  $P + Q$  even. If  $P + Q$  is odd, we have to perform derivatives w.r.t.  $\phi$  and thus we have to treat the  $n$  even/odd cases individually. Let's start with  $n$  even:

$$\begin{aligned} & \frac{\delta}{\delta \bar{\phi}_{y_1}} \langle V[\phi] \rangle \\ &= \frac{\delta}{\delta \bar{\phi}_{y_1}} \mathcal{M}_{x_1 \dots x_{n-1} x_n} \sum_{k=0}^N \left( \frac{n!}{2^k k! (n-n'-2k)!} \Big|_{n'=0} G_{x_1 x_2} \cdots G_{x_{(2k-1)x_{2k}} \bar{\phi}_{x_{2k+1}} \cdots \bar{\phi}_{x_{n-1}} \bar{\phi}_{x_n}} \right) \\ &\stackrel{(*)}{=} \mathcal{M}_{x_1 \dots x_{n-1} y_1} \sum_{k=0}^{N-1} \left( \frac{n!}{2^k k! (n-n'-2k)!} \Big|_{n'=0} G_{x_1 x_2} \cdots G_{x_{(2k-1)x_{2k}} \bar{\phi}_{x_{2k+1}} \cdots \bar{\phi}_{x_{n-1}} (n-2k)} \right) \\ &= \mathcal{M}_{x_1 \dots x_{n-1} y_1} \sum_{k=0}^{N-1} \left( \frac{n!}{2^k k! (n-n'-2k)!} \Big|_{n'=1} G_{x_1 x_2} \cdots G_{x_{(2k-1)x_{2k}} \bar{\phi}_{x_{2k+1}} \cdots \bar{\phi}_{x_{n-1}}} \right) \end{aligned}$$

$$= \mathcal{M}_{y_1 x_2 \dots x_n} \sum_{k=0}^{N-1} \left( \frac{n!}{2^k k! (n - n' - 2k)!} G_{x_{n'+1} x_{n'+2}} \cdots G_{x_{n'+(2k-1)} x_{n'+2k}} \bar{\phi}_{x_{n'+2k+1}} \cdots \bar{\phi}_{x_n} \Big|_{n'=1} \right). \quad (\text{D.18})$$

The main point happened in line (\*) where the fact that we started from even  $n$  played a role. If  $n$  is even,  $k = N$  means that this addend doesn't contain a single factor of  $\bar{\phi}$ , thus its derivative vanishes. This is different in case of  $n$  odd, there the upper boundary is not affected by the first differentiation. It is different if one performs two derivatives w.r.t. to  $\bar{\phi}$  since then the upper limit of the sum changes once altogether independent of whether one starts from  $n$  even or odd. Thus one obtains a relation between derivatives w.r.t. to  $G$  and to  $\bar{\phi}$

$$\boxed{\frac{1}{2} \frac{\delta^2}{\delta \bar{\phi}_x \delta \bar{\phi}_y} \langle V[\phi] \rangle = \frac{\delta}{\delta G_{xy}} \langle V[\phi] \rangle}, \quad (\text{D.19})$$

which will be very useful in proving the equivalence between the generalized RPA using the operator approach and generalized RPA as derived from the time-dependent variational principle. To put this appendix in a nutshell, we have proved that a potential that is an arbitrary polynomial in the field operators can be decomposed into creation and annihilation operators, s.t. upon normal ordering one obtains a sum of subsums where each subsum contains a fixed number of  $c$ 's and  $a$ 's. The subsum consisting of the terms containing  $n'$   $c$ 's and  $a$ 's can be written as a standard polynomial in  $c$ 's and  $a$ 's

$$\left[ \sum_{P=0}^{n'} \frac{1}{P! (n' - P)!} a_{x_1}^\dagger \cdots a_{x_P}^\dagger a_{x_{P+1}} \cdots a_{x_{n'}} \right] \quad (\text{D.20})$$

multiplied by

- if  $n'$  is even,  $n'/2$  derivatives w.r.t. to  $G$  times a factor  $2^{n'/2}$
- if  $n'$  is odd, one derivative w.r.t. to  $\bar{\phi}$  and  $(n' - 1)/2$  derivatives w.r.t. to  $G$ .

We have also shown that each derivative w.r.t. to  $G$  may be traded for two derivatives w.r.t. to  $\bar{\phi}$ .

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