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A time-dependent Gaussian variational description of Lattice Gauge Theories

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Abstract

In this thesis we pursue the novel idea of using Gaussian states for high energy physics and explore some of the first necessary steps towards such a direction, via a time-dependent variational method. While these states have often been applied to condensed matter systems via Hartree-Fock, BCS or generalized Hartree-Fock theory, this is not the case in high energy physics. Their advantage is the fact that they are completely characterized, via Wick's theorem, by their two-point correlation functions (and one-point averages in bosonic systems as well), e.g., all possible pairings between fermionic operators. These are collected in the so-called covariance matrix which then becomes the most relevant object in their description.

In order to reach this goal, we set the theory on a lattice by making use of Lattice Gauge Theories (LGT). This method, introduced by Kenneth Wilson, has been extensively used for the study of gauge theories in non-perturbative regimes since it allows new analytical methods as for example strong coupling expansions, as well as the use of Monte Carlo simulations and more recently, Tensor Networks techniques as well. In spite of being formulated on a lattice, losing then Lorentz invariance, it allows an exact implementation of local gauge invariance and the special consequences of this symmetry. These features have made possible to have a deeper understanding of non-perturbative phenomena like for example the quark-confinement mechanism among others. Moreover we will make use of the Hamiltonian formulation of LGT introduced by Kogut and Susskind.

The aim of this thesis is to test a time-dependent (non)-Gaussian variational ansatz in describing quantum field theories using the framework of LGT. In chapter 2, we firstly introduce the theory of Gaussian states and the time-dependent variational method that will be later applied. Secondly in chapter 3, the framework of LGT will be introduced and how to apply the Gaussian method will become clear. In chapter 4 we apply the Gaussian ansatz to the massless and massive Schwinger models, where the solvability of the first is used to benchmark the method. Later in chapter 5 we will apply the method for a non-Abelian $SU(2)$ gauge theory and finally we will present further ideas in the Outlook.

Contents

1. Introduction

Gauge field theories lie at the heart of our current knowledge in Physics. They appear to be the pillars to all four fundamental interactions in Nature. Moreover they emerge in other branches as Condensed Matter Physics, where they arise as low energy effective descriptions [1]; and in Quantum Information, Kitaev's Toric Code model can be seen as a $\mathbb{Z}_2$ lattice gauge theory. Nevertheless, they take a more prominent essential role in the development of the Standard Model in particle physics. In these theories the so-called *local gauge principle* determines the fundamental interaction between the fermions and the gauge fields. In particular, the gauge theory named after Quantum Chromodynamics (QCD) describing the strong interaction between quarks and gluons is based on a non-Abelian $SU(3)$ group with three colors. QCD is the theory describing the interaction between quarks and gluons [2]. To our current knowledge on particle physics, free isolated quarks and gluons do not appear to exist. In fact their existence has been confirmed indirectly by experiment. They are rather confined forming hadrons —*color confinement*— or maybe glueballs [3]. One is then led to think that the coupling between quarks becomes strong at large distances, being weak at short distances as well —*asymptotic freedom*. So far, the only theories where this surprising behavior appears to happen are those containing a non-Abelian gauge field which gives rise to self interactions for the gluons.

Due to this feature, many of the relevant phenomena in particle physics e.g., whether or not QCD accounts for the observed hadron spectrum and a confirmation that QCD accounts for quark confinement, take place in the strong coupling regime, prohibiting the use of perturbative expansions and requiring new non-perturbative methods to be used [4]. The most powerful approach that has been developed for non-perturbative QCD so far, is *Lattice Gauge Theories* (LGT) introduced by Kenneth Wilson in 1974 [5], where he formulated the gauge theory on an Euclidean spacetime lattice with **exact** gauge symmetry. This formulation opened the way to study non-perturbative phenomena using numerical methods, where the Monte Carlo simulation is the most relevant one, that enable us to study phase diagrams, mass spectra and other phenomena. However, despite the great success of these techniques, there are still many problems which cannot be addressed with them: out of equilibrium dynamics are mostly inaccessible as well as regions of the phase diagram for QCD with nonzero chemical potential where Monte Carlo simulations suffer from the sign problem [6]. Therefore it would be highly desirable to have new tools which overcome these problems. In this context, the alternative Hamiltonian formulation of LGT by Kogut and Susskind [7] has renewly attracted a lot of attention due to its suitability to tackle the problem from a different perspective.

Some of the most recent and promising proposals are Tensor Networks techniques (TN) and Quantum simulators as suggested by Feynmann [8]. Quantum simulation may offer one such alternative route to tackle the problem in gauge theories, and indeed, during recent years there have been several proposals for quantum simulators

using atomic systems [9–11] and even a first experimental realization [12]. Quantum simulation of LGT presents a number of particular features which allow the models to be realized in the experiments corresponding to finite-dimensional or truncated versions of the original gauge groups. On the other hand, new methods based on TN have proved to be powerful approaches in the non-perturbative study of **quantum many-body systems** [13] without suffering from a sign problem. Their main power can be exploited in the Hamiltonian formulation and has attracted a lot of attention [**ROrus**, **otro**, 14–16], thanks to their capability to efficiently describe the relevant states of the theory [17]. Moreover this formulation provides a way to *gauge* global symmetries at the level of individual quantum many-body states, independent of any prescribed Hamiltonian or Lagrangian [18]. Nevertheless the generalization to higher dimensions than one is in general not an easy task.

However in this thesis, we would like to propose an alternative and novel method to tackle gauge theories on a lattice. This is a time-dependent (non)-Gaussian variational ansatz within the family of the so-called Gaussian states. Gaussian states are those which fulfill Wick's theorem, i.e., they are completely characterized by their one and two-point correlators, where these last are usually gathered in the so-called *covariance matrix* [**Bravyi**]. Therefore all higher order correlators can be expressed in terms of those.

On the one hand, bosonic Gaussian states (BGS) are generalizations of the well-known coherent and squeezed states often appearing in Quantum Optics as states saturating the Heisenberg uncertainty principle. BGS are also highly relevant in the study of entanglement properties in Quantum Information Theory via the so called Continuous Variables Quantum Information [19, 20]. On the other hand, fermionic Gaussian states (FGS) are also common in Quantum Information [21] but they are more popular in the Condensed Matter community, since FGS is equivalent to the Slater determinant description in the first quantization, which can be generalized to characterized the BCS state as well [22]. There, they usually appear as ground states of quadratic mean-field Hamiltonians, being also the case for BGS. In fact ground states of quadratic Hamiltonians, either fermionic or bosonic, are in general pure Gaussian states. The possibility to completely characterized a Gaussian state by its covariance matrix (and one point correlators in the bosonic case) motivates the formulation of a time-dependent Gaussian variational ansatz to approximate the ground state of an interacting Hamiltonian within this family of states, considering the covariance matrix elements as a set of variational parameters. Indeed this idea was firstly introduced for FGS in Ref. [23] and later on has been further developed in Ref. [24].

Therefore the relevance of Gaussian states is two-fold. Firstly, they appear as ground and thermal states of quadratic Hamiltonians in creation and annihilation operators and remain so under the evolution governed by quadratic Hamiltonians. These are among the few many-body problems that can be solved exactly, being diagonalized via Bogoliubov transformations. Therefore quadratic (mean-field) approximations, naturally lead to Gaussian states [25]. On the other hand, with the variational principle in mind, the number of parameters in the covariance matrix scales quadratically with the number of fermionic and bosonic modes while one point-correlation functions do it linearly. As a consequence Gaussian states can be efficiently characterized by them, allowing a numerical implementation of the method. Moreover, since in a

lattice the number of modes is automatically finite, these states are expected to be an efficient description of many-body interactions on lattice systems. For that reason, the LGT formulation of High Energy Physics, seems a promising arena for the application of this time-dependent Gaussian variational ansatz. Note that in this case we would be dealing with a system combining both bosonic and fermionic degrees of freedom interacting with each other.

However this ansatz is quite limited by the fact that correlation functions fulfill the conditions of Wick's theorem and so, are very restricted. For example, this ansatz cannot correctly describe the Fractional Quantum Hall Effect, the Kondo model and topological orders [24]. Therefore sometimes to enlarge the family of states becomes necessary, in such a way we can introduce higher order correlations beyond the mean-field theory. In order to do so, one can introduce the so-called non-Gaussian transformations in an efficient way, namely circumventing the exponential dependence of the computational resources in terms of the number of modes. Otherwise the method would not be efficient.

In this thesis we firstly introduce the theory of Gaussian states, being more extensively introduced for FGS since are the ones we will make use of in the last two chapters. We begin by establishing the formalism of FGS in order to then introduce the general formulation of the time-dependent variational method and its possible non-Gaussian extension.

In chapter 3 we begin by reviewing the usual Quantum Field Theory description of non-Abelian gauge theories to later on, being able to compare with the lattice formulation. At this point, we make emphasis on the importance of the charges generating time-independent gauge transformations. In the following, we introduce the Hamiltonian formulation of LGT constructing the Hamiltonian from the gauge principle. We end the chapter introducing the problem of confinement and the suitability of the lattice to consider the strong coupling limit.

In chapter 4 we perform the first necessary step towards the description of lattice gauge theories via the Gaussian ansatz, considering the massless and massive Schwinger model. This is a model for QED in two spacetime dimensions that is exactly solvable in the massless case. Via a unitary transformation, we are able to erase the gauge field, as it's known to happen in this two dimensions. As we will see, this provides a good description via the Gaussian ansatz. The results obtained in this chapter allows us to benchmark the ansatz by comparing to results obtained from MPS calculations in Ref. [26] and [27].

In the last chapter, we attempt to describe non-Abelian gauge theories in two spacetime dimensions applying the same method of unitarily transforming the Hamiltonian. Then we will try to apply the method to the $SU(2)$ gauge theory.

Finally, the interested reader can find in the Outlook, an attempt to describe three spacetime dimensional pure-gauge theories via the Gaussian ansatz, as well as some interesting ideas worthy to be further analyzed.

2. Gaussian states

In this chapter we review the theory of fermionic Gaussian states (FGS) following Ref. [**Bravyi**, **Bravyi2**, 21, 22] and their use as a time-dependent variational ansatz to describe systems on a lattice [23, 24]. Moreover we will give a brief introduction to Bosonic Gaussian states in order to be able to understand the whole variational method that is introduced [19, 20, 24, 25]. Since we work with finite dimensional Hilbert spaces, most of the results can be obtained from [28] or considering the simpler finite case in the proofs given in [22] for infinite-dimensional fermionic systems.

2.1. Introduction

The Gaussian approximation is frequently used in physics when a many-body interacting term appears in the theory. In most cases, the system cannot be analytically solved and one needs to provide an approximation method. In these situations, one describes the theory in terms of two-point correlation functions, as it usually happens in quantum field theory or statistical physics of fields. This means that higher order correlation functions are expressed as products of two-point ones via Wick's theorem.

In the Hamiltonian formulation of Quantum Mechanics this idea can also be applied and in fact has been of great use to study theories with interacting electrons and bosons, like BCS theory (via the so-called pairing channel) and the Hubbard model [23]. As it was explained in the introduction, the method consists on describing the system via FGSs[1], considered to be variational states to approach the ground state of the system under study. FGS can be defined as those states whose density operator ρ can be expressed as an exponential of a quadratic function of creation and annihilation operators. This property implies that they fulfill Wick's theorem and therefore **the state is completely characterized in terms of the second moments of all creation and annihilation operators**, i.e., two-point correlation functions. Those moments are gathered in the so-called —*covariance matrix* (CM), usually denoted as Γ— which then becomes the relevant object in the theory. This formulation is connected to the usual mean field approach but in a broader sense. As we already said, examples of FGSs are Slater-determinants (Hartree-Fock theory) and BCS-states (BCS theory).

The method we will introduce in this chapter, consists on deriving the best Gaussian state approximation, i.e., as explained before a variational state approach, to the ground state of a non-quadratic (interacting) Hamiltonian already discussed in [22] via the numerical minimization [23, 24] of the ground state energy being the covariance matrix Γ the relevant object for the method.

[1] In spite of the fact that we will focus on the discussion of FGS, bosonic Gaussian states have also being extensively discussed in physics literature.

2.2. Fermionic Fock space

Let's consider a M-dimensional, with $M < \infty$, single-particle Hilbert space $\mathcal{H} \cong \mathbb{C}^M$ with orthonormal basis $\{e_i\}_{i=1}^M$. We say M is the total number of considered fermionic modes e_i. From $\mathcal{H}$ we can construct the N-particle fermionic space as $\mathcal{H}^{(N)} := \mathcal{H} \wedge \cdots \wedge \mathcal{H}$ for all $N = 0, 1, \ldots, M$ due to Pauli exclusion principle, where $\mathcal{H}^{(0)} := \mathbb{C}$, $\mathcal{H}^{(M)} := \mathbb{C}$ and $\wedge$ is the antisymmetrized version of $\otimes$. The fermionic Fock space is then defined by

$$\mathcal{F}(\mathcal{H}) := \mathbb{C} \oplus \mathcal{H} \oplus \mathcal{H}^{(2)} \oplus \ldots \mathcal{H}^{(M-1)} \oplus \mathbb{C}, \tag{2.1}$$

with dimension 2^M.

In order to construct $\mathcal{F}(\mathcal{H})$ from $\mathcal{H}$ we can introduce the linear creation operator

$$\phi^\dagger : \mathcal{H} \longrightarrow \mathcal{F}(\mathcal{H}) \qquad \text{such that} \qquad \phi^\dagger(f) : \mathcal{H}^{(N)} \longrightarrow \mathcal{H}^{(N+1)} \tag{2.2}$$

$$f \to \phi^\dagger(f), \tag{2.3}$$

and by linearity $\phi^\dagger(f) = \phi^\dagger(f^i e_i) = f^i \phi^\dagger(e_i)$ define $\phi_i^\dagger := \phi^\dagger(e_i)$. In the same way we can also introduce the (antilinear) annihilation operator ϕ, the adjoint of $\phi^\dagger$, and define $\phi_i = \phi(e_i)$. Annihilation and creation operators fulfill the so-called anticommutation relations (CAR algebra with unital element $\hat{\mathbb{1}}$)

$$\{\phi_i, \phi_j^\dagger\} = \langle e_i |\, e_j \rangle = \delta_{i,j} \hat{\mathbb{1}}, \qquad \{\phi_i, \phi_j\} = 0, \tag{2.4}$$

where as usually $\{A, B\} := AB + BA$. All observables on $\mathcal{F}(\mathcal{H})$ can be expressed in terms of $\{\hat{\mathbb{1}}, \phi_i, \phi_i^\dagger\}$. This representation will be called complex or CAR indistinctly.

Since in the literature, most of the proofs for FGS are given in the so-called *Majorana representation*, let's introduce it now. This alternative representation is generated by $2M$ **Hermitian** operators $\{c_k\}_{k=1}^{2M}$ defined by

$$c_{2j-1} = \phi_i^\dagger + \phi_i, \qquad c_{2j} = i(\phi_i^\dagger - \phi_i), \tag{2.5}$$

with $j = 1, \ldots, M$. Apart from being Hermitian operators, they also satisfy

$$\{c_k, c_l\} = 2\delta_{k,l} \hat{\mathbb{1}}, \tag{2.6}$$

from where we can deduce that $c_k^2 = \hat{\mathbb{1}}$. This algebra is called *Clifford algebra* and it's usually written as $\mathcal{C}_{2M}$. Nevertheless, in our application of the Gaussian approximation in chapters 4 and 5 and the outlook, we will make use of the complex representation given in terms of creation and annihilation operators which provide a clearer physical picture. Therefore we will give the following results in both representations when it's convenient.

As convention we usually denote by Φ and C the column vectors whose components are given by

$$\Phi = (\phi_1, \ldots, \phi_M, \phi_1^\dagger, \ldots, \phi_M^\dagger)^T \tag{2.7}$$

$$C = (c_1, c_3, \ldots, c_{2M-1}, c_2, \ldots, c_{2M})^T, \tag{2.8}$$

calling Φ the *Nambu*-vector(ordering) of the CAR algebra[2]. Moreover $\Phi^\dagger$ will denote the vector

$$\Phi^\dagger = (\phi_1^\dagger, \dots, \phi_M^\dagger, \phi_1, \dots, \phi_M). \tag{2.9}$$

In addition we often collect all annihilation operators in a vector ϕ and all creation operators in a vector $\phi^\dagger$, which are either column or row vectors depending whether they form part of Φ or $\Phi^\dagger$ respectively.

Both vectors are related via

$$C = W\Phi \quad \text{with} \quad W = \begin{pmatrix} \mathbb{1}_M & \mathbb{1}_M \\ -i\mathbb{1}_M & i\mathbb{1}_M \end{pmatrix}, \tag{2.10}$$

such that $WW^\dagger = W^\dagger W = 2\mathbb{1}$. In addition, with this ordering the anticommutation relations (2.4) can be expressed as

$$\{\Phi, \Phi^\dagger\} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix} \hat{\mathbb{1}} = \mathbb{1}_{2M}\hat{\mathbb{1}}. \tag{2.11}$$

2.2.1. Bogoliubov transformations

Linear transformations of fermionic operators $\{\phi_i\}$ and $\{c_k\}$ which preserve the canonical anticommutation relations (2.4) and (2.6) respectively, are called *linear Canonical transformations* and will be denoted by $G_c(M)$. In the complex representation those are given by the unitary group of $2M \times 2M$ matrices $U(2M)$ and $G_c(M) = O(2M)$, i.e., the group of orthogonal $2M \times 2M$ matrices, in the Majorana representation. These transformations

$$\Phi_i \to \sum_j U_{ij}\Phi_j \quad \text{and} \quad C_k \to \sum_l O_{kl}C_l, \tag{2.12}$$

where U could mix both creation and annihilation operators, can be implemented[3] by ***Bogoliubov transformations*** —unitary operators $\mathcal{U}$ on $\mathcal{F}(\mathcal{H})$ that we will take to be generated by quadratic Hamiltonians with no linear terms [28]. In fact, in finite-dimensional Hilbert spaces

Theorem 2.2.1. *Any unitary operator U corresponds to a Bogoliubov transformation $\mathcal{U}$ on $\mathcal{F}(\mathcal{H})$ with*

$$\mathcal{U}\Phi_i\mathcal{U}^\dagger = \Big(U\Phi\Big)_i. \tag{2.13}$$

In order to prove this result one just needs to use Baker-Campbell-Hausdorff formula

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \dots \tag{2.14}$$

with the unitary operator

$$\mathcal{U} = e^{\frac{1}{2}\Phi^\dagger\xi\Phi} \text{ with the hermitian matrix } \xi = \begin{pmatrix} A & B \\ B^\dagger & -A^T \end{pmatrix} \tag{2.15}$$

[2]The ordering chosen for the vector C is know as $q-p$-ordering in the literature [21].

[3]In order to implement rotations in Majorana basis these transformations must fulfill that $\det O = 1$.

such that $A^\dagger = A$ and $B^T = -B$ applied to Φ. Then we find

$$e^{\frac{i}{2}\Phi^\dagger \xi \Phi} \Phi_i e^{-\frac{i}{2}\Phi^\dagger \xi \Phi} = \sum_j \left(e^{-i\xi}\right)_{ij} \Phi_j, \tag{2.16}$$

i.e., the unitary linear transformation is given by $U = e^{-i\xi}$. The same result can be proved for C where in this case ξ is an antisymmetric Hermitian matrix and the generated transformation is orthogonal. The reason why second order polynomials generate Bogoliubov transformations comes from the fact that since $\{\phi_j^\sharp, \phi_k^\sharp\} \in \mathbb{C}$ with $\phi_j^\sharp := \phi_j, \phi_j^\dagger$; then

$$[\phi_i^\sharp \phi_j^\sharp, \phi_k^\sharp] = \phi_i^\sharp \{\phi_j^\sharp, \phi_k^\sharp\} - \{\phi_i^\sharp, \phi_k^\sharp\} \phi_j^\sharp \tag{2.17}$$

is linear in the fields $\phi^\sharp$.

Observation. From equation (2.16) we deduce that time evolutions generated by quadratic Hamiltonians $H^Q(\Phi, \Phi^\dagger) = 1/2 \Phi^\dagger \mathcal{H} \Phi$, simply act as **linear transformations** on creation and annihilations operators

$$\Phi_k \to e^{iH_Q t} \Phi_k e^{-iH_Q t} = \left(e^{-i\mathcal{H}t}\right)_{kl} \Phi_l \tag{2.18}$$

in the Heisenberg picture. This fact is a key point in the formalism of Gaussian states.

2.3. Fermionic Gaussian states

As we briefly exposed in the introduction, fermionic Gaussian states (FGS) are represented by density operators that are exponential of quadratic forms in creation and annihilation operators, that in both Majorana and complex representation take the form

$$\rho = K \cdot \exp\Big[-\frac{i}{4} C^T G C\Big] = K \cdot \exp\Big[-\frac{i}{2} \Phi^\dagger \tilde{G} \Phi\Big], \tag{2.19}$$

with G a real antisymmetric and $\tilde{G}$ antihermitian $2M \times 2M$ matrices and K a normalization constant. From (2.19), it's clear that Gaussian states have the interpretation of thermal Gibbs states for quadratic Hamiltonians. Considering the Hamiltonian

$$H = \frac{1}{2} \Phi^\dagger \left(i\tilde{G}\right) \Phi, \tag{2.20}$$

and diagonalizing $i\tilde{G}$, we show that every FGS has a normal-mode decomposition with the form

$$\rho = K \prod_{k=1}^{M} \exp\Big[-\beta_k a_k^\dagger a_k\Big], \tag{2.21}$$

where the temperatures β_k are the eigenvalues of $i\tilde{G}$ and a_k, $a_k^\dagger$ are related to ϕ and $\phi^\dagger$ by a canonical transformation.

Let's introduce now a more rigorous definition of FGS. Denote

$$\rho_\lambda = \frac{1}{2^M} \prod_{j=1}^{M} \left(\hat{\mathbb{1}} - i\lambda_j c_{2j-1} c_{2j}\right). \tag{2.22}$$

Definition 2.3.1 (FGS)**.** A state ρ is a FGS if and only if it can be represented as

$$\rho = \mathcal{U}\rho_\lambda \mathcal{U}^\dagger \qquad \text{with} \qquad \mathcal{U} = \exp(iH_2 + iH_1), \tag{2.23}$$

where H_2 and H_1 are Hermitian linear combinations of operators $c_p c_q$ and c_p respectively. ρ_λ is called the standard form of a Gaussian state.

This definition for a Gaussian state is more general than the one given in (2.19), since Definition 2.3.1 considers the cases where ρ is the exponential of a quadratic polynomial with linear terms generated by H_1. However as we will explain later, it's convenient to work with *even* FGSs (like the one defined in (2.19)) which corresponds to choose $H_1 = 0$ in Definition 2.3.1.

Definition 2.3.2 (even FGS)**.** A state ρ is even FGS if and only if can be represented as

$$\rho = \mathcal{U}\rho_\lambda \mathcal{U}^\dagger \qquad \text{with} \qquad \mathcal{U} = \exp(iH_2), \tag{2.24}$$

where H_2 is a Hermitian linear combination of operators $c_p c_q$.

From the Definition 2.3.2 one can check that any **pure** FGS has the form

$$|\psi\rangle = e^{iH_2} |0\rangle , \tag{2.25}$$

with H_2 given as above and the vacuum state $|0\rangle$ defined via $\phi_k |0\rangle = 0$ for all k. This means that pure FGS are given by a Bogoliubov transformation applied to the vacuum $\mathcal{U}|0\rangle$. Moreover via Bogoliubov transformations, pure FGS can be transformed to a simple standard form given by

$$\left|\psi^{(\bar{N})}_{\text{Gauss}}\right\rangle = \prod_k (u_k + v_k \phi_k^\dagger \phi_k) |0\rangle , \tag{2.26}$$

where $u_k, v_k \in \mathbb{C}$, $|u_k|^2 + |v_k|^2 = 1$, $\bar{N} = \sum_k \left\langle \phi_k^\dagger \phi_k \right\rangle = 2\sum_k |v_k|^2$. This is for example the case of the BCS-ground state with $k \equiv (\vec{k}, \uparrow)$ and $k \equiv (-\vec{k}, \downarrow)$. The statement and proof of this result can be found in [21].

About parity

The reason to consider even rather than general Gaussian states is related to the *Parity Superselection rule*. A superselection rule is a statement that singles out certain rays in the Hilbert space as not physical realizable states [29]. The parity superselection rule is the widely believed impossibility to prepare a system in a superposition of two states whose total angular momenta are integers and half-integers, respectively [2]. This is like to say that realizable states are eigenstates of the operator $(-1)^F$ where F is even or odd for integer and half-integer states respectively. The usual way to see the inconsistency of not considering this rule goes as follows. If ψ_1 and ψ_2 are states of half-integer and integer spin respectively, the superposition of both given by $\alpha\psi_1 + \beta\psi_2$ transforms under a 2π spin rotation as $-\alpha\psi_1 + \beta\psi_2$. Since these two states are physically indistinguishable this implies that either $\alpha = 0$ or $\beta = 0$. Now in relativistic quantum theories, motivated via spin-statistics theorem one can also deduces that superposition of states with even and odd number of fermions cannot

exist by consistency. Nevertheless, it appears spin-statics theorem is not completely necessary for the proof of this fact in non-relativistic theories [30]. In our case the analogous to the operator $(-1)^F$, is the parity operator

$$P = \prod_k e^{i\pi\phi_k^\dagger\phi_k} = \prod_k e^{i\pi\hat{N}_k}, \tag{2.27}$$

with $\hat{N}_k$ the number operator for the mode k. As before P splits the fermionic Fock space $\mathcal{F}$ into even and odd parity eigenstates, i.e., those with an even or an odd total number of fermions.

Till today, all known physical processes in nature conserves parity [**Bravyi**], i.e., don't mix these two sectors.

Once we have defined what a FGS is, we can also understand why these states are called Gaussian states from the picture of FGS as a thermal state given by (2.21). Indeed, computing averages of polynomial operators A in ϕ and $\phi^\dagger$

$$\langle A\rangle = K\mathrm{Tr}\Big(\exp\Big[-\frac{i}{4}C^TGC\Big]A(C)\Big), \tag{2.28}$$

can be seen as calculating averages with Gaussian distributions for thermal states in the coherent states path integral representation[4]

$$\int D\eta\,\exp\Big(\frac{i}{2}\eta^TG\eta\Big)A(\eta), \tag{2.29}$$

where η are Grassmann variables. It's easy to see that the average of a polynomial operator can be obtained by taking derivatives with respect θ of the integral

$$\int D\eta\,\exp\Big(\eta^T\theta+\frac{i}{2}\eta^TG\eta\Big) = i^n\mathrm{Pf(G)}\cdot\exp\Big(-\frac{i}{2}\theta^TG^{-1}\theta\Big). \tag{2.30}$$

$\mathrm{Pf}(G)$ stands for the Pfaffian of the antisymmetric matrix G, i.e.,

$$\mathrm{Pf}(G) = \sum_\pi{}'\mathrm{sig}(\pi)G_{\pi(1),\pi(2)}\dots G_{\pi(2M-1),\pi(2M)}, \tag{2.31}$$

where $\sum'_\pi$ is the sum over permutations π that satisfy $\pi(1)<\pi(3)<\cdots<\pi(2M-1)$ and $\pi(2j-1)<\pi(2j)$, and $\mathrm{sig}(\pi)$ is the signature of π. For antisymmetric matrices it fulfills $\mathrm{Pf}^2(G)=\det(G)$.

Therefore as in the case of Gaussian probability distributions, that are completely defined by the mean and variance, it makes sense to define the so-called *covariance matrix*(CM) which in the Majorana representation takes the form

$$\Big(\Gamma_M\Big)_{pq} = \frac{i}{2}\mathrm{Tr}\Big(\rho[c_p,c_q]\Big) \tag{2.32}$$

and it's a real antisymmetric matrix, i.e., $\Gamma_M^T=-\Gamma_M$.

Consider the monomial

$$c(\mathbf{x}) = c_1^{x_1}\dots c_{2M}^{x_{2M}}, \tag{2.33}$$

where $\mathbf{x}=(x_1,\dots,x_{2M})$ is a binary string of $2M$ bits with length $|\mathbf{x}|=\sum_k x_k$. An arbitrary linear operator on $\mathcal{F}(\mathcal{H})$ can be represented as a linear combination of these monomials.

[4]This route to define FGS via Grassmann variables is followed in [**Bravyi**], and it's known as Lagrangian formulation of FGS.

Theorem 2.3.1 (Wick's theorem)**.** *Let ρ be an even FGS. Then for any even binary string $\mathbf{x} \in \{0,1\}^{2M}$, $|\mathbf{x}| = 2l$, one has*

$$Tr(\rho c(\mathbf{x})) = i^l Pf(\Gamma_M[\mathbf{x}]), \tag{2.34}$$

where $\Gamma_M[\mathbf{x}]$ is a $2l \times 2l$ submatrix of Γ_M obtained by selecting all matrix elements $\left(\Gamma_M\right)_{pq}$ for which $x_p = x_q = 1$. On the other hand all odd correlators vanish,

$$Tr(\rho c(\mathbf{x})) = 0 \text{ whenever } |\mathbf{x}| = 2l + 1. \tag{2.35}$$

Proof. A discussion of this result can be found in [22] and a proof in [**Bravyi**], in the Lagrangian formulation of fermionic systems. Its proof is also found as a corollary of Wick's product identity expansion for pure Gaussian states explained in Appendix A. □

Remark In order to prove Wick's theorem the assumption of the Gaussian state to be even is not necessary to obtain the first result (2.34) but only for the second.

This result Equation 2.34 motivates an alternative definition of FGS.

Definition 2.3.3. Fermionic Gaussian states are those satisfying Wick's theorem.

2.3.1. Covariance matrix

Let's start reviewing the matrix structure of the already defined Majorana CM, given by (2.32) and its definition in the complex representation. Let's use the notation $\mathrm{Tr}\rho A = \langle A \rangle$ with A an operator. In terms of ϕ's and $\phi^\dagger$'s the covariance matrix is defined as

$$\Gamma = \left\langle \Phi, \Phi^\dagger \right\rangle = \begin{pmatrix} \langle \phi\phi^\dagger \rangle & \langle \phi\phi \rangle \\ \langle \phi^\dagger\phi^\dagger \rangle & \langle \phi^\dagger\phi \rangle \end{pmatrix} \equiv \begin{pmatrix} \mathbb{1}_M - \gamma^T & \alpha \\ \alpha^\dagger & \gamma \end{pmatrix}, \tag{2.36}$$

i.e., a Hermitian matrix where we have defined the $M \times M$ matrices $\gamma := \langle \phi^\dagger\phi \rangle$ with $\gamma^\dagger = \gamma$ and $\alpha := \langle \phi\phi \rangle$ such that $\alpha^T = -\alpha$. Γ_M and Γ are related via

$$\Gamma = \frac{1}{2}\mathbb{1}_{2M} - i\frac{1}{4}W^\dagger \Gamma_M W, \tag{2.37}$$

with W given by (2.10).

Remark. Wick's theorem 2.34 takes the same form when written in terms of creation and annihilation operators

$$\left\langle \phi_1^\sharp \dots \phi_{2l}^\sharp \right\rangle = \sum_\pi {}' \mathrm{sig}(\pi) \left\langle \phi_{\pi(1)}^\sharp \phi_{\pi(2)}^\sharp \right\rangle \dots \left\langle \phi_{\pi(2l-1)}^\sharp \phi_{\pi(2l)}^\sharp \right\rangle, \tag{2.38}$$

where $\left\langle \phi_{\pi(2j-1)}^\sharp \phi_{\pi(2j)}^\sharp \right\rangle$ are elements of Γ. Moreover $\left\langle \phi_1^\sharp \dots \phi_{2l+1}^\sharp \right\rangle = 0$ for even FGS.

In particular we will often use the important formula

$$\left\langle \phi_k^\dagger \phi_l^\dagger \phi_m \phi_n \right\rangle = \left\langle \phi_k^\dagger \phi_l^\dagger \right\rangle \langle \phi_m \phi_n \rangle - \left\langle \phi_k^\dagger \phi_m \right\rangle \left\langle \phi_l^\dagger \phi_n \right\rangle + \left\langle \phi_k^\dagger \phi_n \right\rangle \left\langle \phi_l^\dagger \phi_m \right\rangle, \tag{2.39}$$

which if applied to the expectation value of the two-body potential, these terms correspond to the pairing, exchange and direct channels.

The description of ρ via its covariance matrix is not only convenient due to Wick's result but also because of the observation we made in section 2.2.1. As we saw in (2.18) evolutions generated by quadratic Hamiltonians simply generate a linear canonical transformation $\Phi_i \to \sum_j (e^{-i\mathcal{H}t})_{ij}\Phi_j$ in the Heisenberg picture and therefore because of (2.36)

$$\Gamma \longrightarrow e^{-i\mathcal{H}t}\,\Gamma\, e^{i\mathcal{H}t} \Longrightarrow i\frac{d}{dt}\Gamma = [\mathcal{H}, \Gamma] \tag{2.40}$$

in the Schrödinger picture. Then from the own definition of Gaussian state (2.3.2) and observations 2.2.1 and (2.40) we can deduce

Corollary. *The set of FGS is invariant under Bogoliubov transformations, among which evolutions under quadratic Hamiltonians are contained. This means that Bogoliubov transformations map Gaussian states into Gaussian states. Moreover evolutions under quadratic Hamiltonians can be completely described by the covariance matrix.*

Therefore the covariance matrix plays a really relevant role in the discussion of Gaussian states. Since our goal is to use Gaussian states as variational states, we need to find the set of admissible covariance matrices [**Bravyi2**].

Admissible covariance matrices

Since Γ completely characterized ρ, Γ must be chosen in order to fulfill:

$$(1)\ \rho \geq 0 \text{ non-negativity of } \rho \tag{2.41}$$

$$(2)\ \rho = \rho^\dagger \text{ Hermiticity} \tag{2.42}$$

$$(3)\ \rho^2 = \rho \text{ if } \rho \text{ is a pure FGS.}, \tag{2.43}$$

since $\mathrm{Tr}(\rho) = 1$ can be achieved via a normalization factor. From the standard form ρ_λ of FGS

$$\rho_\lambda = \frac{1}{2^M}\prod_{j=1}^{M}\left(\hat{\mathbb{1}} - i\lambda_j c_{2j-1}c_{2j}\right), \tag{2.44}$$

one can derive from conditions (1) and (2) in (2.41) that

$$\lambda_j \in [-1, 1], \qquad j = 1, \ldots, M, \tag{2.45}$$

and that a state is pure if and only if $\lambda_j = \pm 1$ for all j's. In fact the density operator of the Fock vacuum is given by (2.44) with all $\lambda_j = 1$.[5] The connection to the covariance matrix is given by the following lemma:

[5] Note that in the complex representation

$$\rho_1 = \prod_k^M \phi_k \phi_k^\dagger$$

and therefore is annihilated by al ϕ_k acting from the left and $\phi_k^\dagger$ acting from the right.

Lemma 2.3.2. *A real antisymmetric matrix Γ_M is a covariance matrix of an even FGS if and only if*

$$\Gamma_M^T \Gamma_M \leq \mathbb{1}_{2M} \quad \text{or equivalently} \quad i\Gamma_M \leq \mathbb{1}_{2M} \tag{2.46}$$

The corresponding state is pure if and only if $\Gamma_M^T \Gamma_M = \mathbb{1}_{2M}$. Since $\Gamma_M^T = -\Gamma_M$ this result can also be written as $\Gamma_M^2 = -\mathbb{1}_{2M}$.

Proof. A proof of this result can be found in [**Bravyi**]. □

In terms of Γ the lemma can be stated as follows

Lemma 2.3.3. *A Hermitian matrix Γ is a covariance matrix of an even FGS if and only if*

$$0 \leq \Gamma \leq \mathbb{1}_{2M}. \tag{2.47}$$

The corresponding state is pure if and only if $\Gamma^2 = \Gamma$.

The condition $\Gamma^2 = \Gamma$ implies that Γ is a projector and therefore in general $\det(\Gamma) = 0$[6].

As we have already seen, the description of FGS is efficient via the covariance matrix since it scales quadratically in the number of modes. Moreover in order to further motivate the usefulness of this method, let us prove the already stated result that ground states of (fermionic or bosonic) quadratic Hamiltonians, are **pure** Gaussian states.

2.3.2. Ground state of quadratic Hamiltonians

Let's consider the quadratic Hamiltonian for a finite number of modes M

$$H = \sum_{i,j} A_{ij} \phi_i^\dagger \phi_j + \frac{1}{2} \sum_{i,j} (B_{ij} \phi_i^\dagger \phi_j^\dagger + B_{ij}^* \phi_j \phi_i), \tag{2.48}$$

with $A = A^\dagger$ and $B^T = -B$. We can rewrite it as

$$H = \frac{1}{2} \Phi^\dagger M \Phi + \frac{1}{2} \mathrm{Tr} A, \tag{2.49}$$

where for convenience we neglect the last constant term. Since M is Hermitian, it can be unitarily diagonalized $M = U^\dagger \Omega U$ and therefore H can be diagonalized by a Bogoliubov transformation $\mathcal{U}$, such that

$$\begin{pmatrix} \gamma \\ \gamma^\dagger \end{pmatrix} = U \begin{pmatrix} \phi \\ \phi^\dagger \end{pmatrix} = \mathcal{U} \begin{pmatrix} \phi \\ \phi^\dagger \end{pmatrix} \mathcal{U}^\dagger, \tag{2.50}$$

i.e., $\gamma_k = U_{kl} \Phi_l$. Then

$$H = \frac{1}{2} (\gamma^\dagger, \gamma) \Omega \begin{pmatrix} \gamma \\ \gamma^\dagger \end{pmatrix} \tag{2.51}$$

where Ω is a $2M \times 2M$ diagonal matrix which can be showed to take the form [28]

$$\Omega = \begin{pmatrix} \omega & 0 \\ 0 & -\omega \end{pmatrix} \quad \text{with } \omega \text{ a } M \times M \text{ diagonal matrix.} \tag{2.52}$$

[6] The only projector for which this is not true is for the identity matrix.

Then H can be written in terms of quasi-particle excitations as

$$H = \gamma^\dagger \omega \gamma - \frac{1}{2}\mathrm{Tr}\omega. \tag{2.53}$$

Let's assume ω has non-zero eigenvalues[7]. From (2.53) we see that the ground state of H is the vacuum state for γ_k, called $|\tilde{0}\rangle$, that is related to the vacuum state for ϕ_k via (2.50)

$$0 = \phi_k |0\rangle \Rightarrow 0 = \mathcal{U}\phi_k |0\rangle = \underbrace{\mathcal{U}\phi_k\mathcal{U}^\dagger}_{=U_{kl}\Phi_l}\mathcal{U}|0\rangle = \gamma_k \mathcal{U}|0\rangle \Rightarrow |\tilde{0}\rangle = \mathcal{U}|0\rangle . \tag{2.54}$$

Therefore the ground state of a general quadratic Hamiltonian is given by a Bogoliubov transformation applied to the vacuum, i.e., a pure Fermionic Gaussian state.[8]

2.4. Statement of the problem

With the use of the FGS machinery and the stated results for fermionic quadratic Hamiltonians, we would like to describe more difficult, interacting fermionic (and in general also bosonic) systems on a lattice. We consider Hamiltonians with free and two-body interacting terms of the form[9]

$$H = \sum_{i,j} t_{ij}\phi_i^\dagger \phi_j + \sum_{k,l,m,n} V_{kl;mn}\phi_k^\dagger \phi_l^\dagger \phi_m \phi_n, \tag{2.55}$$

with $t_{ij} = t_{ji}^*$, but in principle different polynomials in ϕ and $\phi^\dagger$ may be considered in the general setting [24].

In order to find the best approximation of the real ground state of H within the family of FGS, one should solve the minimization problem

$$\min_{\rho\in\,\mathrm{Gauss.}} E(\rho) = \min_{\Gamma\leq\mathbb{1}}\Big[\sum_{i,j} t_{ij}\gamma_{ij} + \sum_{k,l,m,n} V_{kl;mn}\Big(\gamma_{kn}\gamma_{lm} - \gamma_{km}\gamma_{ln} + \alpha_{kl}^\dagger\alpha_{mn}\Big)\Big], \tag{2.56}$$

with $E(\rho) = \mathrm{Tr}[H\rho]$.

In [22] it was obtained that the minimum ρ is attained when $\Gamma^2 = \Gamma$, i.e., when ρ is a pure FGS. Therefore characterizing ρ via the covariance matrix Γ, this result motivates to consider the mean-field (quadratic) **state-dependent** Hamiltonian

$$\begin{aligned} H_Q(\Gamma) := &\sum_{i,j} t_{ij}\gamma_{ij} + \sum_{k,l,m,n} V_{kl;mn}\Big(\gamma_{kn}\phi_l^\dagger\phi_m + \gamma_{nl}\phi_k^\dagger\phi_m - \gamma_{ml}\phi_k^\dagger\phi_n \\ &+ \gamma_{nk}\phi_l^\dagger\phi_m + \alpha_{lk}^\dagger\phi_n\phi_m + \alpha_{mn}\phi_k^\dagger\phi_l^\dagger\Big) \end{aligned} \tag{2.57}$$

that is consistent with the previous result and the already acquired knowledge about quadratic Hamiltonians:

[7] In the case where one or more eigenvalues, let's say n, of ω are zero, we would find a degenerate ground eigenspace $\{|\tilde{0}\rangle_i\}_{i=0}^n$. Each of these states are connected via Bogoliubov transformations to the ground states of (2.48).

[8] A similar proof is also valid for bosonic quadratic Hamiltonians [28].

[9] This is the kind of Hamiltonian we deal with in chapters 4 and 5.

Lemma 2.4.1. *If ρ is a FGS minimizer for H, then ρ is a true ground state for the Hamiltonian $H_Q(\Gamma)$.*

Proof. A proof of this result can be found in [22]. □

In general this constrained quadratic (in Γ) minimization problem is difficult to solve. As a first attempt, we could try to obtain the minimum via an imaginary time evolution but because of the exponential growth of the space of states with the number of modes 2^M, this is not efficient for large systems. Instead in [23], the authors proposed the idea to apply a **Gaussian approximation** via Wick's theorem to derive an imaginary-time evolution equation for the covariance matrix. In this way, as we have already explained, we reduced the number of variational parameters to $(2M)^2$. In fact this is the key idea of the Gaussian method and as we will see, it can also be applied to real-time dynamics. Because of Lemma 2.4.1, this method is equivalent to find an effective quadratic state-dependent Hamiltonian $H_Q(\Gamma)$ in such a way we remain within the variational set of Gaussian states. A systematic way to obtain $H_Q(\Gamma)$ via Wick's product identity [31] will be explicitly explained in Appendix A.

2.5. Time-dependent variational ansatz

In this section we present the ideas already introduced in [23, 24].

Even if the physical picture in complex representation is "easier", for simplicity we express the Hamiltonian (2.55) in the Majorana picture which allows quite shorter expressions in terms of c_k's. Moreover we also ease the notation denoting $\Gamma = \Gamma_M$ in this section.

$$H(T,U) = i\sum_{i,j} T_{ij}c_i c_j + \sum_{k,l,m,n} U_{klmn}c_k c_l c_m c_n \tag{2.58}$$

with T_{ij}, $U_{klmn} \in \mathbb{R}$ and $T^T = -T$ while U is anti-symmetric under the exchange of any two adjacent indices. Moreover in this picture the minimization problem (2.56) takes the form

$$\min_{\rho\in \text{Gauss.}} E(\rho) = \min_{i\Gamma\leq \mathbb{1}} \Big[\sum_{i,j} T_{ij}\Gamma_{ij} - 3\sum_{k,l,m,n} U_{klmn}\Gamma_{kl}\Gamma_{mn}\Big] \tag{2.59}$$

and the mean field Hamiltonian (2.57)[10]

$$H_Q(\Gamma) = i\sum_{i,j} T_{ij}c_i c_j + 6i\sum_{i,j,m,n} U_{ijmn}\Gamma_{nm}c_i c_j = i\frac{1}{4}\sum_{i,j} c_i \mathcal{H}(\Gamma)_{ij}c_j, \tag{2.60}$$

with the antisymmetric single particle Hamiltonian

$$\mathcal{H}(\Gamma)_{ij} = 4(T_{ij} + 6\text{Tr}_B[U\Gamma]_{ij}) \tag{2.61}$$

where we have defined $\text{Tr}_B[U\Gamma]_{ij} := \sum_{m,n} U_{ijmn}\Gamma_{nm}$.

In [23] the necessary conditions for a **local minimun** are also derived via Lagrange multipliers and are given by

$$[\mathcal{H}(\Gamma),\Gamma] = 0, \qquad \Gamma^2 = -\mathbb{1}, \tag{2.62}$$

[10] The factor 1/4 appearing in (2.60) is introduced in order to obtain a mean field Hamiltonian in the complex representation of the form $1/2\Phi^\dagger\mathcal{H}(\Gamma)\Phi$.

where the second condition coincides with our previous knowledge. Since (2.62) is in general hard to solve let us introduce the variational method in order to find the ground state.

2.5.1. Imaginary-time evolution: ground state

Consider an arbitrary Gaussian state $\rho(0)$ and evolve it according to

$$\rho(\tau) = \frac{e^{-H\tau}\rho(0)e^{-H\tau}}{\mathrm{Tr}[e^{-2H\tau}\rho(0)]}, \tag{2.63}$$

where τ is the imaginary time. For pure states this equation takes the following form

$$|\psi(\tau)\rangle = \frac{e^{-H\tau}\,|\psi(0)\rangle}{\sqrt{\langle\psi(0)|\; e^{-2H\tau}|\,\psi(0)\rangle}}, \tag{2.64}$$

where the appearance of the denominator is crucial in the following derivation. Note that this doesn't correspond to the usual replacing $it \to \tau$, but as it was proved in [23] leads to the desired ground state.

Observation. Let's give a brief proof to show that one can obtain the ground state of the Hamiltonian H by taking the limit $\tau \to \infty$. Let's assume H has a non-degenerate spectrum $\{E_n\}$ with eigenvectors $\{|\phi_n\rangle\}$ and shift the energy scale such that the ground state energy is shifted to zero, i.e., $H\,|\phi_0\rangle = 0$. Then writing $|\psi(0)\rangle = \sum_n c_n\,|\phi_n\rangle$ restricted to the fact that $\langle\phi_0|\;\psi(0)\rangle = c_0 \neq 0$ we find

$$|\psi(\tau)\rangle = \frac{\sum_n e^{-E_n\tau}c_n\,|\phi_n\rangle}{\sqrt{\sum_n e^{-2E_n\tau}\,|c_n|^2}} \overset{\tau\to\infty}{\longrightarrow} \frac{c_0\,|\phi_0\rangle}{|c_0|}. \tag{2.65}$$

We then obtain the ground state of H if the initial state has non-zero overlap with it. In case the ground state is degenerate we arrive to one or another ground state or a linear superposition of those depending on the choice of the initial state$|\psi(0)\rangle$. As we will see in chapter 4, this fact will be important to characterize quantum phase transitions with the mean field approximation.

In general if we consider a non-quadratic Hamiltonian H, the evolution for the Gaussian state $\rho(0)$ given by (2.63), takes us out of the Gaussian variational family. One possible solution is to use instead the corresponding quadratic Hamiltonian $H_Q(\Gamma)$, that being quadratic will keep us in the Gaussian setting. One could also consider the whole interacting Hamiltonian H and project on each step of the evolution on the Gaussian family by application of Wick's theorem. In [23] the authors proved that these two methods and the direct minimization of (2.59) are equivalent to each other, i.e., one finds the same necessary conditions (2.62) for a steady state of a system under imaginary time evolution.

From (2.63) we can obtain the equation for ρ for any Hamiltonian H

$$\frac{d}{d\tau}\rho(\tau) = -\{H, \rho(\tau)\} + 2\rho(\tau)\mathrm{Tr}[H\rho(\tau)], \tag{2.66}$$

where we can realize that non-quadratic terms in H will leave the tangent space to the Gaussian manifold spanned by quadratic operators as derived in [24]. From here we obtain the equation for the covariance matrix

$$\frac{d}{d\tau}\Gamma_{kl}(\tau) = -i\mathrm{Tr}[\{H, c_k c_l\}\rho(\tau)] + 2\Gamma_{kl}\mathrm{Tr}[H\rho(\tau)]. \tag{2.67}$$

Now either directly applying Wick's theorem or considering H_Q instead of H, one finds

$$\frac{d}{d\tau}\Gamma = -\Big[\Gamma\mathcal{H}(\Gamma)\Gamma + \mathcal{H}(\Gamma)\Big], \tag{2.68}$$

that can be numerically integrated as we have done for the practical analysis in chapter 4.

We can deduce that the evolution equation (2.68) gives a consistent method in order to obtain the approximating FGS of H via imaginary time evolution:

- From (2.68) is easy to show that a **pure state remains pure under the evolution**, i.e., $\Gamma^2 = -\mathbb{1}$.
- On pure Gaussian states, the energy always decreases

  $$\frac{d}{d\tau}E(\rho) = \frac{1}{8}\mathrm{Tr}[([\mathcal{H}(\Gamma), \Gamma])^2] \leq 0 \tag{2.69}$$

  due to the antisymmetry of $[\mathcal{H}(\Gamma), \Gamma]$, Γ and $\mathcal{H}(\Gamma)$. From here we realize the same condition for a local minimum as the one appearing in (2.59), i.e., $[\mathcal{H}(\Gamma), \Gamma] = 0$.

Therefore choosing a pure state as initial seed $\Gamma(0)^2 = -\mathbb{1}$ and numerically integrating (2.68) till verify the energy does not decrease (minimum), one solves the minimization problem (2.59).

2.5.2. Real-time evolution

Following the same ideas and as we already found in the Observation 2.2.1 for the evolution under quadratic Hamiltonians, we can also derive a real-time evolution equation for Γ generated by $H_Q(\Gamma)$ which ensures we remain in the Gaussian manifold. In this case the evolution is given by

$$\frac{d}{dt}\Gamma(t) = [\mathcal{H}(\Gamma), \Gamma], \tag{2.70}$$

as we already found in (2.18). A formal derivation of this result and the equivalence between the evolution under H_Q and the Gaussian approximation can be found in [23].

Moreover this evolution conserves the average energy $E(\rho)$

$$\frac{d}{dt}E(t) = \frac{1}{4}\mathrm{Tr}[\mathcal{H}(\Gamma)[\mathcal{H}(\Gamma), \Gamma]] = 0, \tag{2.71}$$

and the average of the particle-number operator $N = \left\langle \hat{N} \right\rangle_{G.S}$ if the Hamiltonian is number-conserving, i.e., $[H, \hat{N}] = 0$

$$\frac{d}{dt}N(t) = -i\mathrm{Tr}[\rho[\hat{N}, H]] = 0 \tag{2.72}$$

as obtained in [23].

Remark. While the real-time evolution conserves $N(t)$, that's not the case in general for the imaginary time evolution as it can be seen with the following counterexample. Let's consider the one mode Hamiltonian $H = \hat{N} + \hat{N}^2$ with $\hat{N} = a^\dagger a$. Obviously $[H, \hat{N}] = 0$ and its ground state is given by the vacuum state $|0\rangle$ that is a Gaussian state. Let's choose as $|\psi(0)\rangle$ the coherent state $|\alpha\rangle$ with phase $\alpha \neq 0$. Then while $N(0) = |\alpha|^2 \neq 0$ at the beginning of the imaginary-time evolution $N(\infty) = 0$ at the end. The only case where a symmetry U of the Hamiltonian is conserved along the evolution is when considering an eigenstate of such symmetry as the initial state.

2.5.3. Operational approach

Once the method and the mathematical structure has been introduced, its application to a physical system can be done as follows. We work in Nambu representation with creation and annihilation operators[11]. where the evolution equations for the covariance matrix take the form

$$\frac{d}{d\tau}\Gamma = \{\Gamma, \mathcal{H}(\Gamma)\} - 2\Gamma\mathcal{H}(\Gamma)\Gamma, \tag{2.73}$$

$$\frac{d}{dt}\Gamma = [\mathcal{H}(\Gamma), \Gamma]. \tag{2.74}$$

We have proved that the ground state and real-time dynamics of the system can be described within the set of pure Gaussian states:

$$e^{\frac{i}{2}\Phi^\dagger \xi_f \Phi} |0\rangle . \tag{2.75}$$

Elements of the corresponding covariance matrix $\Gamma_{ij} = \left\langle \Phi_i \Phi_j^\dagger \right\rangle$ are considered as the set of variational parameters for which one needs to find the best approximation to the real ground state or dynamics[12]. Therefore in order to apply the Gaussian method one must follow the following steps:

1. Given a non-quadratic Hamiltonian H derive the effective state-dependent Hamiltonian $H_Q(\Gamma)$ and from it the single particle Hamiltonian $\mathcal{H}(\Gamma)$. To do so, one can use the method introduced in the Appendix A or compute $\langle H \rangle$ and take derivatives with respect to Γ such that $\mathcal{H}(\Gamma)_{ij} = -2\partial \langle H \rangle / \partial \Gamma_{ij}$ as stated in [24].

2. Choose an admissible initial seed $\Gamma(0)$ for the evolution equations given by (2.73) and (2.74). If one wants to find the best approximation to the ground state of H, the initial seed should have a non-zero overlap with the real ground state and can be taken to be pure. Otherwise the integration of (2.73) doesn't give the correct result in the limit $\tau \to \infty$. It could happen one gets stuck in a local minimum, reason why one needs to consider different initial seeds and ensure the evolution actually arrives to the global minimum.

[11] We will see the convenience of this picture in chapter 4.

[12] Equivalently one could also consider ξ_f as the variational parameter, since Γ and ξ_f are related via

$$\frac{1}{2}\mathbb{1}_{2M} + \frac{1}{2}U_f(\sigma_z \otimes \mathbb{1}_M)U_f^\dagger$$

with $U_f = e^{i\xi_f}$.

3. On the other hand if the real-time evolution wants to be studied, just fix the initial seed to mimic an initial physical configuration and solve the corresponding initial value problem.

4. As a result one obtains a covariance matrix at a given time τ/t. In the case of imaginary-time evolution this is the covariance matrix describing the ground state $\Gamma(\tau \to \infty)$. From Γ, averages of all observables in the system can be computed.

Therefore the Gaussian ansatz has the advantage to include all the two-point correlators (correlators for all kind of fermionic pairs), thus taking into account all the possible mean-field order parameters characterizing a system, like for example in the superconducting phase where $\Delta_0 = \sum_{\vec{k}} \left\langle c_{\vec{k},\uparrow} c_{-\vec{k},\downarrow} \right\rangle$ is just an element of the covariance matrix. This would be equivalent to consider at the same time different Hubbard-Stratonovich transformations for different channels, maybe coupled to each other in the path integral approach. This advantage has been successfully exploited to the study of the quantum phase transition between the superconducting and charge density wave (CDW) phases in the Holstein model among other systems in [24].

2.6. General variational method

The method we have described so far is part of a more general theory that has been recently formulated "Variational Study of Fermionic and Bosonic Systems with Non-Gaussian States: Theory and Applications" [24], that generalizes the results found in [23]. This theory enlarge the variational ansatz, including all possible fermionic and bosonic Gaussian states as well as the family of states which go beyond the Gaussian setting, non-Gaussian states. Moreover the method can be used to study any Hamiltonian that is an any order polynomial in terms of creation and annihilation, fermionic and/or bosonic operators. In order to do so, the authors derive the evolution equations for the covariance matrix from a geometrical point of view in the variational parameter manifold based on [32]. Apart from the ground state description, for which they also consider equation (2.64), this method also provides a way to study fluctuations around the mean-field Gaussian state both single-particle Bogoliubov excitations and collective ones. The method has been proved to be of great use to describe many physical systems with both fermionic and bosonic degrees of freedom.

Therefore let's briefly introduce the overall picture with the different ingredients which could play a role.

2.6.1. Bosonic Gaussian states

This section will follow the discussion in [19, 20, 25, 28]. Bosonic Gaussian states (BGS) also play an important role in physics. Apart from being eigenstates of annihilation operators —coherent states—, which are usually used in Quantum Optics, Quantum Field Theory and Condensed Matter physics among other branches; they are ground and thermal states of quadratic Hamiltonians like in the fermionic case. Moreover, BGS are also relevant because they admit a powerful phase space description which enables to study quantum many-body problems that are otherwise intractable [25].

This section is thought to provide the minimal mathematical background to understand some related results in chapter 4 and the Outlook. That's the reason we will avoid a technical and detailed discussion (Weyl systems, characteristic and Wigner functions etc) and will focus on the most intuitive explanation along the ideas we've developed in previous sections. Nevertheless a complete introduction to these topics can be found in [20].

The root of this description comes from the "problematic" $[X, P] = i\hbar$ (Weyl representation). Consider a system of M bosonic modes characterized by the operators a_l and $a_l^\dagger$ fulfilling the CCR

$$[a_l, a_k^\dagger] = \delta_{l,k}, \qquad [a_l, a_k] = 0. \tag{2.76}$$

The system can be equivalently described in terms of the quadratures

$$X_l = \frac{1}{\sqrt{2}}(a_l^\dagger + a_l), \qquad P_l = \frac{i}{\sqrt{2}}(a_l^\dagger - a_l), \tag{2.77}$$

with commutation relations

$$[X_k, P_l] = i\delta_{k,l}. \tag{2.78}$$

Defining $R_k = X_k$ and $R_{M+k} = P_k$, these CCR can be written as

$$[R_k, R_l] = i\sigma_{kl}\hat{\mathbb{1}} \quad \text{with} \quad \sigma = \begin{pmatrix} 0 & \mathbb{1}_M \\ -\mathbb{1}_M & 0 \end{pmatrix}. \tag{2.79}$$

Let's define the Weyl operator $\mathcal{W}(\eta)$ with $\eta \in \mathbb{R}^{2M}$ by

$$\mathcal{W}(\eta) = e^{-i\eta^T R}. \tag{2.80}$$

Definition 2.6.1 (Characteristic function)**.** The characteristic function of a state ρ is defined by

$$\chi(x) = \mathrm{Tr}[\rho\mathcal{W}(x)]. \tag{2.81}$$

In fact,

$$\rho = \frac{1}{(2\pi)^M}\int_{\mathbb{R}^{2M}} dx\, \chi(x)\mathcal{W}(-x). \tag{2.82}$$

Definition 2.6.2 (BGS)**.** A state ρ is called Gaussian if its characteristic function is a Gaussian, i.e.,

$$\chi(x) = \exp\Big[-\frac{1}{4}x^T\Gamma_b x + id^T x\Big] \tag{2.83}$$

for a real, strictly positive, symmetric $2M \times 2M$ matrix Γ_b and $d \in \mathbb{R}^{2M}$.

Similar to FGS, bosonic Gaussian states are fully characterized by their second and first moments of quadratures via Wick's theorem, and can be collected in a matrix form

$$\Big(\Gamma_b\Big)_{k,l} = \mathrm{Tr}[\rho\{R_k - d_k, R_l - d_l\}] \equiv \mathrm{Tr}[\rho\{\delta R_k, \delta R_l\}] \tag{2.84}$$

with the displacement d_k given by

$$d_k = \mathrm{Tr}[\rho R_k], \tag{2.85}$$

that in general is different from zero. Examples of bosonic Gaussian states with one mode are given by[13]: the bosonic vacuum state $|0\rangle$ ($\Gamma_b = \mathbb{1}$ and $d = 0$), coherent states $|\alpha\rangle$ with $\alpha \in \mathbb{C}$ ($\Gamma_b = \mathbb{1}$ and $d = \sqrt{2}(\mathrm{Re}\alpha, \mathrm{Im}\alpha)^T$) and squeezed states.

[13] This example is taken from [19].

Remark. Note that all moments in quadratures can be obtained from the characteristic function $\chi(x)$ by taking derivatives w.r.t x and evaluating at $x = 0$. With this observation and via equation (2.83), the proof of Wick's theorem in the bosonic setting is clear.

In this case an admissible covariance matrix must fulfill the condition $\Gamma_b \geq i\sigma$. Moreover a state is pure if and only if $\det(\Gamma_b) = 1$ or equivalently $\Gamma_b = S^T S$ for some symplectic matrix $S \in Sp(2M)$, given by the set of matrices S such that $S\sigma S^T = \sigma$. As in the fermionic case, pure bosonic Gaussian states can be obtained applying a Bogoliubov transformation to the vacuum state

$$e^{\frac{i}{2}\langle R\rangle^T \sigma R} e^{-\frac{i}{4}R^T \xi_b R} |0\rangle , \tag{2.86}$$

with ξ_b a real symmetric matrix. The only difference is the appearance of the displacement operator $e^{\frac{i}{2}R^T\sigma\langle R\rangle}$, generated by linear terms in R. We refer the reader to Ref. [19] for details.

Analogously to the fermionic case, the method described in the Appendix A can also be applied to obtain $H_Q(\Gamma_b, \langle R\rangle)$ where additional linear terms in quadratures may appear unlike in the fermionic case where they were banned by the parity superselection rule:

$$H_Q(\Gamma_b, \langle R\rangle) = \frac{1}{2}\eta_H^T \delta R + \frac{1}{4}\delta R^T \Omega_H \delta R, \tag{2.87}$$

with $\eta_H^i := \partial \langle H\rangle / \partial \langle R\rangle_i$ and $(\Omega_H)_{ij} = 4\partial \langle H\rangle / \partial(\Gamma_b)_{ij}$.

In [24], evolution equations for Γ_b and d for both real and imaginary evolutions have been derived taking the form

$$\frac{d}{d\tau}\Gamma_b = \sigma^T \Omega_H \sigma - \Gamma_b \Omega_H \Gamma, \qquad \frac{d}{d\tau}\langle R\rangle = -\Gamma_b \eta_H \tag{2.88}$$

$$\frac{d}{dt}\Gamma_b = \sigma^T \Omega_H \Gamma_b - \Gamma_b \Omega_H \sigma, \qquad \frac{d}{dt}\langle R\rangle = \sigma \eta_H. \tag{2.89}$$

This has allowed us to attempt the description of (2+1)-dimensional pure gauge theories in the strong coupling limit in the first section of the Outlook.

2.6.2. Non-Gaussian ansatz

Once bosonic Gaussian states have been included one can consider the general Gaussian ansatz

$$|\psi(\xi)\rangle = e^{i\theta} e^{\frac{1}{2}\langle R\rangle^T \sigma R} e^{-\frac{i}{4}R^T \xi_b R} e^{\frac{i}{2}\Phi^\dagger \xi_f \Phi} |0\rangle , \tag{2.90}$$

that is a product state with respect bosonic and fermionic operators.

Therefore (2.90) does not introduce any correlations between bosons and fermions and it's not sufficient to describe many physical situations. Thus we would like to extend the variational manifold in such a way we can include correlations and entanglement between the bosonic and fermionic modes and to go beyond Wick's theorem. In order to do so, we can extend the variational ansatz by multiplying the variational states (2.90) with an operator $\mathcal{U}_S$ that is not Gaussian and can couple fermionic and bosonic degrees of freedom, which will introduce more variational parameters. We will see an example of this kind of transformations in chapters 4 and 5.

2.7. Summary and conclusion

We have introduced Gaussian states which present the remarkable advantage of being completely characterized by their covariance matrix and first order distribution moments which allows to efficiently describe quantum many-body systems. This has let us develop a time-dependent variational approximation method to describe the real and imaginary time evolution of interacting systems. On the one hand we are able to find the best approximation to the ground state via numerical integration and on the other hand, real-time dynamics are also possible. Nevertheless we have assumed a pure Gaussian state that is a product state for bosons and fermions and will in general need a further non-Gaussian transformation on it.

3. Lattice Gauge Theories

In this chapter, we firstly introduce non-Abelian gauge theories in the continuum [2]. Then an introduction to Lattice Gauge Theories [4, 33] in the Kogut-Susskind Hamiltonian formulation will be presented [7]. We will pay special attention to the underlying Hilbert space for both the gauge and fermionic fields and the generators of time-independent gauge transformations in the temporal gauge $A_0 = 0$, that turns out to be the most suitable for this formulation. We will finally study the phenomenon of confinement.

3.1. Introduction

As we explained in the introductory chapter, Lattice Gauge Theories (LGT) provides the most powerful approach to describe non-perturbative phenomena in particle physics. In spite of the fact that the formulation of gauge theories on a lattice loses the continuous spacetime symmetries as Lorentz invariance, it allows an exact implementation of the gauge symmetry for all lattice spacings. This important fact gives rise to the possibility of studying the special consequences of non-Abelian gauge theories, as for example confinement is believed to be.

On the other hand, the alternative Hamiltonian formulation of LGT by Kogut and Susskind [7], gives rise to a second quantized lattice Hamiltonian with fermions living on the sites and gauge fields on the links of the lattice as it happens in Condensed Matter Hamiltonians. This suggests the possibility to apply already known methods from other branches of physics like the time-dependent Gaussian variational method introduced in the previous chapter, that has been so far only applied to condensed matter systems.

Therefore in this chapter, after a brief introduction of the standard formulation of LGT by Wilson, we will focus on the Hamiltonian formulation. In spite of the fact one could obtain one from the other via the transfer matrix method [34], we will construct the quantized Hamiltonian from scratch. We will encounter different subtleties with which one has to deal when placing fermions on a lattice. This formulation will provide us with a way to construct the underlying Hilbert space for both fermionic and gauge degrees of freedom, as well as introduced the concept of confinement via the potential between two static charges. Unlike the standard formulation of LGT, this potential does not need to deduced from the so-called Wilson's loop but it can obtained as the ground state energy for a given configuration of static charges.

3.2. Continuum formulation

In this thesis we will look at theories having a local symmetry under a symmetry transformation described by non-Abelian (or Abelian) compact Lie groups like $SU(N)$,

which appears in gauge theories for particle physics. In fact we will usually make reference and apply results to this specific group that as we will see now is quite suitable. Nevertheless, the analysis we will describe here is also valid for any other compact Lie group. Therefore let's review basic facts before stepping into the theory.

3.2.1. Facts in representation theory

Let's recall some important results from group and representation theory taken from [2, chap.15, App.A] and [35]:

1. A "physical" Lie algebra $\mathfrak{g}$ of a Lie group G, is a direct sum of compact, simple [1] and $U(1)$ subalgebras [2, 35]. Therefore without lost of generality one just needs to focus on compact simple Lie groups like $SU(N)$.

2. $\mathfrak{g}$ is connected to G via the exponential map $\exp : \mathfrak{g} \to G$.

3. We call $T^\alpha \in \mathfrak{g}$ the generators of G.

4. If G is a compact Lie group, every finite-dimensional representation $\Pi : G \to GL(V)$, with $V \cong \mathbb{R}^n, \mathbb{C}^n$ of G is completely reducible, i.e., if $g \in G$, $\Pi(g)$ isomorphic to a direct sum of a finite number of irreducible representations $\oplus_j D^j(g)$, where j denotes the irreducible representations of the group. The representations of the algebra will be denoted by $T^{\alpha,j}$.

5. Finite-dimensional representations of compact Lie groups are unitary, i.e.,
$$D^j_{ab}(g^{-1}) = D^{j,*}_{ba}(g). \tag{3.1}$$

6. For the previous case, there exists a basis for the generators T^α of $\mathfrak{g}$ such that the structure constants $f^{\alpha\beta\gamma}$, defined via
$$[T^\alpha, T^\beta] = i f^{\alpha\beta\gamma} T^\gamma, \tag{3.2}$$
are totally antisymmetric.

7. There is a unique representation π of $\mathfrak{g}$ acting on the same vector space V as Π such that $\Pi(e^X) = e^{\pi(X)}$ for all $X \in \mathfrak{g}$.

8. If G is a connected Lie group then Π is irreducible if only if π is irreducible.

9. The adjoint representation is the **real representation** given by
$$(T^\alpha_{Adj.})^{\beta\gamma} := i f^{\alpha\beta\gamma}, \tag{3.3}$$
and thus $D^{\text{Adj.}}(g)$ is an orthogonal matrix.

10. Spinor fields ψ have two kind of indices: group and spinor indices. Unless it's explicitly said, spinor indices will be omitted and write ψ_a to denote the group components for any spinor index.

[1] *compact* means that the group manifold is compact and *simple* means that there don't exist invariant subalgebras.

11. $SU(N)$ is a simple simply-connected compact Lie group for all N[2]. Moreover $\dim(SU(N)) = N^2 - 1$.

Moreover we also state the conventions and notations that will be used in the remaining of this thesis:

Conventions and notation:

- μ, ν denote spacetime coordinates, e.g., A_μ or $F_{\mu\nu}$.
- The convention for the spacetime metric is mostly negative, i.e., $ds^2 = dt^2 - d\vec{x}^2$.
- i, j, k denote spatial components, e.g., A_i or F_{ij}.
- j can also denotes a given representation of G as we saw.
- When considering non-Abelian gauge groups G, α, β, γ denote either a component of a gauge or strength field, e.g., (A^i_α and E^i_α); or a generator T^α of the associated algebra $\mathfrak{g}$. They will be indistinctly written as subscripts or superscripts.
- Group components in a given representation j are denoted by a, b, $c, \ldots$, e.g., ψ_a and $(T^\alpha)_{ab}$. Nevertheless components in the adjoint representation will be exceptionally denoted by α, β, γ.
- Einstein summation convention is assumed over repeated spacetime, spatial and group indices, i.e., $A^\alpha_\mu T^\alpha := \sum_\alpha^{\dim(\mathfrak{g})} A^\alpha_\mu T^\alpha$.
- The notation $\mathbf{B}$ will be often used to express the collection $\{B^\alpha\}$ when B is either an generator of the algebra, a matrix or an operator which depends on the α-index, e.g., $\mathbf{T} = \{T^\alpha\}$.

The fermionic matter content of the theory is given by spinorial fields $\psi(x)$ which belong to a given irreducible representation j of the group and thus have $dim(j)$ group components $\psi_a(x)$. These are equivalently called group, gauge or color components. Let's consider the Lagrangian density

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi = \bar{\psi}_a(i\gamma^\mu \partial_\mu - m)\delta_{a,b}\psi_b, \tag{3.4}$$

where $\delta_{a,b}$ is the Kronecker delta in group indices. This Lagrangian is invariant under a *global* "rotation" of color indices given by

$$\psi_a(x) \xrightarrow{h \in G} D^j_{ab}(h^{-1})\psi_b(x), \tag{3.5}$$

where $D^j(h)$ is a $dim(j) \times dim(j)$ matrix representation of the group element h. The transformation (3.5) is called global, since $D^j(h)$ does not depend on the space-time point x. As it happens in QED, a (symmetry) gauge principle dictates how to promote this symmetry to a local (gauge) one

$$\psi_a(x) \xrightarrow{h_x \in G} D^j_{ab}(h_x^{-1})\psi_b(x), \tag{3.6}$$

[2]We have non-projective representations of the group.

where now a different color rotation is applied at each spacetime point, leaving the system invariant. We restrict ourselves to unitary representations of the gauge group where $D^j(g)$ can be expressed as

$$D^j_{ab}(h_x) = \Big(\exp[ig\Lambda^\alpha_h(x)T^{\alpha,j}] \Big)_{ab}, \tag{3.7}$$

with $\{\Lambda^\alpha(x)\}$ a set of $dim(\mathfrak{g})$ functions and g a *coupling constant* we introduced for later convenience.

In order to build a (local) gauge invariant Lagrangian density, we introduce the *covariant derivative*

$$\delta_{a,b}\partial_\mu \longrightarrow (D_\mu)_{ab} = \delta_{a,b}\partial_\mu + ig(A_\mu)_{ab},$$

where A_μ is an algebra-valued gauge field — called *connection*— such that

$$A_\mu(x) = A^\alpha_\mu(x)T^\alpha \ \in \mathfrak{g}. \tag{3.8}$$

This procedure gives rise to the invariant Lagrangian density

$$\mathcal{L} = \bar\psi(i\gamma^\mu\partial_\mu - m)\psi - gA^\alpha_\mu j^\mu_\alpha, \tag{3.9}$$

where we have called $j^\mu_\alpha = \bar\psi\gamma^\mu T^\alpha\psi$. However this is not the most general possible Lagrangian density since we could also add invariant pure-gauge terms as well. Defining the *field strength* as

$$F_{\mu\nu} := \frac{-i}{g}[D_\mu, D_\nu] = \partial_\mu A_\nu - \partial_\nu A_\mu + ig[A_\mu, A_\nu] \ \in \ \mathfrak{g},$$

the kinetic term for the gauge fields is fixed by Lorentz, parity[3] and gauge symmetry as well as by renormalizability conditions [2] to be

$$\mathcal{L}_{Kin} = -\frac{1}{4}F_{\alpha,\mu\nu}F^{\mu\nu}_\alpha, \tag{3.10}$$

obtaining the Lagrangian density

$$\mathcal{L} = \bar\psi(i\not{\partial} - m)\psi - gA^\alpha_\mu j^\mu_\alpha - \frac{1}{4}F_{\alpha,\mu\nu}F^{\mu\nu}_\alpha. \tag{3.11}$$

A novel feature of non-Abelian gauge theories in comparison to QED, it's the fact that it is not possible to introduce a kinematic term for the gauge field A_μ without including interaction terms among the gauge fields, arising from the term in $F_{\mu\nu}$ given by $ig[A_\mu, A_\nu]$. This non-linearity is the responsible of many special features of non-Abelian gauge theories.

In order to quantize the theory, we first must derive the canonical conjugate momentum densities for the different fields

$$\Pi^\mu_\alpha = F^{\mu 0}_\alpha, \qquad \Pi_\psi = i\psi^\dagger, \tag{3.12}$$

from where we deduce

$$\Pi^0_\alpha = 0 \text{ and } \Pi^i_\alpha = E^i_\alpha, \tag{3.13}$$

[3] If parity symmetry or CP or T is not assumed one should include an additional quadratic term.

i.e., A^0_α is not a canonical variable and the constraint $\Pi^0_\alpha = 0$ must be fulfilled. For consistency we should also require $\partial_0 \Pi^0_\alpha = 0$, but then using the equation of motion for A^0_α

$$0 = \partial_0 \Pi^0_\alpha = \partial_0 \frac{\delta \mathcal{L}}{\delta(\partial_0 A^0_\alpha)} = -\partial_i \frac{\delta \mathcal{L}}{\delta(\partial_i A^0_\alpha)} + \frac{\delta \mathcal{L}}{\delta A^0_\alpha}. \tag{3.14}$$

and recalling that $\Pi^0_\alpha = 0$ we obtain

$$\begin{aligned} &\partial_i \Pi^i_\alpha - g f^{\gamma\alpha\beta} \Pi^i_\gamma A^i_\beta - g j^0_\alpha = 0 \\ &\Rightarrow \boxed{\partial_i E^i_\alpha = \mathcal{J}^0_\alpha \equiv g f^{\gamma\alpha\beta} E^i_\gamma A^i_\beta + g j^0_\alpha} \quad \alpha = 1, \ldots, dim(G), \end{aligned} \tag{3.15}$$

with i a spatial index.

We realize (3.15) is the non-Abelian version of Gauss' law where the first term on the right hand side is the color charge for the gauge field[4], i.e., it carries it own color charge, and the second is the fermionic color charge. On the other hand the left hand side is the divergence of the electric field related with the *local* rather than global aspect of the gauge symmetry. Note that unlike the Abelian case, there is a Gauss' law for each color component α, which are constraints that any possible field solution must fulfill [5].

In order to apply the canonical quantization procedure one needs to fix a gauge. As we will later see, the use of temporal (Weyl) gauge

$$A'_{0,\alpha} = A_{0,\alpha} - \partial_0 \Lambda_\alpha = 0 \tag{3.16}$$

is convenient for the Hamiltonian formulation of LGT [37]. This choice of gauge leaves remaining unphysical degrees of freedom [38, 39] as we will later see. The canonical variables are the spatial components A^i_α and their conjugate momenta. If the system were unconstrained, we would have just to promote the classical fields to quantum operators by setting equal time canonical commutation relations

$$[A^i_\alpha(x), E^j_\beta(y)] = i\delta^{i,j}\delta_{\alpha,\beta}\delta^{d-1}(x-y), \qquad \{\psi_a(x), \psi^\dagger_b(y)\} = \delta_{a,b}\delta^{d-1}(x-y) \tag{3.17}$$

$$[A^i_\alpha(x), A^j_\beta(y)] = 0, \qquad [E^i_\alpha(x), E^j_\beta(y)] = 0, \qquad \{\psi_a(x), \psi_b(y)\} = 0, \tag{3.18}$$

obtaining the quantum Hamiltonian

$$\begin{aligned} H = &\int d^{d-1}x\, \bar{\psi}\Big(\gamma^i(-i\partial_i) + m\Big)\psi + g A^\alpha_i j^i_\alpha + \frac{1}{2}E^i_\alpha E^i_\alpha + \frac{1}{4}F_{\alpha,ij}F^{ij}_\alpha \\ &- \cancel{A^\alpha_0}^{\,0}(\partial_i E^i_\alpha - g f^{\beta\alpha\gamma} A^i_\beta E^i_\gamma - g j^0_\alpha), \end{aligned} \tag{3.19}$$

[4] Applying Noether's theorem one obtains that the color charge $\mathcal{J}^0_\alpha$ is given by

$$\mathcal{J}^0_\alpha = f^{\gamma\alpha\beta} E^i_\gamma A^i_\beta + j^0_\alpha.$$

[5] This problem is one of constraints as introduced by Dirac [36] where $\Pi^0_\alpha = 0$ and (3.15) are first class constraints and therefore cannot be dealt with via Dirac brackets and therefore one has to fix the gauge.

i.e.,

$$H = \int d^{d-1}x\, \bar{\psi}\Big(\gamma^i(-i\partial_i) + m\Big)\psi + gA_i^\alpha j_\alpha^i + \frac{1}{2}(E_\alpha^i)^2 + \frac{1}{4}F_\alpha^{ij}F_\alpha^{ij}, \tag{3.20}$$

where one can identify the last term in (3.19) to be the non-Abelian Gauss' law (3.15). After fixing the temporal gauge, the Hamiltonian (3.20) is still invariant under *time-independent gauge transformations* which respect $A_\alpha^0 = 0$ and close a symmetry group, that will be called *spatial-gauge transformations*. Imposing Gauss' law as a constraint condition on *physical states* allows us to eliminate these remaining degrees of freedom.[6]. By doing so we are choosing a representative of the equivalence class of states related by gauge transformations.

Remark. Let's insist on the fact that both gauge and strength fields are algebra-value operators where, for example, $\{E_\beta^i\}$ denotes the quantum operator content and $E^i = E_\alpha^i T^\alpha$ would contain both the matrix and quantum operator structure.

Generators of time-independent gauge transformation

As we will see later, the identification of the generators of time-independent gauge transformations, are rather important for the construction of the physical Hilbert space.

In the classical field theory we obtained Gauss' law (3.15) from the equation of motion for A_α^0. Moreover for consistency one should also requires that $\partial_0^2\Pi_\alpha^0 = 0$, i.e., ensures that Gauss' law if fulfilled at all times. Indeed, using the conservation of charge densities $\partial_\mu \mathcal{J}_\alpha^\mu = 0$ one can prove that

$$\partial_0(\partial_i E_\alpha^i - \mathcal{J}_\alpha^0) = 0, \tag{3.21}$$

and then fulfilling (3.15) at $t = 0$ implies Gauss' law will hold at all times. We then see that Gauss' law is a *local constant of motion*, i.e.,

$$\{H, G_\alpha(x)\} = 0 \quad \forall\, x. \tag{3.22}$$

While (3.15) cannot be deduced from Hamilton equations of (3.20) both in classical and quantum field theory, alternatively one finds [39] (or can check) that the set of charge densities generating the spatial-gauge transformations[7] are given by

$$G_\alpha(x) = \partial_i E_\alpha^i - g j_\alpha^0 - g f^{\beta\alpha\gamma} A_\beta^i E_\gamma^i \quad \alpha = 1, \ldots, \dim(G), \tag{3.23}$$

that as we saw, are in fact local constants of motion[8]

$$[H, G_\alpha(x)] = 0 \quad \forall\, x \text{ and } \alpha = 1, \ldots, \dim(G), \tag{3.24}$$

[6] This method is known as Dirac quantization and it was introduced by Dirac in [36].
[7] These charges can be derived applying Noether's theorem to the remaining symmetry group [39].
[8] The proof we just followed is a circular reasoning since from the point of view of Dirac quantization, first class constraints are generators of gauge transformations.

and therefore can be simultaneously diagonalized with H.[9] Therefore the spatial-gauge transformation can be written as

$$\mathcal{V} = \exp\left[i \int d^{d-1}x\, \theta^{\alpha}(x) G_{\alpha}(x)\right], \tag{3.25}$$

as one can check by using (3.17). We will further discuss the interpretation of gauge symmetries and transformations in the discrete formulation of gauge theories, where the previously introduced concept of connection becomes clear. Therefore in order to erase the remaining gauge degrees of freedom we need to restrict the Hilbert space to gauge invariant states $|\psi\rangle$ fulfilling

$$\mathcal{V}\,|\psi\rangle = |\psi\rangle\,, \tag{3.26}$$

usually called *physical states*. These condition is equivalent to set

$$G_{\alpha}(x)\,|\psi\rangle = 0 \qquad \forall\, \alpha, \tag{3.27}$$

which defines a linear subspace known as *physical space of states*.

Remark. Using (3.17) one can check as an easy exercise applying the Baker-Campbell-Hausdorff formula that for the Abelian case, the gauge field $A_i(x)$ transforms under the spatial-gauge transformation as

$$e^{i\int d^{d-1}y\,\theta(y)\left(\partial_j E^j(y) - j^0(y)\right)} A_i(x) e^{-i\int d^{d-1}y\,\theta(y)\left(\partial_j E^j(y) - j^0(y)\right)} = A_i(x) \tag{3.28}$$
$$-\int d^{d-1}y\,\theta(y)\delta^{i,j}\partial_{y^j}\delta^d(x-y) = A_i(x) + \int d^{d-1}y\,\partial_{y^j}\theta(y)\delta^{i,j}\delta^d(x-y) = A_i(x) + \partial_i\theta(x).$$

3.3. Gauge theories on a lattice

In the standard formulation of LGT by Wilson [5], one replaces the continuum spacetime of a *Euclidean* quantum field theory with a d-dimensional hypercubic lattice ($\mathbb{Z}^d$) of spacetime points and links with lattice spacing a, which provides an ultraviolet cutoff. Although analytically the existence of such a cutoff is not really appealing, it allows strong-coupling calculations via, for example, simulation methods. This provides a way to understand non-perturbative phenomena like: quark confinement, hadronic spectrum and spontaneous breakdown of chiral symmetry in QCD; whose analytical understanding is still lacking. The lattice formulation of gauge theories, while losing spacetime symmetries of the original action, like Lorentz symmetry, allows to study the special effects of exact gauge invariance in strongly coupled theories [7], being the reason why it has attracted so much attention in other branches of physics like condensed matter. In fact this is also one of the goals of this thesis.

The idea is to discretize the original (Euclidean)[10] action in such a way one recovers the continuum theory as $a \to 0$ —keeping $V = a^d \cdot N$ constant being $N \to \infty$ the

[9] In spite the fact all charges commute with H, different $G'_{\alpha}s$ do not commute.

[10] By Euclidean action one means the obtained action after a Wick's rotation, i.e., from real to imaginary time, has been applied. This procedure allows the use of Monte Carlo techniques as well as further connections to Statistical Physics.

number of point in the lattice—

$$a^d \sum_{x \in \mathbb{Z}^d} \mathcal{L}(ax) \xrightarrow{a \to 0} \int d^d x \, \mathcal{L}(x) \tag{3.29}$$

with the restriction that for any value of the lattice spacing a, the **discrete action is gauge invariant**. This limit is called *classical continuum limit* as one assumes the fields are slowly varying on a length scale of the order of a [33][11]. There is also a necessary condition that the discretized action confines quarks in the strong coupling limit.

Let us set some conventions. An arbitrary point on the lattice is denoted by x and it's a Bravais lattice vector. On each site x, $2d$ lattice directions enter and leave the site. For example in 3 spatial dimensions, $\hat{x}$, $\hat{y}$, $\hat{z}$ and $-\hat{x}$, $-\hat{y}$, $-\hat{z}$. They will be called positive ($i > 0$) and negative ($i < 0$) orientated respectively and usually denoted with μ, ν if a spacetime lattice is considered or i,j if only a spatial lattice is considered as already explained in the adopted conventions section 3.2.1. Finally the spaces between neighboring lattice points (*links*) are denoted by a position and a lattice vector (x, μ). The same interval can be denoted $(x + \mu, -\mu)$.

On the lattice the fermionic fields ψ_x, $\bar{\psi}_x$ live on the sites while the gauge fields $A_\mu(x)$ lives on the links, being x a d-vector with integer components. Since the action must be gauge invariant, the simple naive discretization of directional derivatives $\partial_\mu \psi(x)$ by finite differences $1/2a(\psi_{x+\hat{\mu}} - \psi_{x-\hat{\mu}})$ with $\hat{\mu}$ a unit vector along the axis μ, cannot be applied. This is due to the fact that the product $\bar{\psi}_x \psi_{x \pm \hat{\mu}}$ is not gauge invariant.[12] Instead the so called "naive" gauge invariant discretization is given by

$$\begin{aligned} S_W = &\frac{a^{d-1}}{2} \sum_x \sum_\mu \left[\bar{\psi}_x \gamma^\mu U_\mu(x) \psi_{x+\hat{\mu}} - \bar{\psi}_{x+\hat{\mu}} \gamma^\mu U_\mu^\dagger(x) \psi_x \right] - m a^d \sum_x \bar{\psi}_x \psi_x \\ &+ \frac{1}{2g^2} a^{d-4} \sum_x \sum_{\mu,\nu>0} \left[U_\mu(x) U_\nu(x+\mu) U_\mu^\dagger(x+\nu) U_\nu^\dagger(x) + h.c. \right], \end{aligned} \tag{3.30}$$

where as before g is defined to be the coupling constant, $\mu, \nu > 0$ means that the sum must be taken along positive orientated links and $U_\mu(x)$ is a unitary operator given by

$$U_\mu(x) = e^{igaA_\mu(x)}, \tag{3.31}$$

in such a way one can recover the classical continuum limit from (3.30). There is not over-all factor of i in (3.30) due to the Euclidean metric. This action is called "naive" since still suffers from the technical issue of placing fermions on a lattice, known as *doubling problem*, that will be introduced later. Note that from the last term in (3.30) one recovers the kinetic term (3.10) for the gauge field where the factor $1/2g^2$ is needed to recover the continuum limit in its conventional notation. In fact this discretization

[11] This condition could not hold and the classical continuum limit could differ from the real one [40].

[12] This product was once already found by Schwinger when trying to regulate the ultraviolet divergences of quantum electrodynamics and he considered point-split products of fermionic fields [34]. He fixed the non invariance by inserting a phase of the form

$$\bar{\psi}(r+\xi)\gamma_\mu e^{ie\int_r^{r+\xi} dx^\mu \, A_\mu(x)} \psi(r)$$

.

is not unique, in the sense that there exist other configuration of closed loops apart from the chosen "plaquettes" operators which recover the same limit. However recall the fact one usually considers the simplest admissible discretization. The operator $U_\mu(x)$ is often called *connector*, and despite the reason why is so it will be argued once the Hamiltonian formulation has been introduced, let's give a brief idea about it.

Let's consider the case of QED, i.e where the gauge group is the Abelian $U(1)$. In that case the connector $U_\mu(x)$ can be interpreted as a Aharonov-Bohm phase picked by the fermions when hopping from site to site on the lattice. Therefore, when the fermion closes a loop, picks up a gauge invariant phase proportional to the magnetic strength. In this way we can understand the last term in (3.30) as the magnetic contribution to the action.

Remark. Note the fact that the coupling g appears as an inverse power in the pure-gauge dynamical term in (3.30). Therefore in the lattice the natural perturbative expansion is around the strong-coupling limit [4]. This fact is one of the key ideas of LGT.

3.4. Hamiltonian formulation of LGT

In many problems in physics it's interesting to look at wavefunctions, estimate energies, masses and shapes of bound states of the system, i.e understand the underlying Hilbert space structure of the system. Sometimes these are difficult to be obtained from a path integral formulation but not so much from a Hamiltonian quantum-mechanical formulation. Being so, one could either obtain the quantum Hamiltonian from the path integral formulation by calculating the system's transfer matrix [5] or construct the Hamiltonian from scratch [7].

This second option was presented by Kogut and Susskind in 1974 [7], months later Wilson published his seminal paper on LGT [5]. As in the Euclidean formulation, the key is the requirement that local gauge invariance is an exact symmetry of the system for all lattice spacing a. In this formulation we consider a spatial lattice and leaves the time to be a continuous variable. Since the gauge transformations could depend in principle both in time and spatial directions, the formalism would be highly simplified if choosing the temporal gauge, i.e $A_0 = 0$, since then the only remaining gauge symmetry group is formed by the time-independent gauge transformations, whose arguments are evaluated on points of the spatial lattice.

Because of we will only apply the formalism to (1+1)-dimensional theories with both matter and gauge fields (chapters 4 and 5) and (2+1)-dimensional pure-gauge theories (Outlook), let us only introduce the gauge theory for the later case (where the former appears as an example) and the fermionic sector for the (1+1)-dimensional case. Now x will denote a point in the spatial lattice. Moreover as abuse of notation, we will omit the chosen representation for the gauge group and call

$$D^j(g_x) \to V(x), \tag{3.32}$$

keeping $U_i(x)$ for the gauge field when the representation is not explicitly necessary. Moreover, from now on by gauge transformations we will mean time-independent

gauge ones. Finally, we will develop the theory for non-Abelian gauge theories, being the $U(1)$ case (analyzed in chapter 4) a simplified case of them with only a small different technicality and focus on the case $SU(2)$, when a explicit and intuitive computation needs to be done.

Note. Let's note the fact than in the non-Abelian quantum version

$$U(x,i) = e^{iagA_i(x)} = e^{iagA_i^\alpha(x)T^\alpha} \tag{3.33}$$

is a matrix, due to the matrix structure of T^α and as gauge operators because of A_i^α and therefore two kind of commutation relations can be meant. Moreover, like the matter fields ψ, the gauge fields will depend on the choice of representation j for the generators of G. This dependence will be expressed in the form $U^j(x,i)$, following the notation by Kogut and Susskind. Finally, the notation U^j will be used when the given result holds for every link of the lattice.

Gauge transformations on the lattice

As we saw in (3.30), in order to construct an invariant action one needs to introduce unitary operators connecting the different matter fields. It's the aim of this section to derive and interpret this result. In order to do so let's start reviewing how the different mathematical ingredients change under gauge transformations. As it's known from the continuum theory, the generators of gauge transformations for the fermionic fields are given by the conserved charges $\int dx\, j^0$. As it couldn't be other way, this is also true in the discrete case. Calling $Q_x^\alpha = \psi_x^\dagger T^\alpha \psi_x$ the discretized charge, which being a quantum representation of the algebra $\mathfrak{g}$ holds

$$[Q^\alpha, Q^\beta] = if^{\alpha\beta\gamma}Q^\gamma, \tag{3.34}$$

and denoting Λ_x the parameters representing a specific group element $h \in G$, we see that

$$\Theta_h^Q = \exp\left[i\sum_x \Lambda_x^\alpha Q_x^\alpha\right] \Rightarrow \Theta_h^Q \psi_x \Theta_h^{Q,\dagger} = V^\dagger(x)\psi_x, \qquad \Theta_h^Q \psi_x^\dagger \Theta_h^{Q,\dagger} = \psi_x^\dagger V(x), \tag{3.35}$$

with

$$V(x) = \exp[i\Lambda_x \cdot \mathbf{T}] \equiv \exp[i\Lambda_x^\alpha T^\alpha], \tag{3.36}$$

where we have introduced the notation $\Lambda_x \cdot \mathbf{T} := \sum_\alpha \Lambda_x^\alpha T^\alpha$ that will be used from now on.

On the other hand we have to consider the group elements $U(x,i) \in G$ living on a link. Since in general G is non-Abelian, one has to distinguish between left and right multiplications **on each link**

$$\text{Left:} \quad U(x,i) \to V(x)U(x,i) \tag{3.37}$$

$$\text{Right:} \quad U(x,i) \to U(x,i)V(x+i), \tag{3.38}$$

which are generated by two different kind of generators, also defined on the link, namely left $\mathbf{L} = \{L_\alpha\}$ and right $\mathbf{R} = \{R_\alpha\}$ which hold the commutation relations

$$[-L^i_\alpha(x), -L^i_\beta(x)] = -if^{\alpha\beta\gamma}L^i_\gamma(x), \qquad [R^i_\alpha(x), R^i_\beta(x)] = if^{\alpha\beta\gamma}R^i_\gamma(x)$$
$$[L^i_\alpha(x), R^i_\beta(x)] = 0, \tag{3.39}$$

on every link $(x, \hat{i})$ and equal zero if evaluated on different links [7, 9, 40]. As it will be explained, they **can be interpreted as left and right electric fields**. As in the standard formulation of LGT, we want the product

$$\psi^\dagger_x U(x,i)\psi_{x+\hat{i}} \tag{3.40}$$

to be gauge invariant. Since the product $\psi^\dagger_x\psi_{x+\hat{i}}$ transforms as

$$\psi^\dagger_x\psi_{x+\hat{i}} \to \psi^\dagger_x V(x)V^\dagger(x+i)\psi_{x+\hat{i}}, \tag{3.41}$$

this implies that $U(x,i)$ should transform

$$U(x,i) \to V^\dagger(x)U(x,i)V(x+\hat{i}), \tag{3.42}$$

Now defining the unitaries generated by $\mathbf{L}$ and $\mathbf{R}$ on the link $(x, \hat{i})$

$$\Theta^L_h = \exp[-i\Lambda_h(x)\cdot\mathbf{L}^i_x], \qquad \Theta^R_h = \exp[i\Lambda_h(x)\cdot\mathbf{R}^i_x] \tag{3.43}$$

we find

$$\Theta^L_h U(x,i)\Theta^{L,\dagger}_h = V^\dagger(x)U(x,i), \qquad \Theta^Q_h U(x,i)\Theta^{Q,\dagger}_h = U(x,i)V(x+\hat{i}), \tag{3.44}$$

i.e the spatial-gauge transformation (3.42) is given by [41]

$$\Theta^L_h\Theta^R_h U(x,i)\Theta^{R,\dagger}_h\Theta^{L,\dagger}_h = V^\dagger(x)U(x,i)V(x+\hat{i}). \tag{3.45}$$

Remark. We just prove that the product

$$\psi^\dagger_x U(x,i)\psi_{x+\hat{i}}, \tag{3.46}$$

i.e product of group elements along open loops bounded by fermionic operators, as well as

$$\mathrm{Tr}\Big[U(x,i)U(x+\hat{i},k)\dots U^\dagger(x,l)\Big], \tag{3.47}$$

i.e traces of products of group elements along closed loops —*Wilson loop*— are gauge invariant. In fact these two possibilities are the only ones and will be used to construct the gauge-invariant Hilbert space.

Finally, choosing a specific representation j for the transformations matrices $V(x)$ the following commutation relations

$$[L_\alpha, (U^j)^l{}_r] = (T^{\alpha,j})_{lk}(U^j)^k{}_r \qquad [R_\alpha, (U^j)^l{}_r] = (U^j)^l{}_k(T^{\alpha,j})_{kr} \tag{3.48}$$

hold for every link of the lattice [7], as one can prove considering the infinitesimal versions of the finite transformations in (3.44). Note that (3.48) and (3.39) can be obtained from each other via Jacobi identity, i.e using the relation

$$[L_\alpha, [L_\beta, (U^j)^l{}_r]] - [L_\beta, [L_\alpha, (U^j)^l{}_r]] = [[L_\alpha, L_\beta], (U^j)^l{}_r] \tag{3.49}$$

between quantum operators.

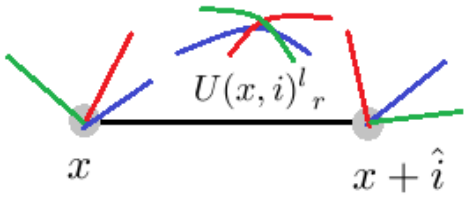


Figure 3.1.: The picture shows two different color frames at different sites of the lattice, connected by the group element $U(x,i)$ in order to relate different reference frames.

Interpretation.

Let's start with the simple Abelian case. In such a situation the group is Abelian and left and right element multiplication coincide. Therefore there is only one generator and the group element are phases. In the $U(1)$ case the commutation relations (3.44) simplify to $[E^i(x), A^j(y)] = -i\delta_{x,y}/a\delta^{i,j}$, i.e as the gauge field $A_i(x)$ the conjugate momenta $E^i(x)$ also live on the links.

On the other hand, we find that in the non-Abelian case, two kind of generators exist on a link fulfilling the canonical commutation relations (3.48) and multiplying either from the right or from the left to $U(x,i)$. Moreover via the transformation (3.35), one can **independently** "rotate" the color indices on each site of the lattice. Therefore we can think of independent color reference frames at each site x, which can be freely orientated. However it's our aim to construct a (local) gauge invariant (colorless) Hamiltonian, since physics does not depend on the orientation of these frames. In order to relate different reference frames as we move from site to site and get a gauge invariant system, we **connect** those via the connector $U(x,i)$ as it's shown in the Figure 3.1 whose color frame can also be orientated via (3.44)[13].

From (3.44) we know that on the given link, **L** and **R**, generate left and right rotations of $U(x,i)$ respectively. Now the question is how to interpret them as two different kind of electric fields on a link. In order to do so we can write the complete expression for the gauge time-independent transformation defined on each site x for $h \in G$ as

$$\Theta_h = \prod_{i>0} \Theta^L_{h,i} \prod_{i<0} \Theta^R_{h,i} \Theta^Q_h, \tag{3.50}$$

i.e, the transformation acting on the site x and all links going in $i<0$ and out $i>0$ from x. Since the different factors in the products commute with each other we can obtain that the generator of gauge transformations is given by

$$G^\alpha_x = \sum_{i>0} L^\alpha_i(x) - \sum_{i<0} R^\alpha_i(x) - Q^\alpha_x, \tag{3.51}$$

where we recognize the discrete version of the continuum charge densities (3.23). Once again imposing gauge invariant physical states one finds the discretized quantum Gauss' law

$$G^\alpha_x |\psi\rangle = \Big(\sum_{i>0} L^\alpha_i(x) - \sum_{i<0} R^\alpha_i(x) - Q^\alpha_x \Big) |\psi\rangle = 0. \tag{3.52}$$

[13]This interpretation is due to Yang and Mills [42].

From (3.52) and using $(x, \hat{i}) = (x - \hat{i}, \hat{i})$ for the right generator, we observe that on a given site x the difference —not sum over i is implied—

$$L_i^\alpha(x) - R_i^\alpha(x - \hat{i}) = Q_x^\alpha \sim \partial_i E_\alpha^i = j_\alpha^0(x) + g f^{\beta\alpha\gamma} A_\beta^i E_\gamma^i, \tag{3.53}$$

is not only the fermionic color charge Q_x^α due to the fact that the gauge boson carries its own color charge, and therefore unlike in the Abelian case, the "electric field" can change from site to site on a given link. In fact one can prove [7] that the classical continuum limit of such difference is the left hand side of the continuum result in (3.53).

Now we will construct the Hamiltonian for both the gauge and matter fields in such a way we can recover the Hamiltonian (3.20) in the continuum limit. In order to do so we will look for the simplest and local gauge invariant form of the Hamiltonian, i.e commuting with the G^α operators.

Static charges

So far we introduced gauge and fermionic content in the theory. Sometimes is interesting to insert some (colored) impurities to study the behavior of the system on their presence. In LGT, these impurities are called *static charges* and they appear as non-zero eigenvalues of the charge generator. As we have seen the generators of spatial-gauge transformations are constants of motion, i.e

$$[H, G_x^\alpha] = 0 \quad \forall\, \alpha\, x, \tag{3.54}$$

and in the non-Abelian case they also hold the algebra

$$[G_x^\alpha, G_x^\beta] = i f^{\alpha\beta\gamma} G_x^\gamma, \tag{3.55}$$

with $f^{\alpha\beta\gamma}$ the structure constants of the gauge group.

Therefore the Hamiltonian, one chosen generator $G_n^{\bar{\alpha}}$ and the possible Casimir operators of the given algebra, can be simultaneously diagonalized. This fact allows to subdivide the Hilbert space into sectors of eigenvalues of $G_n^{\bar{\alpha}}$

$$\mathcal{H} = \bigoplus_{\{q_x^{\bar{\alpha}}\}} \mathcal{H}(\{q_x^{\bar{\alpha}}\}), \tag{3.56}$$

where $q_x^{\bar{\alpha}}$ are the eigenvalues of $G_x^{\bar{\alpha}}$ and their possible values depend on the chosen representation for the gauge group.

Each sector $\mathcal{H}(\{q_x^{\bar{\alpha}}\})$ corresponds to a configuration of a set of eigenvalues $\{q_x^{\bar{\alpha}}\}$ called *static charges* and can change from site to site on the lattice.

The reason why these are called static charge goes as follows. Suppose that in (3.20) we couple the gauge field to an external current $J_{\text{ext}} = q^\alpha \delta(x - x_0)$. There is a subtlety since one should treat the group components (spin) of the external charges quantum mechanically, considering an additional Hilbert space as we will see in chapter 5. Gauss' law is now given by

$$G^\alpha(x) = \partial_i E_\alpha^i - \mathcal{J}_\alpha^0 = J_{\text{ext},\alpha}^0, \tag{3.57}$$

whose quantum version is the eigenvalue problem

$$G_x^\alpha \left|\psi(\{q_x^\alpha\})\right\rangle = q_x^\alpha \left|\psi(\{q_x^\alpha\})\right\rangle. \tag{3.58}$$

Therefore different spatial eigenvalue configurations of G^α just describe different physical situations corresponding to different spatial configurations of static charges. A clarifying description of the insertion of static charges can be found in [40, pag. 45] and will be discussed in 5.2.2.

3.4.1. Fermionic sector

In the previous subsection we already saw that the combination $\bar{\psi}_x U(x,i)\psi_{x+\hat{i}}$ is gauge invariant, therefore we just need to copy from (3.30), eliminating the temporal direction and the gauge field component $A_0 = 0$. It's also clear that the mass term is invariant as well since both fermionic fields are evaluated on the same point of the lattice. One obtains

$$H = a^{d-1}\sum_x \sum_k \frac{-i}{2a}\left[\bar{\psi}_x \gamma^k e^{iagA_k(x)}\psi_{x+\hat{k}} - \bar{\psi}_{x+\hat{k}}\gamma^k e^{-iagA_k(x)}\psi_x\right] + ma^{d-1}\sum_x \bar{\psi}_x\psi_x. \tag{3.59}$$

One can read (3.59) as formed by two terms: a hopping term, where the hopping excitation acquires a phase depending on the position; and a mass term.

Classical continuum limit

Let us compute the classical continuum limit of the fermionic Hamiltonian (3.59). In order to do so we need the assumption of slowly varying fields and use the limit

$$a^d \sum_x f(ax) \overset{a\to 0}{\longrightarrow} \int d^d x\, f(x). \tag{3.60}$$

From here it's clear one can easily recover the mass term. Moreover expanding the exponential factors to first power in a, writing the directional derivative as

$$\psi(ax + a\hat{k}) - \psi(ax - a\hat{k}) = 2a\partial_k\psi(ax) + \mathcal{O}(a^2), \tag{3.61}$$

and rewriting the hopping term as[14]

$$H = a^{d-1}\sum_x \sum_k -i\bar{\psi}_x\gamma^k\left[\frac{\psi_{x+\hat{k}} - \bar{\psi}_{x-\hat{k}}}{2a}\right] + ag\frac{\bar{\psi}_x\gamma^k A_k(x)\psi_{x+\hat{k}} + \bar{\psi}_{x+\hat{k}}\gamma^i A_k(x)\psi_x}{2a}, \tag{3.62}$$

we recover its continuous form.

It could look like we have finished the discussion for the discretization of fermionic fields. However our current discretized version of the theory has double fermionic content. This technical problem is known as the *doubling problem* or *species doubling* and is a specific case of a more general kind of phenomena studied by Nielsen and Ninomiya in 1981.

Doubling problem

Nielsen-Ninomiya No-Go theorem [43, 44] states that there can be no net chirality in a lattice model of fermions in which the Hamiltonian satisfies the following conditions:

[14] In order to rewrite it in this way, we assume an infinite system or periodic boundary conditions.

it is quadratic in the fields, invariant under change of the phase (at least global) of the fields, invariant under translations of the (cubic) lattice and local, meaning that the dispersion relation is a smooth function on the momentum.

Let's discuss the (1+1)-dimensional Dirac Hamiltonian, since it's the case that will be used for the description of the Schwinger model in terms of the Gaussian method and since we can already understand the doubling problem in its simplest form. A discussion for higher dimensional cases can be found in [45]. In a one-dimensional spatial lattice we can name both points and links with only one integer n, in such a way that the link between the sites n and $n+1$ will be also denoted by n. Let us consider the second quantized Hamiltonian

$$H = \int dx\, \bar{\psi}(x)(-i\gamma^1\partial_x + m)\psi(x) \tag{3.63}$$

where

$$\gamma_0 = \sigma_z, \qquad \gamma^1 = \sigma_z\sigma_x, \qquad \gamma_5 = \sigma_x, \tag{3.64}$$

since in (1+1)-dimensions the Clifford algebra can be chosen to be of dimension two. In the massless case

$$H = \int dx\, \psi^\dagger(x)\gamma_5(-i\partial_x)\psi(x), \tag{3.65}$$

the eigenstates of the Hamiltonian $\psi_\pm$ are chiral eigenstates, i.e

$$\gamma_5\psi_\pm = \pm\psi_\pm, \tag{3.66}$$

which in one dimension coincides with the group velocity $v = \partial E/\partial k$, i.e the **slope of the dispersion relation**. In fact their dispersion relations are given by

$$E_\pm(k) = \pm k, \quad -\infty < k < \infty. \tag{3.67}$$

Let's place the Dirac quantum Hamiltonian on a one-dimensional chain of N sites, placing $\psi = (\psi_1, \psi_2)^T$ on each site of the lattice and replacing ∂_x by a discrete difference as before.

$$H_N = \frac{-i}{2a}\sum_n \psi_n^\dagger\gamma_5[\psi_{n+1} - \psi_{n-1}]. \tag{3.68}$$

As a consequence of the Bloch theorem, the first Brillouin zone is given by $[-\pi/a, \pi/a]$ where $k = -\pi/a$ and $k = \pi/a$ are identified, being the energy periodic with period $2\pi/a$. Fourier transforming (3.68)

$$H_N = \sum_k \frac{\sin(k\cdot a)}{a}\psi_k^\dagger\gamma_5\psi_k, \tag{3.69}$$

we observe the eigenstates $\psi_\pm$ are still chiral eigenstates with eigenvalues depending on k. In fact

$$E_\pm^N(k) = \pm\frac{\sin(ka)}{a}. \tag{3.70}$$

Let's focus on the eigenstate ψ_+ for the continuous and the discrete case. It describes the excitation shown in Figure 3.2. The continuum theory (red line) describes a right mover (chirality +1) for all values of k. On the other hand in the discrete theory (curved blue line) there are a right-mover around $k = 0$ and a left-mover around

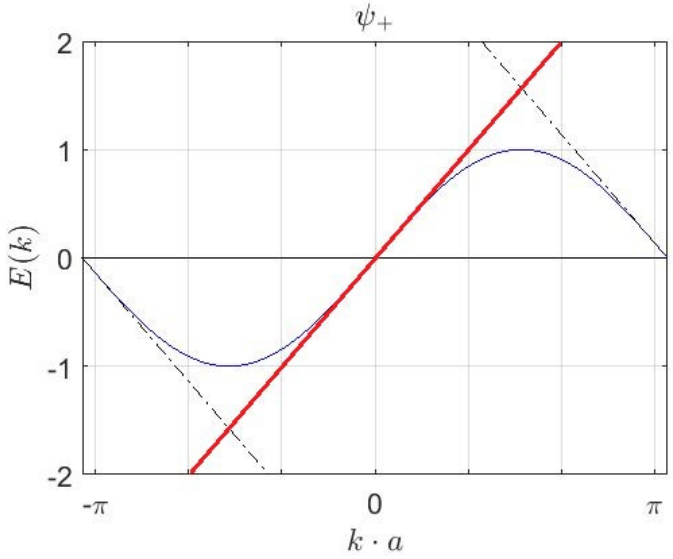


Figure 3.2.: Positive branch of dispersion relation (3.71) for $m = 0$.

$k = \pi/a$. However since the continuum limit is given by the combination of both the straight-red and dashed-black lines, we find that we can identify 2 two-component Dirac particles in the continuum limit. Therefore the finite energy content of the lattice field ψ_+ is a pair of fermions with net chirality zero [46]. We could also have deduced this result from the non-injective of the dispersion relation of the discrete Hamiltonian for ψ_+

$$E_+(k) = \sqrt{m^2 + \frac{\sin^2(k \cdot a)}{a^2}}, \tag{3.71}$$

since then

$$E_+(0) = E_+(\pi/a) = m, \tag{3.72}$$

i.e the discrete Hamiltonian doubles the fermionic content of the field ψ since there are two particles of mass m for every ψ.

In spite of the fact we have not considered the gauge field interaction in our example, this problem still remains as long as one does not break one of the assumptions of Nielsen-Ninomiya theorem. Among the different known possibilities [4] like for example *Wilson fermions*, lift the energy at the edges of the Brillouin zone, we will work with *Staggered fermions* [45], reducing the number of degrees of freedom by placing a single component spinor on each site of the lattice. This strategy is usually adopted in Quantum Simulation protocols [10, 11] and Tensor Network calculations [14, 15, 26].

The staggering consists on place single-component fermionic fields ϕ_n[15] on each site such that

$$\{\phi_n, \phi_m\} = 0 \qquad \{\phi_n, \phi_m^\dagger\} = \delta_{nm}, \tag{3.73}$$

and describe its dynamics with the Hamiltonian

$$H_S = \frac{-i}{2a} \sum_n [\phi_n^\dagger \phi_{n+1} - \phi_{n+1}^\dagger \phi_n] + m \sum_n (-1)^n \phi_n^\dagger \phi_n. \tag{3.74}$$

[15] In order to avoid non-necessary constants we use dimensionless fields $\phi_n = \phi'_n/\sqrt{a}$.

Note. Note that the doubling problem comes from the existence of several spinor components on a site of the lattice but not because of group multiplets. Therefore after the staggering the fields ϕ_n are still in a given representation of the gauge group G.

In order to identify the two-component Dirac field, one needs to decompose the lattice into an even sublattice (those points for which $(-1)^n = 1$) and an odd one (points with $(-1)^n = -1$) such that

$$\psi(n) = \begin{pmatrix} \psi_1(n) \\ \psi_2(n) \end{pmatrix} \longrightarrow \begin{cases} \psi_1(n) = \phi_n, & n \text{ even} \\ \psi_2(n) = \phi_n, & n \text{ odd} \end{cases} \tag{3.75}$$

Doing this identification one can recover the continuum theory. In fact the factor $(-1)^n$ in the mass term comes from the fact that

$$\int dx\, \bar{\psi}(x)\psi(x) = \int dx \left(\psi_1^\dagger \psi_1 - \psi_2^\dagger \psi_2\right) \longrightarrow \sum_n (-1)^n \phi_n^\dagger \phi_n,$$

while the hopping term is obtained from the fact that $\gamma_5 = \sigma_x$.

Note that this Hamiltonian is invariant only under translation by an **even number of sites** and therefore the **unit cell is doubled**. Due to Bloch theorem this means that the first Brillouin zone (1BZ) is half the size of the initial one, i.e $k \in [-\pi/2a, \pi/2a]$. Equivalently we can consider that we have two different Bravais lattices with lattice spacing $2a$. Fourier transforming we can write ϕ_n for even and odd n in terms of its Fourier components ϕ_k and $\tilde{\phi}_k$

$$\phi_n = \sum_k e^{ikn} \phi_k \qquad n \text{ even} \tag{3.76}$$

$$\phi_n = \sum_k e^{ikn} \tilde{\phi}_k \qquad n \text{ odd}, \tag{3.77}$$

where we distinguish by a $\sim$ between them. Applying it to H_S we obtain

$$H_S = \frac{1}{2ia} \sum_n \phi_n^\dagger [\phi_{n+1} - \phi_{n-1}] + m \sum_{n \text{ even}} [\phi_n^\dagger \phi_n - \phi_{n+1}^\dagger \phi_{n+1}] \tag{3.78}$$

$$= \sum_k \frac{\sin(k \cdot a)}{a} [\phi_k^\dagger \tilde{\phi}_k + h.c.] + m \sum_k [\phi_k^\dagger \phi_k - \tilde{\phi}_k^\dagger \tilde{\phi}_k] = \sum_k \Phi^\dagger \mathcal{H}_k \Phi_k, \tag{3.79}$$

with $\Phi = (\phi_k, \tilde{\phi}_k)^T$ and $\mathcal{H}_k$ given by

$$\mathcal{H}_k = \frac{\sin(ka)}{a} \sigma_x + m\sigma_z. \tag{3.80}$$

As before we obtain the dispersion (3.71). However now the 1BZ is just $(-\pi/2a, \pi/2a]$ and therefore (3.71) is injective in this domain giving a unique chiral state in the continuum limit.

Therefore once the gauge "phases" are introduced our target Hamiltonian takes the form

$$H_F = \frac{-i}{2a} \sum_n [\phi_n^\dagger e^{iagA_1(n)} \phi_{n+1} - \phi_{n+1}^\dagger e^{-iagA_1(n)} \phi_n] + m \sum_n (-1)^n \phi_n^\dagger \phi_n. \tag{3.81}$$

Staggered gauge charges

We already saw the form of Q^α when the whole spinor multiplet is placed on a site of the lattice. However due to the staggering it's shape may change. The explanation of this part will be entirely based on the publication [41]. The staggering allows us to define a lattice analogy of the Dirac sea, which is a state in which all even (particle) sites are empty, while the odd (antiparticle) ones are occupied. This picture is supported by the mass term in (3.81), which punishes the existence of particles. In addition, due to the decomposition of the Dirac field on different sites, the charges could also change sign alternately. It's the aim of this part to give a formal derivation of the staggered charges.

Consider the (group-multiplet) fermionic field ϕ_n on a given site. A gauge transformation on ϕ_n is the result of acting with an operator $\Theta_h^{Q,j}$ on it such that ϕ_n transforms as ψ_n in (3.35)

$$\Theta_h^{Q,j}\phi_n\Theta_h^{Q,j\dagger} = D^{j\dagger}(h)\phi_n, \qquad \Theta_h^{Q,j}\phi_n^\dagger\Theta_h^{Q,j\dagger} = \phi_n^\dagger D^{j\dagger}(h). \tag{3.82}$$

For the gauge groups we are considering, $SU(N)$ and $U(1)$, $\Theta^{Q,j}$ can be easily written as the exponential of some quadratic fermionic generator depending on the corresponding representation $T^{\alpha,j}$. However the transformation laws (3.82), fixed the form of Θ^Q up to a phase which can be freely chosen. Therefore we can define it via

$$\Theta_h^{Q,j} = \exp\left[i\phi_a^\dagger q(h)_{ab}\phi_b\right]\det(h^{-1})^S, \tag{3.83}$$

with $S = 1/2(1-(-1)^n)$ where n is the site index, i.e $S = 0$ for even vertices and $S = 1$ for the odd ones, $\det(h^{-1}) := \det(D^{j\dagger}(h))$ since we are considering unitary representations and

$$q(h) = \begin{cases} 1 & \text{if } G = U(1) \\ \sum_\alpha \Lambda_h^\alpha T^\alpha & \text{if } G = SU(N) \end{cases}. \tag{3.84}$$

Now for $SU(N)$ all determinants are one and the **staggering plays no role** in the definition of charges finding

$$Q^\alpha_{SU(N),n} = \phi_n^\dagger T^\alpha \phi_n, \tag{3.85}$$

as we found before. Nevertheless for $U(1)$, since $\det(h) = e^{i\theta}$ with $\theta \in \mathbb{R}$ the gauge transformation is given by

$$\Theta^Q_{\theta,n} = e^{i(\phi_n^\dagger\phi_n - S)\theta}, \tag{3.86}$$

which implies that the Abelian staggered charge reads

$$Q_{U(1),n} = \phi_n^\dagger\phi_n - \frac{1}{2}(1-(-1)^n). \tag{3.87}$$

This construction of the Abelian charge let us to support the physical picture of Dirac sea [9]. With staggered fermions, even sites represent *particles* with positive mass m, while odd sites represent "holes" with negative masses $-m$. If now we measure the energy on odd sites with respect $-m$, occupied sites will contribute with zero energy (occupied hole) while empty ones would acquire a mass m (free hole in the

Dirac sea). Therefore applying a particle-hole transformation on odd sites ($\phi_n \leftrightarrow h_n^\dagger$ and $\phi_n^\dagger \leftrightarrow h_n$) we can interpret the system as formed by particles and holes in the even and odd places respectively. Now in the Abelian case, i.e QED we can use the expression for the staggered charge to further support this picture. From (3.87) we observe that an occupied even site acquires a charge $+1$ while an empty odd site n has a charge -1, i.e an empty odd place plays the role of a hole.

3.4.2. Gauge sector

So far we just introduced dynamics for the matter fields. Now we need to add a gauge-invariant pure-gauge term in order to give non-trivial dynamics for the gauge field. By non-trivial we mean a term which does not commute with the already constructed fermionic part (3.81) of the Hamiltonian. That would lead us to consider terms obtained from gauge invariant combinations of the gauge group elements U and its canonical conjugate variables $\mathbf{L}$ and $\mathbf{R}$.

Gauge invariance forces us to consider (group) traces of product elements along closed paths [9]. The simplest and "most local" of such products are given by plaquettes operators p (Wilson loops) terms considered already in (3.30),

$$H_B = -\frac{1}{2g^2} a^{d-5} \sum_p \Big[U_1 U_2 U_3^\dagger U_4^\dagger + h.c. \Big], \tag{3.88}$$

where the subscripts 1, 2, 3 and 4 represents the counter clockwise order of the product around the plaquette. This term is know as magnetic term since its classical continuum limit gives raise to the magnetic contribution to the energy. Nevertheless H_B commutes with (3.59) and give non-trivial dynamics for U. We could then try to write the lattice version of the electric energy. Considering the interpretation of $\mathbf{L}$ and $\mathbf{R}$ in section 3.4 as electric fields on a link, the electric term must be given as a function of the Casimir operators of the corresponding gauge group, since it must be invariant. In order to recover the continuum limit

$$\frac{1}{2} a^{d-1} \sum_x \sum_{\alpha,i} (E_\alpha^i(x))^2 \longrightarrow \frac{1}{2} \int d^d x \sum_{\alpha,i} (E_\alpha^i(x))^2 \tag{3.89}$$

we consider the quadratic Casimir operator (the only one for $SU(2)$)[16]

$$H_E = \frac{g^2}{2a^{d-3}} \sum_{x,i} (\mathbf{L}_x^i)^2, \tag{3.90}$$

where E_α^i and the dimensionless generator L_α^i are related via $E_\alpha^i = g a^{2-d} L_\alpha^i$.

The Kogut-Susskind gauge term in the Hamiltonian formulation of LGT is given by

$$H_G = H_E + H_B = \frac{g^2}{2a^{d-3}} \sum_{x,i} (\mathbf{L}_x^i)^2 - \frac{1}{2g^2} a^{d-5} \sum_p \Big[U_1 U_2 U_3^\dagger U_4^\dagger + h.c. \Big], \tag{3.91}$$

[16] The same result can be obtained from the Euclidean path-integral formulation as explained in [46].

for $d > 2$ spacetime dimensions, since in $d = 2$ the last term does not exist. Recall that $A_i = A_i^\alpha T^\alpha$.

In the Abelian case for $(d-1)$-spatial dimensions the Hamiltonian takes the form

$$H_{U(1)} = \frac{1}{2a^{d-3}} \sum_{x,i} (E_x^i)^2 - \frac{1}{2g^2} a^{d-5} \sum_p \cos\Big[ag(\underbrace{A_1 + A_2 - A_3 - A_4}_{\nabla \times A_p})\Big], \tag{3.92}$$

where $\nabla_p \times A$ is the discrete rotational operator on the plaquette p such that in the continuum limit one recovers the magnetic field

$$\cos(\nabla_p \times A) \longrightarrow 1 - B_p^2/2. \tag{3.93}$$

Further comments about QED in (1+1)-dimensions will be given on chapter 4. Therefore we have constructed the discrete Hamiltonian for gauge theories on a lattice with the correct classical continuum limit avoiding the doubling problem via staggering, at least in (1+1) dimensions.

Remark. Note the fact on each link, left and right generators are related via the group elemente U on the link in the adjoint representation

$$R^\alpha = (U^{\text{Adj.}})_{\alpha\beta} L^\beta, \tag{3.94}$$

and therefore $\mathbf{L}^2 = \mathbf{R}^2$.

Proof. In order to prove that $\mathbf{L}$ and $\mathbf{R}$ can be related by a linear transformation in the generator-index, we need to make use of the commutation relations (3.48). Let's express $R^\alpha = M_{\alpha\beta} L^\beta$ where we suppose M is an invertible matrix and substitute this relation in (3.48) for the commutation relation for $\mathbf{R}$[17]

$$M_{\alpha\beta} L_\beta \otimes U^j - U^j \otimes M_{\alpha\beta} L_\beta = U^j T_a^j,$$

multiplying by $M^{-1}_{\delta,\alpha}$

$$L_\alpha \otimes U^j - U^j \otimes L_\alpha = U^j M^{-1}_{\alpha\beta} T^j_\beta,$$

and comparing with the commutation relation for $\mathbf{L}$ in (3.48) we find

$$U^{j,\dagger} T^j_\alpha U^j = M^{-1}_{\alpha\beta} T^j_\beta \Rightarrow M^{-1} = U^{\text{Adj.},\dagger} \Rightarrow \mathbf{R} = U^{\text{Adj.}} \mathbf{L} = U^j \mathbf{L} U^{j\dagger}, \tag{3.95}$$

where we have used the fact that $\mathbf{T}^j$ transforms as a 3-vector under color rotations since $(T^{\alpha,\,\text{Adj.}})_{\beta,\gamma} = i f^{\alpha\beta\gamma}$. Relation (3.95) means that $\mathbf{L}$ and $\mathbf{R}$ are equivalent representations of the gauge algebra.

□

This relation helps us to give a different interpretation to $\mathbf{L}$ and $\mathbf{R}$ that can be found in [7]. On each link one can interpret the space of states as different configurations of a quantum rotator, where $\mathbf{L}$ generate space-fixed rotations and $\mathbf{R}$ body fixed rotations, being the connection between both given by $\mathbf{R} = U^{\text{Adj.}} \mathbf{L}$. Due to local gauge invariance requirements such rotator should be spherical since must be independently invariant under body and space rotations. Therefore the gauge sector of a lattice can be understood as a collection of spherical quantum rotators whose configuration is given by U.

[17] In order to avoid indices the notation $[\,,\,]_\otimes$ has been used to make reference to the matrix structure contained in U, that was not explicitly written in (3.48).

Note. Consider a (1+1)-dimensional system. The non-Abelian Gauss' law (3.51) takes the form

$$L_n^\alpha - R_{n-1}^\alpha = Q_n^\alpha. \tag{3.96}$$

Because of the relation (3.94) and using the expression (3.33) in the adjoint representation

$$U^{\text{Adj.}} = e^{iagA_n(x)^\gamma T^\gamma_{\text{Adj.}}}, \tag{3.97}$$

one can write (3.96) as

$$Q_n^\alpha = L_n^\alpha - \left(e^{iagA_n(x)^\gamma T^\gamma_{\text{Adj.}}}\right)_{\alpha\beta} L_{n-1}^\beta, \tag{3.98}$$

and expanding to first order in a one obtains

$$\begin{aligned} Q_n^\alpha/a &= \frac{L_n^\alpha - L_{n-1}^\alpha}{a} - igA_n(x)^\gamma (T^\gamma_{\text{Adj.}})_{\alpha\beta} L_{n-1}^\beta + \mathcal{O}(a^2) \\ &= \frac{L_n^\alpha - L_{n-1}^\alpha}{a} + gA_n(x)^\gamma f^{\gamma\alpha\beta} L_{n-1}^\beta + \mathcal{O}(a^2), \end{aligned} \tag{3.99}$$

which reproduces (3.23) in the limit $a \to 0$. The difference in the sign for the color charge is due to the sign convention for the adjoint representation.

3.5. Hilbert space

We already said that one of the advantages to follow the Hamiltonian formulation is the fact that one can have an easy access to the underlying Hilbert space. In this section we follow the analysis of the physical Hilbert space done in [7]. We consider separately the Abelian case $U(1)$, that will be studied in chapter 4.

3.5.1. Abelian theory: $U(1)$ case

The Kogut-Susskind Hamiltonian for QED (3.92), introduces the gauge field as an angular variable with period 2π. This kind of formulation of Abelian theories on a lattice are called *compact* due to the boundedness of the interval where the gauge field takes different values. Therefore let's emphasize this fact by introducing the dimensionless fields

$$\phi'_x = \phi_x/\sqrt{a}, \qquad \theta_x^i = -agA_x^i, \qquad L_x = E_x/g, \tag{3.100}$$

such that θ_x^i is taken to live in the bounded interval $[0, 2\pi)$.

The canonical commutation relations with this new definition of the fields take the form

$$\{\phi'(x), \phi'^\dagger(y)\} = \delta(x-y) \longrightarrow \{\phi'_x, \phi'^\dagger_y\} = \frac{\delta_{x,x}}{a} \Rightarrow \{\phi_n, \phi_m^\dagger\} = \delta_{n,m} \tag{3.101}$$

$$[E(x), A(y)] = i\delta(x-y) \longrightarrow [E_x^i, A_m^j y] = i\delta^{i,j}\delta_{x,y}/a \Rightarrow \boxed{[\theta_x^i, L_y^j] = i\delta^{i,j}\delta_{x,y}}. \tag{3.102}$$

Therefore due to the periodicity of θ_x^i, its canonical conjugate variable L_x^i is an angular momentum operator [11, 34] with unbounded discrete integer spectrum

$$L_x^i |m\rangle = m |m\rangle \text{ with } m \in \mathbb{Z}, \tag{3.103}$$

which implies that on each link **the electric field is quantized in integer multiples of** g, i.e electric flux quanta m

$$E_x^i |m\rangle = mg |m\rangle \text{ with } m \in \mathbb{Z}, \tag{3.104}$$

where the sign of m refers to the direction of the E_x^i along the link. Therefore the ground state of the electric Hamiltonian is given by the product of all vacuum states $|0\rangle$ on the links, that is a gauge invariant state.

Moreover the operators $U_i(x)$ and $U_i(x)^\dagger$ behaves like raising and lowering operators (ladder operators) of electric flux quanta, since

$$[L_x^i, U_i(x)] = U_i(x) \Rightarrow L_x^i U_i(x) |m\rangle = (m+1) U_i(x) |m\rangle \tag{3.105}$$

$$[L_x^i, U_i(x)^\dagger] = -U_i(x)^\dagger \Rightarrow L_x^i U_i(x)^\dagger |m\rangle = (m-1) U_i(x)^\dagger |m\rangle , \tag{3.106}$$

and then

$$U_i(x) |m\rangle = |m+1\rangle \quad \text{and} \quad U_i(x)^\dagger |m\rangle = |m-1\rangle , \tag{3.107}$$

add and subtract flux quanta from the links.

3.5.2. Non-Abelian theory

This subsection will follow the publication [7]. Let's consider the case $G = SU(2)$ with a given representation j. Since there are two kind of generators L^α and R^α, and one Casimir operator $\mathbf{L}^2$, we can label the states with the quantum numbers for $\mathbf{L}^2$, L^z and R^z, i.e

$$|\psi\rangle_G = |j, m_1, m_2\rangle . \tag{3.108}$$

These states are eigenstates of the electric Hamiltonian on each link with energy

$$H_E |j, m_1, m_2\rangle = \frac{g^2}{2} j(j+1) |j, m_1, m_2\rangle , \tag{3.109}$$

with degeneracy $(2j+1)^2$. In particular the ground state is the gauge invariant state given by $|0\rangle = |0, 0, 0\rangle$, from which we can construct the rest of the states. Consider the state $(U^j)^l{}_r |0\rangle$ on a link. Using (3.48) we can prove that

$$H_E (U^j)^l{}_r |0\rangle = \frac{g^2}{2} \sum_\alpha (T^{\alpha,j} \cdot T^{\alpha,j})^l{}_i (U^j)^i{}_r |0\rangle = \frac{g^2}{2} j(j+1) (U^j)^l{}_r |0\rangle , \tag{3.110}$$

due to the fact that $\sum_\alpha (T^{\alpha,j} \cdot T^{\alpha,j})^l{}_i = j(j+1)\delta_i^l$ is the Casimir operator for the algebra $\mathfrak{su}(2)$.

Now Gauss' law $G^\alpha |\psi\rangle_G = 0$ should be imposed, in order to obtain the physical Hilbert space. From (3.110) we obtained that we can construct the Hilbert space starting from the gauge vacuum and applying group elements U. Since both the fermionic $|0\rangle_F$ and the gauge vacua $|0\rangle_G$ are gauge invariant, in order to construct gauge-invariant states we just need to apply gauge invariant operators to them. This

will be the case if and only if all group indices in such operators are contracted. In order to do so there are two possibilities: (1) trace of product of group elements along closed loops $\mathcal{C}$ on the lattice

$$\mathrm{Tr}U^j(\mathcal{C}) = \mathrm{Tr}\Big[U_i^j(x)U_k^j(x+i)\dots U_m^{\dagger,j}(x)\Big], \tag{3.111}$$

or (2) open loops as was proved in (3.46), given by an open path $\mathcal{C}$ between two fermionic operators $\psi_x^\dagger$ and ψ_y of products of group elements known as *string*

$$U^j(x,y;\mathcal{C}) = \psi_x^\dagger U^j(\Gamma)\psi_y. \tag{3.112}$$

3.6. Confinement

One of the most interesting and not yet well understood phenomenon in Quantum Chromodynamics is the confinement of color charge. This belongs to the general phenomena of confinement of quantum numbers. As explained in [47], a theory is said to be *confining* if all **finite-energy** states are invariant under global gauge transformations, i.e they are color singlets in the non-Abelian case or chargeless in QED. For example, QED in (3+1)-dimensions is not confining since the electron is a finite-energy state with nonzero electric charge. In fact it's one of the main features of non-Abelian gauge theories and it's thought to be related to the highly nonlinear dynamics of the pure-gauge sector [33].

In 1974 Kenneth G. Wilson [5] (inspired by Schwinger [48]), proposed a new way to understand the mechanism which could keep quarks bound. One of the conclusions of this seminal paper is that one could focus on the static aspect of confinement, namely test the theory with a static quark-antiquark pair and study the dependence of the ground state energy as a function of the interquark distance. A potential example of this situation holding the definition of confinement given by [47] is given by the string

$$\psi_x^\dagger U^j(\mathcal{C})\psi_y\,|0\rangle\,, \tag{3.113}$$

connecting two quarks as we will see in subsection 3.6.2.

3.6.1. Charge confinement in Abelian lattice theories

The phenomena of confinement is usually discussed in non-Abelian gauge theories in 3+1 dimensions for color confinement. However its appearance depends on both the dimensionality of the considered spacetime and whether we are dealing with a continuous or a lattice model. In the former case, one can already study confinement for QED in 1+1 dimensions as we will study in chapter 4, where the electric potential grows linearly with the distance, i.e one finds confinement to all regimes in the coupling constant g. In the lattice however, confinement for Abelian theories appears when considering *compact* formulations as the one presented in (3.92), where the gauge field appears as an angular variable, i.e the Hamiltonian is constructed from group elements of $U(1)$ instead of elements of the algebra. This gives rise to self-interacting photons which lead, in some regimes, to confinement. This model is usually called *compact QED* (cQED) and it's defined in correspondence to the lattice

gauge formulation for non-Abelian theories. Nevertheless QED admits many inequivalent formulations [49], with different behaviors in the strong coupling regime. In fact compact formulations of Abelian theories show confinement for all non-vanishing coupling $g > 0$ in 2+1 dimensions, while in 3+1 a phase transition takes place at a finite g between a confining ($g >> 1$) and a non-confining phase ($g << 1$) [49].

3.6.2. Is there confinement?

Here we follow the exposition given by [7]. Usually one introduces the Wilson loop to discuss confinement [5, 40]. Nevertheless one of the advantages of using the Hamiltonian formulation is the possibility to compute directly the potential energy between two widely [18] separated **static** quarks [19]. To ensure a confining result is obtained, let's restrict ourselves for simplicity to $SU(2)$ non-Abelian case in the fundamental representation $j = 1/2$[20]. Let's consider both particles are placed over the same edge of the lattice at a distance L [21]. In the strong coupling limit $g >> 1$, $H \sim H_E$ and the minimun-energy gauge invariant state is given by the string (gauge invariant) state with potential energy

$$V_Q(L) = \frac{g^2}{2}\left[\frac{1}{2}\left(\frac{1}{2}+1\right)\right] \cdot \frac{L}{a}, \tag{3.114}$$

where one observes there is a distance-independent attractive force between the quarks. Whether or not is enough to confine the quarks depends on the value of g and other considerations. Considering the magnetic term H_B as a perturbation, one realizes that may generate closed loops on top of the vacuum or deform the line of electric flux. The vacuum becomes a soup of closed flux loops [7]. When higher orders in perturbation theory are considered, $V_Q(L)$ is still proportional to the distance, for large distances.

Finally when considering the hopping term, a string is no more an eigenstate of the Hamiltonian. This term allows the production of pairs $\bar{q}q$ out of the vacuum allowing the string to break. This phenomenon will be studied in chapter 4, and it's know as *string breaking*.

3.7. Summary and conclusion

The Kogut-Susskind Hamiltonian formulation of Lattice Gauge Theories gives as a result a **second quantized Hamiltonian** (3.81) + (3.91), written in terms of fermionic ϕ_x,$\phi_x^\dagger$ and gauge degrees of freedom $U_i(x)$. This allows us to apply the method introduced in chapter 2, to describe High Energy Physics, hopefully like QCD in 3+1 dimensions, in the Gaussian approximation via two-point correlation functions with the advantage of having a clear description of the underlying Hilbert space. However in this Hamiltonian, the only quadratic term which does not need to be approximated via Wick's theorem is the mass term. The remaining three terms must be handled

[18] to avoid problems in the perturbation expansion at short distances.

[19] The term quarks will refer to representation of the gauge group. In the case of $U(1)$ are $U(1)$-charged particles and for $SU(2)$ "spins".

[20] For integer representations of the group the theory is non-confining [40, pag. 46].

[21] This avoids problems of degeneracy of the ground state, since several paths could have the same energy.

—via approximations, Schwinger representation, unitary transformations or other analytical tools— in such a way one gives the best description the Gaussian approach can in fact gives. It will be the goal of the last two chapters to apply this method to (1+1)-dimensional lattice gauge theories with gauge and fermionic degrees of freedom in the case of $U(1)$ (chapter 4) and $SU(2)$ (chapter 5) gauge groups.

4. The Schwinger model

In this chapter we will study the Schwinger model [48] on a lattice [16] via the Gaussian method. In order to test the time-dependent Gaussian variational method, we will compare our results to those obtained for the exactly solvable massless case as well as to other numerical results obtained for the massive model via Matrix Product States [26, 27].

4.1. Introduction

As we already explained chapter 3, many relevant phenomena in QCD appear in the non-perturbative regime, for which not much can be computed analytically in four dimensions. Therefore in order to get some intuition as well as try to develop new analytical methods, simpler models like QED_2 or QCD_2, models in two spacetime dimensions, have been considered for a long time playing the role of labs for Quantum Field Theory methods [50].

In particular the Schwinger model, also known as QED_2, is often used for testing new methods of QFTs like for example Bosonization, lattice computations or new numerical approaches like ours. Nevertheless, the Schwinger model is interesting per se being the simplest non-trivial gauge theory displaying interesting phenomena like: a nontrivial vacuum structure, chiral anomaly, confinement, no fermions in the physical particle spectrum etc; also appearing in Quantum Chromodynamics.

The massive Schwinger model [51] has been proved to be equivalent to the massive sine-Gordon model through Bosonization being exactly solvable in the massless case [52].

Moreover during the last few years this model has become relevant in his own due to the fact it could be realized by quantum simulators [9, 12] and has been used as a benchmark to test Tensor Networks (TN) methods [14, 15, 26, 27] which have supplied, in some cases, a better description than that made by Monte Carlo simulations, due to the fact it allows us to deal with fermions avoiding the otherwise problematic "sign problem" [6].

4.2. Continuum theory

The Schwinger model is thus (1+1)-dimensional QED described by the Lagrangian density

$$\mathcal{L} = \bar{\psi}(i\partial\!\!\!/ - gA\!\!\!/ - m)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} \tag{4.1}$$

where as always $B\!\!\!/ := \gamma^\mu B_\mu$ with $\mu = 0, 1$. In order to clarify ideas, we follow the general procedure presented in chapter 3 for the Abelian case, where the formalism

becomes simpler. From equation (4.1) we obtain the Hamiltonian density

$$\mathcal{H} = -i\bar{\psi}\gamma^1(\partial_x + igA_1)\psi + m\psi^\dagger\psi + \frac{1}{2}E^2 - \cancelto{0}{A^0}(\partial_x E - g\psi^\dagger\psi) \tag{4.2}$$

where with our metric convention $\eta = \mathrm{Diag}(1,-1)$, the electric field is given by $E = F^{1\,0} = -F^{0\,1} = \Pi^i$. Working on the temporal gauge ($A_0 = 0$) and integrating over the space we obtain the Hamiltonian

$$H = \int dx \left\{ -i\bar{\psi}\gamma^1(\partial_x - igA^1)\psi + m\bar{\psi}\psi + \frac{1}{2}E^2 \right\} \tag{4.3}$$

where the relation $A_1 = -A^1$ has been used. Recall that A_0 is not a canonical variable and that the last term in (4.2) is a constant of motion.

Once the canonical quantization procedure has been applied, we impose Gauss' law (in its usual Abelian form) as explained in section 3.4

$$(\partial_x \hat{E} - g\hat{\psi}^\dagger\hat{\psi})\,|Phys\rangle = 0, \tag{4.4}$$

i.e., restrict the Hilbert space to the space of gauge-invariant states $|Phys\rangle$.

4.2.1. Dimensional analysis

Before continuing, let's review the dimensionality of the different fields and parameters that appear in the (1+1)-dimensional theory. Since $\hbar = c = 1$, we express all fields and parameters in units of energy

$$[\mathcal{L}] = 2 \Longrightarrow \begin{cases} 2 = [i\bar{\psi}\partial_\mu\psi] \Rightarrow [\psi] = 1/2,\ [m] = 1 \\ 2 = [F_{\mu\nu}F^{\mu\nu}] \Rightarrow 2 = 2 + 2[A_\mu] \Rightarrow [A_\mu] = 0 \\ 2 = [\bar{\psi}gA_\mu\psi] \Rightarrow [g] = 1 \\ [E] = 1 \end{cases} \tag{4.5}$$

Therefore in (1+1) dimensions the gauge field A_μ is dimensionless and the **coupling constant g has units of energy**.

4.2.2. Solving the continuum theory

This section will follow and develop the explanations given in Ref. [33, 53–55]. Moreover, in the interest of simplicity and clarity and trying to avoid a lengthy introduction to the topic, we will provide a constructive derivation and skip a formal introduction to Bosonization.

Massless Schwinger model

The massless Schwinger model, i.e., QED with massless fermions in (1+1) dimensions, is an **exactly solvable** theory showing interesting features. As in the 4-dimensional case [47], we can express the photon propagator in the form

$$D_{\mu\nu}(k^2) = \frac{g_{\mu\nu} - k_\mu k_\nu/k^2}{k^2(1 - \Pi(k^2))}, \tag{4.6}$$

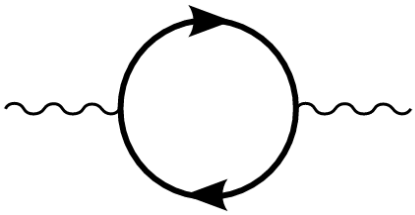


Figure 4.1.: Vacuum-polarization loop in the two-dimensional Schwinger model. Public picture from Wikipedia.

and evaluate it in the one-loop correction, shown in Figure 4.1, to the self-energy giving the finite value

$$\Pi(k^2) = \frac{g^2/\pi}{k^2}. \tag{4.7}$$

Substituting back in the photon propagator (4.6), we find

$$D_{\mu\nu}(k^2) = \frac{g_{\mu\nu} - k_\mu k_\nu/k^2}{k^2 - g^2/\pi}, \tag{4.8}$$

i.e., the photon has picked up a mass $M = g/\sqrt{\pi}$ due to vacuum polarization effects. In fact further analysis shows that $M = g/\sqrt{\pi}$ is an exact result. Now that the photon is massive, the potential between static external charges is short ranged and behaves as $\sim Q^2 e^{-M|x|}$, where Q is the charge of the impurities and can take any value. Therefore an arbitrary charge is **screened** to zero in this model and that's the reason why it is said that this is not true confinement as in Ref. [52], in the sense that it does not imply a long-range potential for any Q.

In (1+1) dimension the gauge field is not a physical dynamical degree of freedom and therefore it can be eliminated. It's usually said that this is the case since there is not space for tranversal photons. For this introduction let's set $A_1 = 0$ (axial gauge) instead of the previous temporal $A_0 = 0$ gauge, which does not erase spatial-gauge invariance. The equation of motion for A_0 is given by

$$\frac{\partial^2 A_0}{\partial_x^2} = -g\psi^\dagger(x)\psi(x) = -gj^0(x), \tag{4.9}$$

which can be integrated to give

$$A_0(x) = -\frac{1}{2}g \int dx' \, |x - x'| \, j^0(x') - Fx - C, \tag{4.10}$$

i.e., Coulomb potential in two spacetime dimensions plus linear contributions, where C is an irrelevant parameter that it does not enter into the expression for the electric field. Since $F_{01} = -\partial_x A_0$ we find that the electric field is given by

$$F_{01}(x) = g \int dx' \, \partial_x \Big(\frac{1}{2} \, |x - x'| \, \Big) j^0(x') + F. \tag{4.11}$$

The advantage of working with one-dimensional fermionic systems is that they can be described by one-dimensional boson fields in a method known as bosonization [56]. In the following we list the main relations we will later need:

$$: j_\mu :=: \bar{\psi}\gamma_\mu\psi :\longleftrightarrow \epsilon_{\mu\nu}\partial_\nu\phi/\sqrt{\pi}, \tag{4.12}$$

$$: j^5_\mu :=: \bar{\psi}\gamma_5\gamma_\mu\psi :\longleftrightarrow \partial_\mu\phi/\sqrt{\pi}, \tag{4.13}$$

$$: \bar{\psi}\psi :\longleftrightarrow c : \cos(2\sqrt{\pi}\phi) :, \tag{4.14}$$

$$: \bar{\psi}\gamma_5\psi :\longleftrightarrow c : \sin(2\sqrt{\pi}\phi) :, \tag{4.15}$$

$$: i\bar{\psi}\not{\partial}\psi :\longleftrightarrow \frac{1}{2}\partial_\mu\phi\,\partial_\mu\phi, \tag{4.16}$$

where ϕ is a scalar field, $c = \pi^{-3/2}e^\gamma$ with γ Euler's constant and $::$ normal order with respect to the vacuum of the Dirac field for the fermionic operators and the vacuum for the massive field ϕ with mass $g/\sqrt{\pi}$ on the right hand side. From the last identification we learn that a free massless Dirac field is equivalent to a free massless bosonic field. Restricting ourselves to states of total zero charge

$$\int dx\, j^0(x) = \sqrt{\pi}(\phi(\infty) - \phi(-\infty)) = 0, \tag{4.17}$$

and making use of (4.12), we can express F_{01} as

$$F_{01} = \frac{g}{\sqrt{\pi}}\phi(x) + \underbrace{\frac{g}{\sqrt{\pi}}\phi(\infty) + F}_{\equiv F'}, \tag{4.18}$$

where $\phi(\infty)$ is a constant, fixing the boundary conditions of ϕ at the boundaries of the system. Then we can think of F as a boundary term of ϕ at infinity and reabsorb it in $\phi(\infty)$ or equivalently, we can think about $\frac{g}{\sqrt{\pi}}\phi(\infty)$ as a background electric field and reabsorb this constant in the background field F. We will use one picture or the other depending on the interpretation we want to discuss.

Let's introduce both the fermionic and bosonic representation in order to match the different terms. Note the fact that the Hamiltonian density can be written as

$$\mathcal{H} = -i\bar{\psi}\gamma^1\partial_x\psi + \frac{1}{2}(F_{01})^2. \tag{4.19}$$

The fermionic representation can be found using (4.18) with the charge zero restriction (4.17) and integrating by parts to be

$$H = \int dx\,\bar{\psi}(x)\gamma^1(-i\partial_x)\psi(x) + \frac{1}{2}\int dx dx'\, j^0(x)V(x-x')j^0(x') - g\int dx \underbrace{Fx}_{-A_0^{ext}(x)} j^0(x), \tag{4.20}$$

i.e., a Dirac fermion with a potential energy given by the interaction of charges via the potential $V(x-x') = -g^2/2\,|x-x'|$ and with a background field F. On the other hand, applying the Bosonization identities (4.12) to (4.1), Legendre transforming and inserting (4.18) one finds

$$H = \frac{1}{2}\int dx \left[(\partial_t\phi)^2 + (\partial_x\phi)^2 + \frac{g^2}{\pi}\left(\phi + \frac{\sqrt{\pi}}{g}F\right)^2\right], \tag{4.21}$$

i.e., a Hamiltonian for a free massive bosonic field ϕ "interacting" with a background field F. Note that in the massless case, the Hamiltonian density (4.19) is chirally

invariant and so must be (4.21). In the bosonic representation a global chiral transformation transforms $\phi \to \phi + \alpha$ with $\alpha \in \mathbb{R}$, i.e., acts as a translation changing ϕ's boundary value $\phi(\infty)$ or equivalently $\sqrt{\pi}/gF$. Therefore in order to make (4.21) chirally invariant, we need to consider the chiral invariant field $\hat{\phi} = \phi - \phi(\infty)$ instead of ϕ [54]. This can be achieved by shifting $\phi \to \phi - \sqrt{\pi}/gF$, obtaining

$$H = \frac{1}{2}\int dx \left[(\partial_t\phi)^2 + (\partial_x\phi)^2 + \frac{g^2}{\pi}\phi^2\right], \tag{4.22}$$

where we can understand why F does not play any important role in the massless case. It costs no energy, since the fermionic excitations are massless, to screen any external field to zero and therefore only $F = 0$ is a physical possibility [1]. Note also that the mass term for the bosonic field ϕ is the mass acquired by the photon in the fermionic picture (4.8).

Massive Schwinger model

Unlike the massless model, the massive one is not exactly solvable and as we will see the Hamiltonian depends on F. In this case due to the mass term, when we apply (4.12) we obtain

$$H = \frac{1}{2}\int dx \left[(\partial_t\phi)^2 + (\partial_x\phi)^2 + \frac{g^2}{\pi}\left(\phi + \frac{\sqrt{\pi}}{g}F\right)^2\right] - mc\int dx \ :cos\left(2\sqrt{\pi}\phi\right): \tag{4.23}$$

Now if we shift the ϕ-field as before we find

$$H = \frac{1}{2}\int dx \left[(\partial_t\phi)^2 + (\partial_x\phi)^2 + \frac{g^2}{\pi}\phi^2\right] - mc\int dx \ :cos(2\sqrt{\pi}\left(\phi - \frac{\sqrt{\pi}}{g}F\right)):, \tag{4.24}$$

F appears as a periodic variable in the Hamiltonian and therefore we can define $\theta = 2\pi F/g$ with $\theta \in [0, 2\pi)$, i.e., the Hamiltonian is periodic in F with period one (taking $g = 1$). The constant field θ is usually called θ-field and has relation with the chiral symmetry breaking and the ground state structure of the system. In this case the model is sensitive to θ, and one expects different kind of behavior from that realized in the massless case, like for example confinement rather than screening. In order to confirm this intuition we can set two opposite static charges on the system, via the insertion of $j^0_{ext} = Q/\sqrt{\pi}\phi_{ext}$ in the mass term of (4.24), placed at a distance L and compute the extra average energy with respect to the absence of charges. Doing so one obtains [2] for two **widely** separated charges on first order of m-perturbation theory the result

$$V_Q(L,\theta) = \frac{mcg}{2}\left[\cos(\theta) - \cos(\theta)\cos\left(2\pi\frac{Q}{g}\right) + \sin(\theta)\sin\left(2\pi\frac{Q}{g}\right)\right]L. \tag{4.25}$$

We learn from (4.25) that: (1) there is a linear confining energy for any external charge that is not a multiple the fundamental charge g, (2) the non-zero mass prevents from "screening" in the sense we saw before, (3) when $Q/g \in \mathbb{Z}$ this confining force

[1] In this case the ground state of the theory is given by the so called "θ-vacua".

[2] One can find an exact computation of the string tension with widely separated charges for the massive case in [53].

does not exist anymore and (4) the theory is sensitive to the value of θ we consider. As we will see observation (3) is related to the phenomenon of string breaking that we will analyze later. Sometimes the string tension is a useful quantity that is defined as

$$\sigma_Q = V_Q(L)/L, \tag{4.26}$$

i.e., the slope of the function $V_Q(L)$.

4.3. Schwinger model on a lattice

In order to place the theory on the lattice we must rewrite the Hamiltonian (4.3) as a lattice Kogut-Susskind Hamiltonian with staggered fermions as explained in chapter 3. Then the theory is described via

$$H = -\frac{i}{2a}a\sum_n \left\{\phi_n'^{\dagger} e^{-igaA^1_n}\phi'_{n+1} - h.c.\right\} + ma\sum_n (-1)^n \phi_n'^{\dagger}\phi'_n + \frac{1}{2}a\sum_n E_n^2, \tag{4.27}$$

where as always g is the coupling constant for QED, taking to be the fundamental charge. Introducing the dimensionless operators

$$\phi = \sqrt{a}\phi', \qquad \theta_n = -agA^1_n, \qquad E_n = gL_n \tag{4.28}$$

we find the commutation relations

$$\{\phi_n, \phi_m^{\dagger}\} = \delta_{n,m}, \qquad [\theta_n, L_m] = i\delta_{n,m}, \tag{4.29}$$

and the Hamiltonian can be written as

$$H = -\frac{i}{2a}\sum_n \left\{\phi_n^{\dagger} e^{i\theta_n}\phi_{n+1} - h.c.\right\} + m\sum_n (-1)^n \phi_n^{\dagger}\phi_n + \frac{ag^2}{2}\sum_n L_n^2 \tag{4.30}$$

where the dimensionless electric field L_n is fixed by the (staggered) discrete Gauss' law

$$L_n - L_{n-1} = \phi_n^{\dagger}\phi_n - \underbrace{\frac{1}{2}(1-(-1)^n)}_{=\pi_n}. \tag{4.31}$$

Now the goal is to analyze the theory given by (4.27) and (4.31) applying the method studied in chapter 2.

4.3.1. Trial 1: Schwinger bosons representation

The first idea we tried in order to apply the Gaussian method was motivated by the quantum simulation perspective for the Schwinger model introduced in [57]. It's showed that this model can be simulated using two fermionic and two bosonic species arranged in an optical lattice. Following this picture our first approach was to give a Schwinger boson representation of the Schwinger algebra [58] on each link, truncating the spectrum of $L_n \equiv L$ to the region $-l < L < l$ equally on all links, giving rise to an

integer representation l of a (artificial) $SU(2)$ group on the link with $2l+1$ (internal) levels for the bosonic species.

As we saw in section 3.5, U and $U^\dagger$ act like ladder operators of electric flux in the Abelian case. Nevertheless

$$[U, U^\dagger] = 0 \quad \text{while} \quad [L_+, L_-] = 2L_z, \tag{4.32}$$

i.e., U is unitary while L_+ and L_- raising and lowering generators of the $\mathfrak{su}(2)$ algebra are not.

As explained before, the idea [9] is to substitute the $U(1)$ angular momenta by the artificial $SU(2)$ in an integer representation l by the following mapping for each link

$$L \longrightarrow L_z \tag{4.33}$$

$$U \longrightarrow \tilde{L}_+ = \frac{1}{\sqrt{l(l+1)}} L_+ \tag{4.34}$$

$$U^\dagger \longrightarrow \tilde{L}_- = \frac{1}{\sqrt{l(l+1)}} L_- \tag{4.35}$$

In this case

$$\tilde{L}_\pm |l, m\rangle = \sqrt{1 - \frac{m(m \pm 1)}{l(l+1)}} \, |l, m \pm 1\rangle \quad \text{and} \quad [\tilde{L}_+, \tilde{L}_-] = \frac{2}{l(l+1)} L_z, \tag{4.36}$$

therefore if $|m| \ll l$, i.e., we consider the "bulk" of a given representation l, then in the limit $l \to \infty$ we recover the $U(1)$ gauge group fulfilling (3.107) and (4.32).

This map was checked in [10] for pure-gauge theories, where the authors showed the rapidly convergence of this truncated theory to the standard Abelian Kogut-Susskind model for different values of l, for both the weak and strong coupling regimes. Thus we can now deal with the truncated Hamiltonian for a finite representation l that takes the form

$$H_l = \frac{-i}{2a\sqrt{l(l+1)}} \sum_n \left\{ \phi_n^\dagger (L_+)_n \phi_{n+1} - h.c. \right\} + m \sum_n (-1)^n \phi_n^\dagger \phi_n + \frac{ag^2}{2} \sum_n L_n^{z2}, \tag{4.37}$$

As a result, we have obtained a Hamiltonian (4.37) that depends on the generators of this artificial $\mathfrak{su}(2)$ algebra that will be represented by means of the Schwinger boson representation [58]. In order to do so we need to consider two species of bosonic creation/annihilation operators a and b on each link. Calling $\hat{N}_a$ and $\hat{N}_b$ their corresponding number operators on this specific link and $\hat{N} = \hat{N}_a + \hat{N}_b$, one obtains

$$L_z = \frac{1}{2}(\hat{N}_a - \hat{N}_b), \quad L_+ = a^\dagger b, \quad L_- = b^\dagger a, \quad L^2 = \frac{1}{2}\hat{N}(\frac{1}{2}\hat{N} + 1) \tag{4.38}$$

thus

$$m = \frac{1}{2}(n_a - n_b) \quad \text{and} \quad l = \frac{1}{2}N = \frac{1}{2}(n_a + n_b) \tag{4.39}$$

where n_a, n_b and N are the eigenvalues of $\hat{N}_a$, $\hat{N}_b$ and $\hat{N}$ respectively, meaning the number of bosons of both species **on each link of the lattice**. Since the electric

field is quantized, i.e., $m \in \mathbb{Z}$, N must be even as $l = N/2$. Moreover l **must be fixed and equal on all links of the lattice**, since otherwise it has not been proven one can recover the Kogut-Susskind Hamiltonian in the limit $l \to \infty$.

In this new representation the Hamiltonian takes the form

$$H_l = \frac{-i}{2a\sqrt{l(l+1)}} \sum_n \left\{ \phi_n^\dagger (a^\dagger b)_n \phi_{n+1} - h.c. \right\} + m \sum_n (-1)^n \phi_n^\dagger \phi_n + \frac{ag^2}{2} \sum_n \left[\frac{1}{2} (\hat{N}_a - \hat{N}_b) \right]^2, \tag{4.40}$$

which commutes with $\hat{N}$ and therefore it's a number preserving Hamiltonian for the sum of both bosonic species.

Gaussian method

Following the operational method described in subsection 2.5.3, we should now compute the Mean Field Hamiltonian of (4.40), but in this case a list of subtleties must be considered:

1. The number of bosons in a link must be **even and constant** during the Gaussian evolution. In spite of the fact $\langle N \rangle$ is conserved under the real time dynamics as we saw in subsection 2.5.2, this does not hold under the imaginary evolution (counterexample2.5.2). Moreover Gaussian states are not eigenstates of the number operator $\hat{N}$, and the condition $\hat{N} |G.S\rangle = 2l |G.S\rangle$ is too restrictive to be imposed.

2. Gauss' law must be imposed and preserved during the evolution.

3. The appearance of an interaction term between fermionic and bosonic degrees of freedom on the hopping term is being approximated by a pure Gaussian ansatz in bosons and fermions independently, i.e., we are just considering a Mean fermionic field acting on bosons and in the other way around. This looks to be a rather crude approximation.

The first two constraints could be imposed dynamically introducing additional terms in the Hamiltonian (4.40) in the form of chemical potentials which punish energetically their non-fulfillment. This could be achieved via the minimization of $\langle H \rangle$ with the additional terms

$$\langle H_G \rangle = \mu_G \sum_n \langle G_n \rangle^2 \qquad \text{with } \mu_G > 0 \tag{4.41}$$

in order to impose Gauss' law and

$$\langle H_N \rangle = \mu_N \sum_n \left(\left\langle \hat{N} \right\rangle_n - 2l \right)^2 \qquad \text{with } \mu_N > 0, \tag{4.42}$$

to implement the constant dimension of the representation l, taking both μ_G and μ_N to be much bigger than any other energy scale appearing in the Hamiltonian in order to ensure both constraints are fulfilled. As it can be observed we are imposing

the constraints in the weak sense, i.e., on average. This fact will be commented and further developed in section 6.1 for the (2+1)-dimensional formulation for pure-gauge theories where will be applied. Nevertheless the insertion of such different scales in the evolution will not usually allow a numerically efficient or accurate way to obtain the ground state of the system via imaginary-time evolution.

Moreover the requirement of minimizing (4.41), implies that the gauge symmetry is broken, since linear combination of states with different charges would fulfill the weak condition $\langle G_n \rangle = 0$, against parity superselection rule [29], already introduced in section 2.3. In addition, despite not being $\left\langle \hat{N} \right\rangle$ a constant value, we just need to worry about the fact that the ground state fulfills the condition $\left\langle \hat{N} \right\rangle = 2l$. On the other hand one also realizes that the use of the Schwinger boson representation gives rise to quartic terms in creation and annihilation operators that should be approximated by a mean field. We would like to find a way to better study the system avoiding so many approximations to give a more accurate description.

4.3.2. Trial 2: Erasing the gauge field

As we saw in the previous section the main difficulties to deal with the Schwinger model are the interactions between fermionic and gauge fields and Gauss' law. However as we saw in section 4.2, due to the absence of transversal directions, one can solve Gauss' law and write the Hamiltonian only with fermionic fields. In this section we will use this fact to erase the gauge phases living on the links of the lattice, by a unitary transformation giving rise to a *unitarily equivalent* Hamiltonian therefore describing the same physical phenomena. As in the continuum, this unitary transformation will result in a long-range potential term between charges.

In previous studies of the Schwinger model on a lattice a Jordan-Wigner transformation was performed, arriving to an equivalent spin system [16]. In our case we continue working with a second quantized Hamiltonian.

As we saw in Equation 3.35, fermionic operators transform under a local gauge transformation by a phase factor

$$\phi_n \to e^{i\Lambda_n} \phi_n,$$

where Λ_n is an operator acting on the gauge sector. This linear transformation is generated by some unitary operator $\mathcal{U}$, generated by a quadratic form in ψ and $\psi^\dagger$ as we saw in subsection 2.2.1, acting on the fermionic Fock space and therefore in order to erase the gauge phases one needs to apply a gauge transformation imposing

$$\theta_n = \Lambda_n - \Lambda_{n+1} \qquad \forall n, \tag{4.43}$$

i.e., the discrete analogue of $A_1(x) = -\partial_x \Lambda(x)$.

Let's fix open boundary conditions for the gauge field[3]. This means that (4.43) must be fulfilled for all $n = 1, \cdots, N-1$ where as before N is the number of sites in the chain and there is one less link. Solving this set of linear equations one finds that

$$\Lambda_n = \sum_{k=n}^{N-1} \theta_n + \Lambda_N, \tag{4.44}$$

[3]This boundary condition is suitable to benchmark the Gaussian ansatz in comparison to MPS results where open boundary conditions are often used.

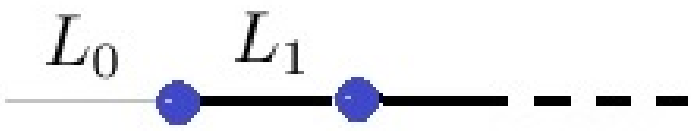


Figure 4.2.

where Λ_N can be freely chosen since (4.43) just imposes $N-1$ conditions. Let's choose $\Lambda_N = 0$.

Now we need to find the form of $\mathcal{U}$, which can be easily checked to be the Bogoliubov transformation

$$\mathcal{U} = \exp\Big[-i\sum_n \Lambda_n \phi_n^\dagger \phi_n\Big]. \tag{4.45}$$

Under this transformation the Hamiltonian takes the form

$$H \to \mathcal{U}H\mathcal{U}^\dagger = -\frac{i}{2a}\sum_n \{\phi_n^\dagger \phi_{n+1} - h.c.\} + m\sum_n (-1)^n \phi_n^\dagger \phi_n + \frac{ag^2}{2}\sum_n \mathcal{U}L_n^2\mathcal{U}^\dagger, \tag{4.46}$$

where we used the fact that $[\mathcal{U}, \phi_m^\dagger \phi_m] = 0$ for all m. Let's explicitly compute how the electric field transforms:

$$\mathcal{U}L_n\mathcal{U}^\dagger = L_n - i\sum_m \phi_m^\dagger \phi_m [\sum_{k\geq m} \theta_k + \cancelto{0}{\Lambda_N}, L_n] = L_n + \sum_{k\leq n} \phi_k^\dagger \phi_k, \tag{4.47}$$

then the Hamiltonian results in

$$H \to \mathcal{U}H\mathcal{U}^\dagger = -\frac{i}{2a}\sum_n \{\phi_n^\dagger \phi_{n+1} - h.c.\} + m\sum_n (-1)^n \phi_n^\dagger \phi_n + \frac{ag^2}{2}\sum_n \big(L_n + \sum_{k\leq n} \phi_k^\dagger \phi_k\big)^2, \tag{4.48}$$

that is a fermionic Hamiltonian of the kind discussed in section 2.4, with a quadratic and a quartic interacting term.

On the other hand Gauss' law (4.31) is mapped to

$$L_n - L_{n-1} = -\pi_n, \tag{4.49}$$

i.e., the electric field is fixed in this new picture via a recursive relation. Eq. (4.49) determines the electric field L_n entirely, up to an arbitrary additive constant L_0. In order to solve it we can consider an additional open link to the left of site 1 with electric field L_0 as represented in Figure 4.2.

Then fixing L_0[4] we solve (4.49) giving

$$L_n = L_0 - \sum_{k\leq n} \pi_k. \tag{4.50}$$

[4] As a convention we will choose the left boundary.

Remark. We could also have eliminated the π_n-term in the equation (4.50) by a gauge transformation of the form

$$\tilde{\mathcal{U}} = \exp\Big[-i\sum_n \Lambda_n(\phi_n^\dagger\phi_n - \pi_n)\Big]. \tag{4.51}$$

Note also that both $\mathcal{U}$ and $\tilde{\mathcal{U}}$ supposed a **non-Gaussian transformation**, i.e., an exponential of order higher than two in creation/annihilation operators, which in this case couples gauge and fermionic degrees of freedom on a cubic term of the form

$$\sum_n (\sum_{k=n}^{N-1}\theta_n + \Lambda_N)\phi_n^\dagger\phi_n.$$

This fact makes the difference between the method introduced in subsection 4.3.1 and the one presented now, since correlations between both degrees of freedom are taken into account.

With the same procedure one could also erase the phase factor $-i$ multiplying the first term of the Hamiltonian without changing neither Gauss' law nor the Hamiltonian. Therefore its final form turns out to be

$$H = \varepsilon\sum_n\{\phi_n^\dagger\phi_{n+1} + h.c.\} + m\sum_n(-1)^n\phi_n^\dagger\phi_n + \frac{ag^2}{2}\sum_n\Big(L_0 + \sum_{k\le n}Q_k\Big)^2 \tag{4.52}$$

where we have defined $\varepsilon := 1/2a$, the hopping parameter which turns out to be a relevant parameter in purely lattice considerations [14]. In fact the last term in (4.52) corresponds to the long range potential and background interaction terms appearing in the continuum case (4.20) as explained in section 4.3.2.

In order to explore the continuum limit of this theory on a lattice with lattice spacing a it's useful to introduce the parameter $x = 1/a^2g^2$ following the ideas from [26]. The continuum limit then corresponds to $x \to \infty$. The Hamiltonian (4.52) takes the form

$$H = \frac{g}{2\sqrt{x}}\Big[\underbrace{x\sum_n\{\phi_n^\dagger\phi_{n+1} + h.c.\}}_{H_{int}} + \underbrace{\frac{2\sqrt{x}}{g}m\sum_n(-1)^n\phi_n^\dagger\phi_n}_{H_M} + \underbrace{\sum_n\Big(L_0 + \sum_{k\le n}Q_k\Big)^2}_{H_E}\Big] \tag{4.53}$$

with $L_0 \in \mathbb{R}$ a real free parameter. The interpretation of L_0 can be followed from (4.50) and Figure 4.2. In the new frame the electric field on all the links have the constant contribution of L_0. Therefore we can understand L_0 as a constant background electric field, in an equivalent way as θ-field appeared in the continuum formulation of the theory, in fact its relation should be given by $\theta = 2\pi L_0/g$ as it happened for F.

Conclusion. In conclusion, we have transformed the Hamiltonian to a different frame where: Gauss' law has been already considered inside the Hamiltonian **giving rise to a long range force interaction between fermionic charges**, the gauge field has been erased allowing us to just consider Fermionic Gaussian states as an ansatz and a truncation of the exact Kogut-Susskind Hamiltonian has been avoided.

Recovering the continuum limit

In order to obtain (4.20) we used the restriction

$$\int dx\, j^0(x) = 0, \tag{4.54}$$

which allowed us to use the equality

$$\int dx \int_{-\infty}^{x} dy\, j^0(y) = -2 \int dx\, x j^0(x) \tag{4.55}$$

and obtain the electric term in the fermionic representation. Relation (4.55) can be used to express the electric term in a way that can be compared to the discretized case

$$\frac{1}{2}g^2 a \sum_n \left(E_0/g + a \sum_{k\leq n} Q'_k \right)^2 \xrightarrow{a\to 0} \frac{1}{2}g^2 \int dx \int_{-\infty}^{x} dy\, j^0(y) \int_{-\infty}^{x} dz\, j^0(z) + gF \int dx \int_{-\infty}^{x} dy\, j^0(y) \tag{4.56}$$

proving that the discrete formulation after erasing the gauge field tends to the continuum one as $a \to 0$. We have used the dimensional operators $aQ' = Q$ and $E_0 = gL_0$ as defined in (4.28). The missing term is a constant value $\sim F^2 \cdot \text{Vol}$, proportional to the volume of space that can be erased by redefining the vacuum energy. Therefore the long-range force appearing in (4.52) is in fact the discrete version of the one encountered in the continuum theory.

Ground state in strong-coupling limit

Consider the dimensionless Hamiltonian $W = \sqrt{x}/gH$ as in [16]. In the strong-coupling limit $x \to 0$, the only remaining terms are H_M and H_E. Since H_E is strictly positive, the ground state of the system will fulfill $L_n = 0$ for all n. On the other hand due to the staggered mass appearing in H_M, odd sites of the lattice will be occupied while even ones will be empty

$$\phi_n^\dagger \phi_n = \frac{1}{2}(1 - (-1)^n), \tag{4.57}$$

supporting the interpretation of the Dirac sea picture, presented in section 3.4.1, that particles (antiparticles) occupy even (odd) sites of the lattice. This state $|\Omega\rangle_f$ will be called indistinctly Dirac sea or "free vacuum". In fact this allows a different, more physical derivation of the staggered charge Equation 3.87 as explained in [16].

Insertion of static chargers

Interesting physical phenomena in the Schwinger model is related as we saw to the interaction of two static charges placed on different sites of the lattice. Therefore we should introduce an external fermionic charge density in Gauss' law describing those. The mathematical insertion of these static charges is via enlarging the fermionic Hilbert space with an additional static one, i.e., adding a non-dynamical massive fermionic field. This only implies the modification of the charge density in Gauss' law

$$L_n - L_{n-1} = Q_n + Q_n^{\text{ext}}. \tag{4.58}$$

As explained before, one could also erased the external charge density by a unitary transformation that takes the form

$$\mathcal{U} = \exp\Big[- i \sum_n \Lambda_n (Q_n^{\text{ext}} + Q_n)\Big], \tag{4.59}$$

where in the new frame this gives as a result the Hamiltonian

$$\boxed{H = \varepsilon \sum_n \{\phi_n^\dagger \phi_{n+1} + h.c.\} + m \sum_n (-1)^n \phi_n^\dagger \phi_n + \frac{ag^2}{2} \sum_n \Big(L_0 + \sum_{k \leq n} \{Q_k + Q_k^{\text{ext}}\} \Big)^2} \tag{4.60}$$

4.3.3. Gaussian approach for the Schwinger model

In this section we will apply the Gaussian approach to the Hamiltonian (4.70) in order to describe the physics of the Schwinger model. As we said, it's important to realize the unitary transformation given by (4.59) is non-Gaussian which, not only erases the gauge field but also allows us a better description of the system by applying **the Gaussian approach in the rotated frame** (unitarily equivalent) frame.

In order to apply the Gaussian ansatz, we use the Nambu representation $\Phi = (\phi, \phi^\dagger)^T$ for which the Covariance Matrix takes the form

$$\Gamma = \begin{pmatrix} \langle \phi \phi^\dagger \rangle & \langle \phi \phi \rangle \\ \langle \phi^\dagger \phi^\dagger \rangle & \langle \phi^\dagger \phi \rangle \end{pmatrix} \tag{4.61}$$

with the restrictions given by Lemma 2.3.3.

Mean Field Hamiltonian

Since H_M and H_{int} in (4.70) are already quadratic in creation and annihilation operators[5] then they are already in Mean Field form. We just need to apply the normal order $:\,:$ with respect to the pure FGS ansatz. The electric term H_E however is a long-range quartic operator. After applying Wick's theorem the state dependent quadratic Hamiltonian reads

$$\boxed{H_Q(\Gamma) = \langle H \rangle + \frac{1}{2} :\Phi^\dagger \Big[\sigma_z \otimes (mD + \varepsilon T) + \frac{ag^2}{2} \sum_n \Big\{ 2(L_0 - \sum_k^n \pi_k)\sigma_z \otimes id_n + H_4(n) \Big\} \Big] \Phi :,} \tag{4.62}$$

where: σ_z is the diagonal Pauli matrix, D the diagonal matrix $D = \text{Diag}((-1)^n)$, T the tridiagonal matrix with $1's$ on the ± 1 diagonals and 0 on the main one, Tr^n trace over the $n \times n$ first entries of the respective matrix and $H_4(n)$ is given by

$$H_4(n) = 2 \begin{pmatrix} Tr^n(\langle \phi \phi^\dagger \rangle) - \frac{1}{2} + \langle \phi \phi^\dagger \rangle & - \langle \phi \phi \rangle \\ - \langle \phi^\dagger \phi^\dagger \rangle & -Tr^n(\langle \phi \phi^\dagger \rangle) + \frac{1}{2} - \langle \phi \phi^\dagger \rangle^T \end{pmatrix}. \tag{4.63}$$

[5] It's on this point where the Unitary transformation $\tilde{U}$ took its most important role.

Computation of the energy

As we saw in chapter 2, the average energy plays an important role in the Gaussian approach since it should decrease during the imaginary time evolution allowing us to know the rate at which the system tends to the ground state. Therefore its analytical computation it's an important calculation in this method. Applying as always Wick's theorem we find the expression

$$\begin{aligned}\langle H\rangle = mTr(D\left\langle\phi^\dagger\phi\right\rangle) + \varepsilon(Tr^{+1}(\left\langle\phi^\dagger\phi\right\rangle) + h.c) + \frac{ag^2}{2}\sum_n\Big(L_0^2 - 2L_0\sum_k^n\pi_k \\ + \big(\sum_k^n\pi_k\big)^2\Big) + ag^2\sum_n\Big\{(L_0 - \sum_k^n\pi_k)Tr^n(\left\langle\phi^\dagger\phi\right\rangle)\Big\} \\ + \frac{ag^2}{2}\sum_n\Big\{Tr^n(\left\langle\phi^\dagger\phi\right\rangle)^2 + Tr^n(\left\langle\phi^\dagger\phi^\dagger\right\rangle \underbrace{\langle\phi\phi\rangle}_{-\langle\phi\phi\rangle^T}) + Tr^n(\left\langle\phi^\dagger\phi\right\rangle\left\langle\phi\phi^\dagger\right\rangle^T)\Big\},\end{aligned} \tag{4.64}$$

where Tr^{+1} is defined as the sum over the upper-first diagonal's elements. The derivation of (4.62) and (4.64) can be found in section B.1 of the Appendix.

Another relevant observable that will allow us to characterize the system is the electric field on a link. Since all our observables are measured on the ground state of the system $|\Omega\rangle$, that we are approximating by a Gaussian state, the average of L_n reads

$$\begin{aligned}\langle\Omega|L_n|\Omega\rangle_{O.F} = \left\langle\Omega\middle|\tilde{L}_n\middle|\Omega\right\rangle_{R.F} = \left\langle\Omega\middle|\mathcal{U}L_n\mathcal{U}^\dagger\middle|\Omega\right\rangle_{R.F} = \left\langle\Omega\middle|L_n + \sum_{k\le n}\phi_k^\dagger\phi_k\middle|\Omega\right\rangle_{R.F} \\ = \left\langle\Omega\middle|L_0 + \sum_{k\le n}\{\phi_k^\dagger\phi_k - \pi_k\}\middle|\Omega\right\rangle_{R.F} \approx L_0 - \sum_{k\le n}\pi_k + Tr^n\Big(\left\langle\phi^\dagger\phi\right\rangle\Big),\end{aligned} \tag{4.65}$$

where the subscripts $O.F$ and $R.F$ stand for "Original frame" and "Rotated frame" respectively, the vacuum state transforms as $|\Omega\rangle_{R.F} = \mathcal{U}|\Omega\rangle_{O.F}$ and in $\approx$ the Gaussian approximation has been applied being the last average evaluated on the Gaussian ground state.

4.4. Physics in the Schwinger model: Screening and confinement

From our analysis in section 3.6, one expects an electric flux tube connecting the particle-antiparticle —string— and the potential $V_Q(L)$ growing linearly with the distance. However, due to the consideration of dynamical fermions, there exists a critical distance L_c at which the string breaks, being the static charges completely screened. The way this screening appears depends on whether we consider massless or massive fermions as we stated while solving the continuum theory in subsection 4.2.2.

In the next section we will study the Schwinger model for both massless and massive fermions in order to establish the validity of the Gaussian approach. Since an analytical expression for $V_Q(L)$ can be exactly obtained for the massless Schwinger model, we will make use of it in order to check the results obtained via the Gaussian approximation.

Recall that $V_Q(L)$ is computed as the ground state energy $E_Q(L)$ for a configuration of a static particle-antiparticle pair $\bar{q}q$ at a distance L

$$V_Q(L) = E_Q(L) - E_{\text{vac}} \tag{4.66}$$

where E_{vac} is the energy of the (interacting) vacuum and on the lattice, distances are given by $L = k/\sqrt{x}$ (in physical units $g = 1$) with $n \in \mathbb{Z}^+$.

Moreover depending on the physics we would like to analyze, we will consider different boundary conditions for the string, either —static charges— or excitations of the fermionic field at the corresponding site —dynamical charges. Finally as a **convention** we denote by Q the positive external charge measured in units of the fundamental one g.

4.4.1. Massless Schwinger model

In section 4.2.2 we saw that due to the finite mass acquired $M = g/\sqrt{\pi}$ by the photon, the potential between impurities should be a screening one, depending on M. In fact placing external charges into the system one obtains that the potential energy "between" them is given by [52]

$$V_Q(L) = \frac{\sqrt{\pi} g Q^2}{2}\left(1 - e^{-gL/\sqrt{\pi}}\right), \tag{4.67}$$

with $g/\sqrt{\pi}$ the mass acquired by the photon.

Classically, one would expect this potential to rise linearly with the inter-charge separation but vacuum polarization can shield these impurities giving rise to the screening potential (4.67), which saturates to a constant value for long distances for any either integer or not integer charge Q.

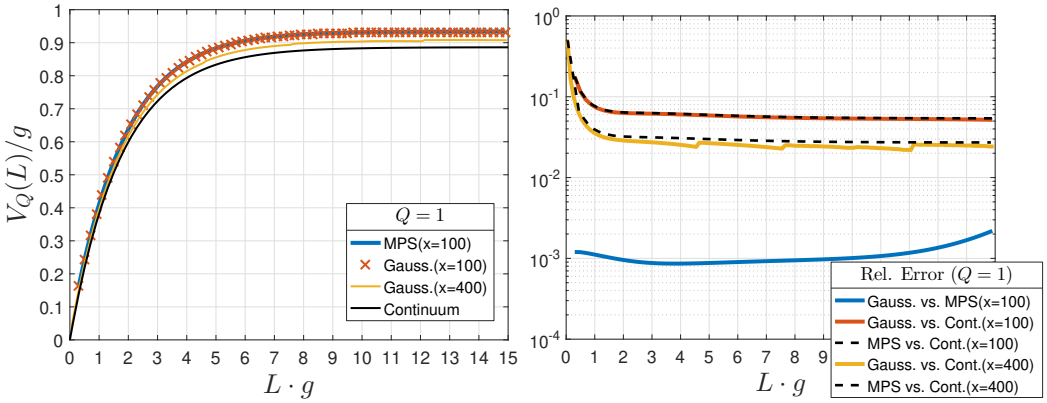
Since (4.67) is an exact result obtained for the continuum theory, we need to consider the continuum limit of our discrete Hamiltonian. In order to do so, we will consider (4.53) for different values of $x = 1/g^2a^2$ and compute the ground state energy of the system for different distances L between the static charges. In Figure 4.3a $V_Q(L)$ has been plotted for $x = 100$ and 400, in comparison to the analytical result and the result obtained from MPS in Ref. [26]. We observe, as expected, that larger values of x give more accurate results to obtain the continuum limit. Moreover in Figure 4.3b a more quantitative analysis has been given for both parameters $x = 100$ and $x = 400$. In Figure 4.3b we have plotted the relative error comparing two results for different values of x in logarithmic scale. The relative error is calculated as follows

$$\Delta(\text{M1,M2}) = \frac{\left|V_Q^{\text{M1}}(L) - V_Q^{\text{M2}}(L)\right|}{\left|V_Q^{\text{M2}}(L)\right|},$$

where M1 and M2 stand for the first and second arguments in the legend written as "M1 vs. M2". In this way we consider the continuum theoretical result as the most

exact result while we consider the Gaussian ansatz as the least accurate, since it's the one we want to analyze.

Therefore in Figure 4.3b we observe that for $x = 100, 400$, both MPS and the Gaussian ansatz recover the continuum analytical result with the same level of accuracy. In fact the relative error between MPS and the Gaussian ansatz is bounded by $\Delta < 0.3\%$. For $x = 100$ the relative error is bounded by $\Delta < 8 \cdot 10^{-2}$ except for distances $L \cdot g < 1$, where the continuum limit does not work so well. In fact this is a problem of the discretization that cannot be solved by just taking x larger, as can be also realized in the Figure 4.3b. Then as long as we consider distances $L \cdot g > 1$, we will only make a relative error of less than 8%. Since the agreement with the analytical result for $V_Q(L)$ is already good enough in the case $x = 100$ and in order to compare with the results obtained in $x = 100$, we will restrict ourselves from now on to $x = 100$.



(a) Qualitative comparison: Gaussian ansatz, MPS and exact continuum exact.

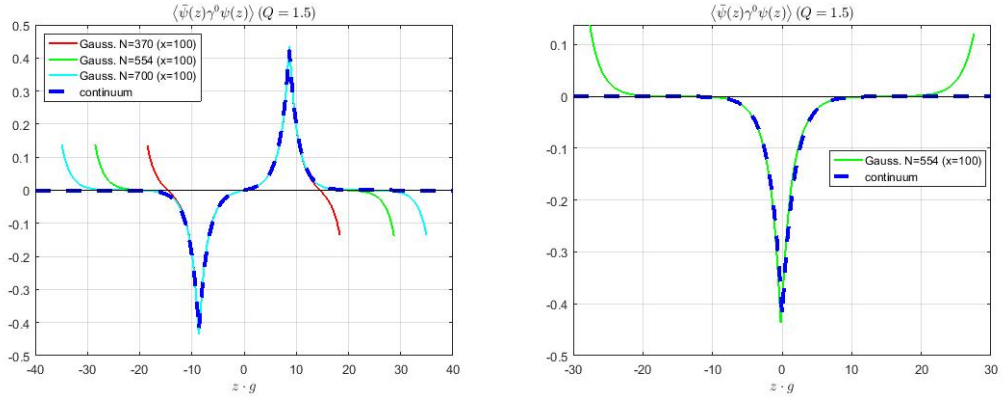
(b) Comparison in logarithmic scale with MPS and exact continuum result for $x = 100, 400$.

Figure 4.3.: Comparison among exact continuum result, Gaussian ansatz and MPS [26] for $Q = 1$ and $x = 100, 400$.

In order to visualize the screening mechanism, we would like to plot the distribution of the dynamical fermionic charge density $\langle \bar{\psi}(z)\gamma^0\psi(z) \rangle$ on the ground state of such configuration. To do so we need to consider the (continuous) charge density distribution $\langle \bar{\psi}(z)\gamma^0\psi(z) \rangle$ for which an analytical result was also obtained in [52]

$$\langle \bar{\psi}(z)\gamma^0\psi(z) \rangle (x_0, y_0) = \frac{Qg}{2\sqrt{\pi}} \left(e^{-g|z-y_0|/\sqrt{\pi}} - e^{-g|z-x_0|/\sqrt{\pi}} \right) \tag{4.68}$$

where x_0 and y_0 are the positions of the positive and negative external charges $\pm Q$ respectively. In order to compare with the exact result (4.68), we have to recover the staggered formulation of locating fermions ϕ'_n on the lattice. Remember the fact that particles of positive (negative) charge live on the even (odd) nodes of the lattice, whose combination gives rise to the appearance of a two-component Dirac field in the continuum limit. Therefore in order to recover the continuum limit, we consider the intermediate points between an odd (to the left) and an even (to the right) sites giving $z = a(2n - 1/2)$ with $n \in \mathbb{Z}$. In these points the dynamical charge density takes the form



(a) Evaluation of finite-size effects. (b) Screening of a isolated charge $Q = 1.5$.

Figure 4.4.: For $Q = 1.5$ and $m/g = 0$, we test the Gaussian approximation via the exact result for charge density.

$$\left\langle \bar{\psi}(z)\gamma^0\psi(z)\right\rangle (x_0, y_0) = \frac{1}{2}\left\langle \underbrace{Q'_{2n-1}}_{\text{antipart.}} + \underbrace{Q'_{2n}}_{\text{particle}} \right\rangle = \frac{1}{2a}\left\langle Q_{2n-1} + Q_{2n}\right\rangle \tag{4.69}$$

where we have used the relation $\phi_n = \sqrt{a}\phi'_n$ and the definition of charge density $Q_n = \phi_n^\dagger\phi_n - 1/2(1-(-1)^n)$.

In Figure 4.4a we have plotted $\left\langle \bar{\psi}(z)\gamma^0\psi(z)\right\rangle$ for two static charges $Q = 1.5$ at a distance $L \cdot g = 17.3$ computed via the Gaussian approximation and the exact result (4.68). We observe two symmetrical accumulations of charge around the static ones which completely screens them. Indeed the solution we obtained coincides with the analytical result except on the boundaries, due to **finite-size effects**. This effect can be observed in Figure 4.4a, where we have plotted the result for different chains of length $N = 370, 574$ and 700, where we observe a better agreement for larger N's. Moreover Figure 4.4b shows screening is independent of the existence of other charges in the massless case.

4.4.2. Massive Schwinger model

Being not solvable, it's a known exact result [53] that as long as the external charges are integer multiples of the fundamental charge, these will be completely screened by the creation of particle-antiparticle pairs out of the vacuum (Schwinger mechanism) giving rise to the breaking of the string. This will be studied in the next sections. Once this has happened one would expect a flattening of the potential $V_Q(L)$ for L greater than some critical distance L_c, where the excited pairs screen the external charges creating **two isolated (mesons) color singlets**. Therefore one realizes two different phases: a confining phase where opposite charges are joined by an electric flux tube and string-breaking phase where these charges are screened by the creation of pairs.

Structure of the vacuum

As it was explained in section 4.2.2, the massive model is sensitive to the chosen value for the θ-field (L_0 in the discretized case), that as we saw is interpreted as a background field. Charges are "confined" [6] in the model for any value of θ but, as it was pointed out by Coleman [55] and later on confirmed in [59], there is a special phenomenon appearing for $\theta = \pi$ known as "half-asymptotic" particles. Nevertheless we will focus on the case $\theta = L_0 = 0$ following previous studies like the ones done in [15, 16, 26] in order to test the Gaussian method. We leave the study of the θ-vacuum as part of the Outlook 6.3.

Confining/string breaking quantum phase transition

In Figure 4.5 the Gaussian approach results are showed in comparison to those obtained with MPS in Ref. [26], whose authors have kindly shared their data with us. In Figure 4.5a the potential $V_Q(L)$ is displayed for several values of the ratio $m/g = 0, 0.125, 0.25, 0.75, 1, 2$. At the critical length $L = L_c$, a quantum phase transition takes place between the confining and string breaking phases. Moreover, as expected from the semiclassical results obtained in the bosonized theory [26], this transition happens more suddenly for larger values of m/g and L_c is a function of m/g. There is a linear confining potential for $L << L_c$ and a flattening of $V_Q(L)$ for large distances $L >> L_c$ corresponding to the string breaking phase where the two mesons have been formed.

In Figure 4.5b a comparison between both methods is showed via the computation of the relative error

$$\Delta = \frac{\left| V_Q^{\text{Gauss.}}(L) - V_Q^{\text{MPS}}(L) \right|}{\left| V_Q^{\text{MPS}}(L) \right|}$$

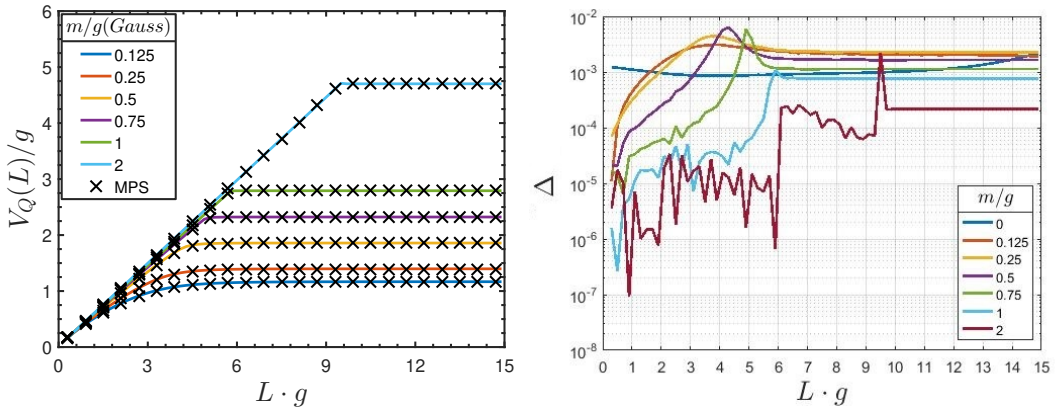
in logarithmic scale, where Gauss. and MPS stand for Gaussian and MPS methods respectively. We can appreciate that the relative difference between both methods is given for the case $m/g = 0.5$ and it's bounded by $\Delta \sim 7 \cdot 10^{-3}$ (i.e., a percent error of 0.7%) near the critical distances $L \sim L_c$, at which the appearance of peaks take place being $V_Q^{\text{Gauss.}}(L)/g > V_Q^{\text{MPS}}(L)/g$ for all values of m/g. The appearance of these peaks is related to the fact that at $L = L_c$ the quantum phase transition takes place.

At these points the confining and string-breaking phases have the same energy for the exact Hamiltonian H. However since we are using a mean-field approximation $H_Q(\Gamma)$, these two could correspond to different energies. Therefore near L_c, one needs to initialize the imaginary time evolution with seeds corresponding to a string and two mesons configurations, which are orthogonal to each other, taking the lowest energy at the end of the evolution[7]. In fact it could also happen that a linear superposition of both states have a lower energy in the Gaussian approximation. Nevertheless recall the fact that Gaussian states do not close a linear space and therefore linear superpositions of Gaussian states are in general not Gaussian. Thus since we are using

[6] By "confined" we mean that one can see either confinement or the confining/ string breaking transition.

[7] Remember that the imaginary time evolution could get stuck in a local minimum.

a mean-field Hamiltonian the description at L_c where the quantum phase transition takes place is in principle not as reliable as other techniques.



(a) Gaussian computation vs MPS

(b) Comparison in logarithmic scale.

Figure 4.5.: Comparison Gaussian approximation with MPS [26] for $Q = 1$ and $x = 100$ for the massive Schwinger model.

We can conclude that the Gaussian approach correctly describes the quantum phase transition and the confining and string breaking phase separately, for different values m/g. Moreover, we should ensure for distances near the critical one that the imaginary time evolution has arrived to a global rather than to a local minimum.

Characterization via imaginary-time evolution The characterization of the string-breaking phase, can be already realized in the imaginary time evolution calculation that is done in order to find the ground state of the system.

Figure 4.6 shows the energy and the electric flux configuration of the system as a function of the imaginary time in the string breaking phase for $L \cdot g = 12.1$ and $m/g = 2$. Starting with an initial seed of a string, we as usually observe a fast exponential decay of the energy at the begining of the imaginary time evolution followed by a flattening. As it was explained in [14], this metastable plateau corresponds to the interacting string state. For a later time we again observe a decrease in the energy of the configuration which coincides, as it can be seen in the (imaginary) dynamical electric flux configuration plot, to the breaking of the string. At this moment the mesons have been formed as can be seen in the evolution of the dynamical fermionic charge density in Figure 4.7. On the other hand, using the identical initial seed, the previous metastable plateau becomes a stable one for the confining phase.

Partial screening

Unlike the massless case, it's also known that for the case of charges that are non-integer multiples of the fundamental charge g, the string tension σ_Q does not vanish, i.e., the string does not break, and therefore only the integer part of a static charge $\lfloor Q \rfloor$ can be screened [53]. While this result is known to be true in the weak (mass-perturbative) coupling limit $m/g \to \infty$, we will now analyze its behavior for different finite ratios of m/g. In Figure 4.8a we have plotted the potential for the values

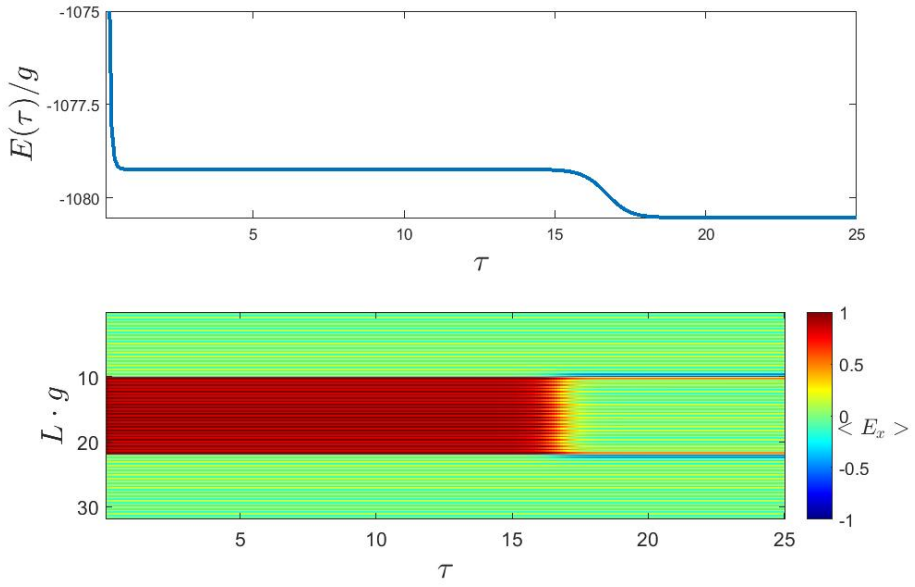


Figure 4.6.: Energy and flux imaginary evolution for string-breaking phase for an external charge $Q = 1$ and $x = 100$ for $m/g = 2$.

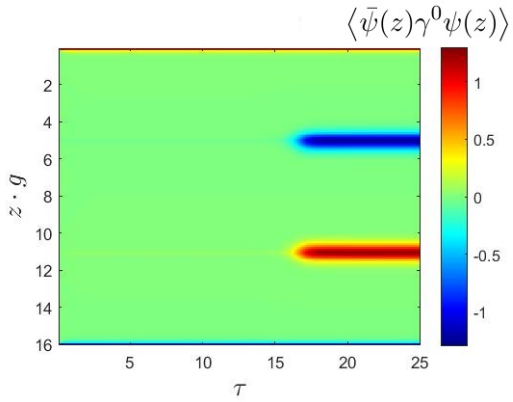
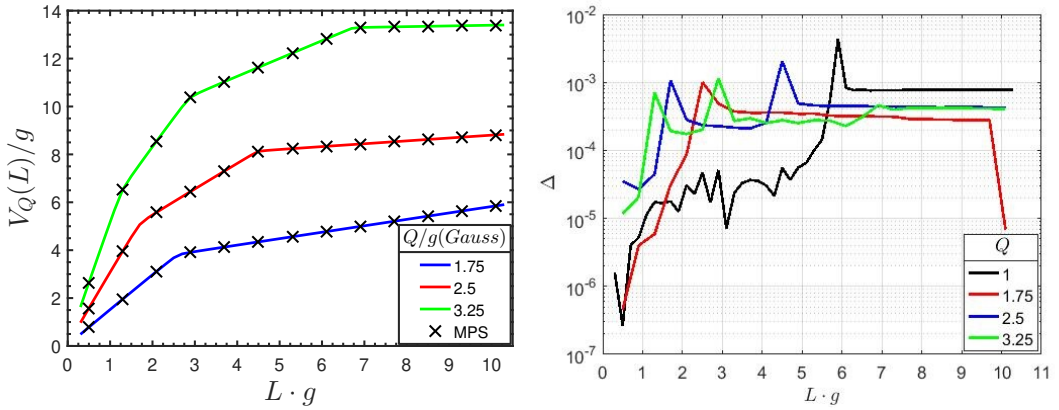


Figure 4.7.: Charge density imaginary evolution for string-breaking phase for an external charge $Q = 1$ and $x = 100$ for $m/g = 2$

$Q = 1, 1.75, 2.5, 3.25$ with the Gaussian method (straight lines) in comparison to MPS results ($*$ scatter plot). We observe as many changes in the string tension σ_Q, as the integer part of the static charges, therefore creating $\lfloor Q \rfloor$ dynamical pairs which screen them. The resulting "mesons" are connected by the remaining electric flux tube. This phenomenon is known as *partial string breaking* and it's been deeper discussed in [26]. In Figure 4.8b we compare the Gaussian to the MPS results from [26] as before. In this case we observe as many peaks in $\Delta(L)$ bounded by $\Delta < 4 \cdot 10^{-3}$ with maximum in the case $Q = 1$, as $\lfloor Q \rfloor$ for each case, since at each of these points a "string breaking" phenomenon is taking place.

Again we can conclude that the Gaussian method is able to describe this phe-



(a) Gaussian computation versus MPS results. Qualitative comparison.

(b) Comparison in logarithmic scale between Gaussian and MPS.

Figure 4.8.: Partial screening $m/g = 1$. Comparison between Gaussian and MPS calculation from [26].

nomenon with a surprisingly good accuracy.

4.4.3. Real time dynamics

Finally let's analyze the dynamical properties of the theory, where we will focus on the understanding of the string breaking mechanism. Most of our understanding of this effect is related to static properties as we saw in the previous section. In fact Tensor Networks techniques are being developed nowadays, due to its advantage over conventional Monte Carlo simulations of avoiding the "sign problem" [6] that appears in some parameters regime when considering dynamical fermions [14, 26, 27]. Moreover Quantum Simulation protocols are also being developed [10]. In fact last year (2016) the first experimental demonstration of a digital quantum simulation of a lattice gauge theory was realized [12] by the use of trapped ions. Similar to them, the Gaussian approach allows us to consider the real time evolution of a system. Therefore this method open new possibilities to study the dynamics of gauge theories, like for example understand the dynamical breaking from the creation of particle-antiparticle pairs on top of each other and their subsequent dynamical separation in order to screen the static charges.

In [52] the real time evolution of the charge density was already study for the massless Schwinger case. However no much is known about the real time dynamics of the string breaking. In fact it wasn't till 2013 when a first attempt to describe the space-time picture of string breaking phenomenon [60] was made, and 2016 when a more detailed discussion was given [27] by means of Tensor Network techniques.

Moreover in order to be able to compare with the results obtained by MPS in [14, 27], we will consider the Hamiltonian form

$$H = -\varepsilon \sum_n \left\{\phi_n^\dagger \phi_{n+1} + h.c.\right\} + m \sum_n (-1)^n \phi_n^\dagger \phi_n + \frac{ag^2}{2} \sum_n \left(L_0 + \sum_{k \leq n} \left\{\phi_k^\dagger \phi_k - \pi_k\right\}\right)^2, \tag{4.70}$$

where $\varepsilon \in \mathbb{R}$ will be consider a free hopping parameter therefore focusing in the (exact) gauge symmetry implemented in the lattice Hamiltonian (4.70) rather than on the continuum limit. In addition we will consider two different scenarios: an initial dynamical string configuration whose extremes can freely propagate (dynamical fermions) and an inital static configuration where the extremes are fixed by placing two static particles. Both states must be constructed on top of what we will call **interacting vacuum state**, i.e., the ground state of the total Hamiltonian, different from the "free vacuum" or the Dirac sea $|\Omega\rangle_f$ we obtained in section 4.3.2. Therefore, we start obtaining the interacting vacuum state $|\Omega\rangle$ of the system via an imaginary time evolution and in the case of a free string, we will afterwards apply the gauge invariant operator whose form in the original frame is

$$S_{n,k} = \phi_n^\dagger U_n \dots U_{n+k-1} \phi_{n+k}, \tag{4.71}$$

for odd k and in the rotated frame via (4.51) takes the form

$$\mathcal{U}^\dagger S_{n,k} \mathcal{U} \longrightarrow \tilde{S}_{n,k} = \phi_n^\dagger \phi_{n+k}, \tag{4.72}$$

therefore generating a particle-antiparticle pair at sites n and $n+k$.

Moreover because we are not interested in recovering the continuum limit and since we will allow to independently change m and g, we consider the integer distances $L/a = k$ unlike the previous sections ($L = k/\sqrt{x}$ in units of g), where k names a site on the lattice.

Static string breaking:

As we have seen, the usual way of proving string breaking is via the analysis of the static potential energy $V_Q(L)$. In this way, we can focus on the string breaking phenomenon and ease the complications coming for the different possibilities in which the string can freely propagates. Therefore, in this part we study the scenario where two static external charges are placed on the lattice at a distance greater than the critical one. At this point one would expect to see how the string gets broken as the system evolves. We consider a model with $\varepsilon = 2$ and $m/g = 1$ which results in a critical distance $L_c/a \sim 10$ and therefore we place the static charges at a distance $L/a = 33$ that is greater than L_c, since we are interested in studying the string breaking dynamics. Since we set $\hbar = g = 1$, time is given in units of $\hbar/g$.

In Figure 4.9 we observe the evolution of the string, surrounded by the interacting vacuum and where the electrix flux tube gets broken and it oscillates between different flux configurations without recovering the complete string configuration, i.e., we are realizing the dynamical breaking of the string.[8] Therefore the Gaussian approach could provide a method to understand the dynamical features of gauge theories, and more specifically of the string breaking phenomenon.

Free string breaking:

A different approach can also be considered. In order to test our results we compare them with [27]. In [27] the authors considered the Quantum Link Model formula-

[8] The real-time dynamics needs a high precision. That's the reason of using a time step equals to $\Delta t = 5 \times 10^{-4}$ in the numerical solution, while testing the state at each time is still a pure fermionic Gaussian state.

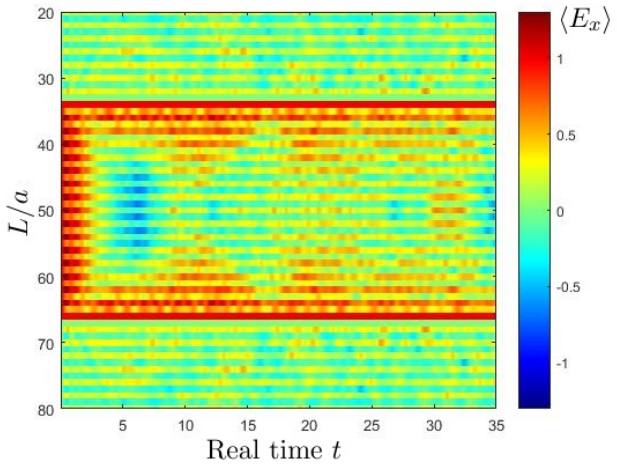


Figure 4.9.: Real time dynamics for a distance between static charges equals to $z \cdot g = 33a$ and $\varepsilon = 2$, $m/g = 1$.

tion where a truncation of the infinite-dimensional gauge Hilbert space on a link is performed [61]. On the other hand, due to the applied unitary transformation to the Hamiltonian (4.70), we avoid to perform such a truncation, giving the Gaussian method an exact description of the system when $g = 0$. In this part, in order to be able to compare our results with [27], we will consider the case $\varepsilon = 1$ and therefore time is measured in units of $\hbar/\varepsilon$. Let me highlight the fact that in [27], the operator (4.72) is applied to the free vacuum $|\Omega\rangle_f$ instead to the interacting one $|\Omega\rangle$. Therefore this initial state looks like a global quench in the considered system, unlike our previous case where we considered a string on top of the real interacting vacuum (local quench) evolving under the Hamiltonian (4.70).

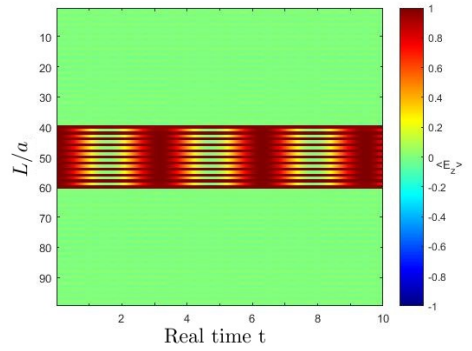
In Figure 4.10 we compare the Gaussian method to results obtained by MPS in [27]. We observed the perfect agreement for the case $m = 3$ and $g = 3.5$ (while $\varepsilon = 1$) plotted in Figure 4.10a and Figure 4.10d where the dynamical fermions are basically motionless out of the string since the mass term is quite bigger than the hopping interaction. The case $m = 0.25$ and $g = 1.25$ is given in Figure 4.10b and Figure 4.10e where the first part of the evolution is quite similar but it starts to differ around $t \sim 4$. The last two plots Figure 4.10c and Figure 4.10f show the evolution for the case $m = g = 0$ that is exactly solved by the Gaussian ansatz due to the fact that (4.70) becomes a quadratic Hamiltonian in creation/annihilation operators. As it can be clearly seen, both plots do not coincide.

In order to identify which of both results is correct, let's solve the problem analytically. In this case $m = g = 0$, the Hamiltonian takes the form

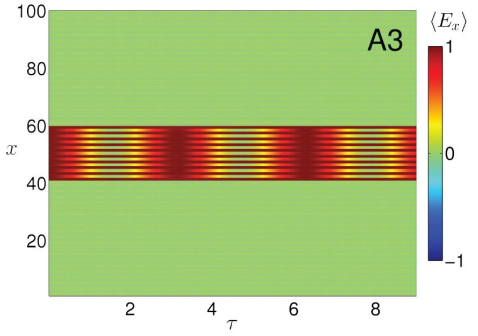
$$H = \varepsilon \sum_{n=1}^{N} \{\phi_n^\dagger \phi_{n+1} + \phi_{n+1}^\dagger \phi_n\} \equiv \phi^\dagger \mathcal{H} \phi, \tag{4.73}$$

where ϕ is a column vector defined by $\phi = (\phi_n)_n$ and $\phi^\dagger$ is Hermitian conjugate formed by creation operators. Then in the Heisenberg picture $\phi(t)$ is given by

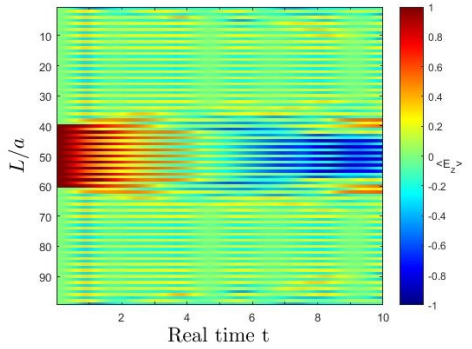
$$\phi(t) = e^{-i\mathcal{H}t}\phi(0) \Longrightarrow \phi^\dagger(t) = \phi^\dagger(0)e^{i\mathcal{H}t}, \tag{4.74}$$



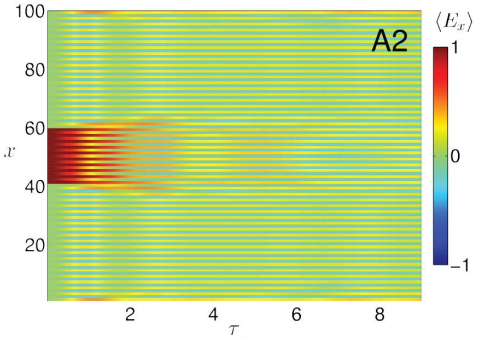
(a)



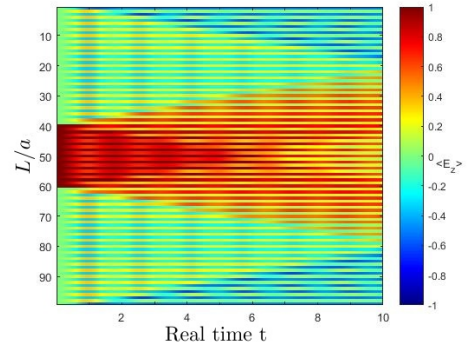
(b)



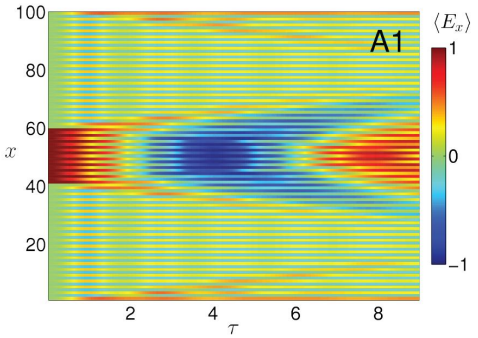
(c)



(d)



(e) Gaussian approximation.

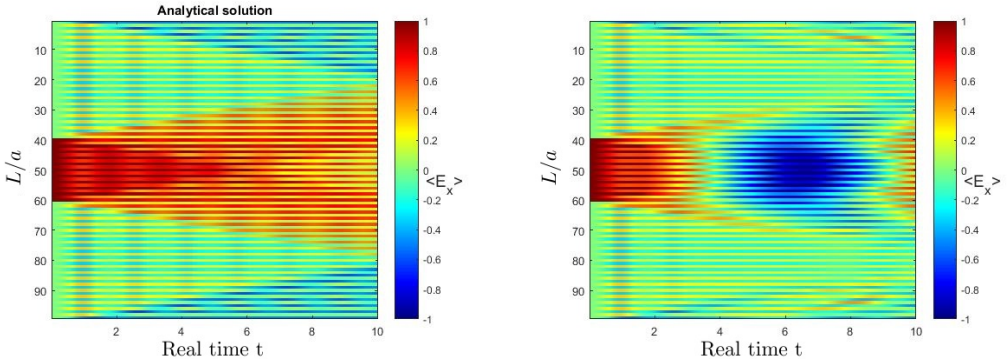


(f) MPS calculation [27].

Figure 4.10.: Comparison Gaussian approximation (first column) vs. MPS [27] (second column) for real time dynamics with $Q = 1$: $m = 3$, $g = 3.5$ (first line) and $m = 0.25$, $g = 1.25$ (second line) and $m = 0$, $g = 0$ (third line) .

i.e., the evolution is just a linear transformation mixing annihilation operators on different sites due to the fact the Hamiltonian is quadratic (Observation 2.2.1).

Let's call $U(t) = \exp(-i\mathcal{H}t)$. Since $\langle L_n \rangle$ is given by elements of the form $\left\langle \phi_n^\dagger \phi_n \right\rangle$, let's compute the evolution of



(a) Alternative method: analytical solution for the case $m = g = 0$.

(b) Real time evolution for $m = 0$ and $g = -\varepsilon = 1$.

Figure 4.11.

$$\left\langle (\phi^\dagger(t))^T \phi(t)^T \right\rangle = \left\langle \begin{pmatrix} \phi_1^\dagger \\ \phi_2^\dagger \\ \vdots \\ \phi_N^\dagger \end{pmatrix} (\phi_1, \phi_2, \dots \phi_N) \right\rangle = U^*(t) \left\langle (\phi^\dagger(0))^T \phi(0)^T \right\rangle U^T(t). \tag{4.75}$$

Now diagonalizing $\mathcal{H}$ and solving the evolution in MATLAB we obtain Figure 4.11a for $\langle L_n \rangle (t)$.

In Figure 4.11a we see the similarity of the result with that obtained in the Gaussian approach Figure 4.10c. In fact we have verified that $|\langle L_n \rangle_{Gauss.} - \langle L_n \rangle_{Alt.}| (t) = 0$ for any time t and any link n. We therefore conclude that, as expected, the Gaussian method is exact in this situation and differs from the result obtained in [27]. Moreover we have observed that $\max_{n,t} |\langle L_n \rangle| > 1$ during the evolution and therefore it could happen that a truncation of the gauge field for $l = 1$ is not totally justified. Moreover in Figure 4.11b, we show a similar evolution with the different string breaking and anti-string formation appearing in Figure 4.10f. As explained in [27], the electric field oscillates between the string $(\bar{q}q)$ and anti-string $(q\bar{q})$ configurations while creating two electric field excitation wavefronts where the formation of mesons also takes place.

A possible explanation for the similarity of both methods in the large mass and coupling limit $m = 3$ and $g = 3.5$ and the big difference in the massless case could be the following. In [27], a Quantum Link Model with spin-1 is considered. This only allows to the electric field to take three different values on a link $m = 0, \pm 1$. However in the limit $m = g = 0$ fermionic excitations can be freely created out of the vacuum. Since $g = 0$ as well, these excitations can make the electric flux to fluctuate on the different links and take any possible value in the infinite dimensional Hilbert space. Therefore a truncation with $l = 1$ in this situation is not justified. Another way to express the same problem can be to consider the Schwinger representation as explained in subsection 4.3.1. In this case m takes values $|m| \sim l$ and therefore the convergence as in the $l \to \infty$ case is not justified.

Remark. In addition to study the dynamics in the purely discretized version of the Schwinger model, we would like to consider the dynamics in the continuum limit in such a way one can extrapolate some conclusions to the continuum model. However, due to the high precision needed for the real-time dynamics and the additional cost that suppose to consider big enough system sizes, this task results numerically expensive.

4.5. Conclusion

In this chapter we have successfully applied the Gaussian method to Quantum Electrodynamics in two spacetime dimensions with both massless and massive fermions. In the massless case this method is able (1) to recover the continuum theory by tuning, as in standard LGT and TN techniques, the lattice spacing a. Moreover (2) the Gaussian ansatz gives a description of the massless case, as accurate as MPS does. We have being able (3) to identify the screening of external charges as obtained in [52], but realizing finite size effects problems which should be taken into account. Finally we have (4) verified that the Gaussian method correctly describes the dynamics of a theory for massless fermions without gauge field. Nevertheless the better description given by the Gaussian ansatz in comparison to MPS, just allows us to evaluate the suitability of the considered model rather than the method to describe the system since in ours we have eliminated the gauge field.

In the massive case the method is (5) able to realize the quantum phase transition between a confining and a string breaking phase, having relatively small numerical deviations from MPS calculations near the critical points. We believe this is a drawback of the mean field theory we are applying. Nevertheless the Gaussian ansatz gives a surprisingly accurate solution despite of the fact that a non-quadratic long-range interaction terms appears in H. The method also realizes (6) the phenomenon known as partial string breaking, with the same numerical problems founded in (5). As an important advantage this method also allows us to analyze dynamical aspects of the theory where no much is known from the analytical solution. Therefore, the Gaussian method looks a promising method to study LGT.

5. Non-Abelian groups in two spacetime dimensions

Due to the success describing Abelian gauge theories, in this chapter we will go one step further and will benchmark the ability of the Gaussian approximation to describe non-Abelian theories. In order to do so we will try to deduce a unitary transformation which again allows us to forget about the gauge field.

5.1. Introduction

While the massless Schwinger model is exactly solvable, QCD in two spacetime dimensions (gauge group $SU(3)$) for massless fermions is not [62]. However, this 2-dimensional model has allowed the development of important tools to understand realistic quantum field theories that are expected to appear in 4-dimensional QCD. QCD_2 has been used to study the bound-state spectrum, algebraic structure and duality properties of QFTs [50]. Nevertheless in order to realize some physical phenomena like confinement and its dynamical analysis, is enough to consider a smaller gauge group like $SU(2)$ as in the studies done in [**otro**, 7, 9, 14, 63]. In fact Kogut and Susskind introduced in [7] the Hamiltonian formulation of LGT using the $SU(2)$ as an easier example where one can use the usual addition of angular momenta.

5.2. Erasing the gauge field

As we explained in subsection 4.3.2, in two spacetime dimensions the gauge field can be erase via an unitary transformation. It's also commonly known the fact that this does not depend on whether the group is either Abelian or not. In this section following the same motivation as in the $U(1)$ Abelian case, we get rid of the gauge degrees of freedom for any $SU(N)$ gauge group. This will give us a similar structure as the one found in the Abelian case. In general we can extend this transformation to any non-Abelian group as long as there exist Unitary representations of the group.

The Kogut-Susskind Hamiltonian with gauge group $SU(N)$ in (1+1)-dimension and hopping parameter ε takes the form

$$H = \varepsilon \sum_n \{(\phi_n^\dagger)_a (U_n)_{ab} (\phi_{n+1})_b + h.c.\} + m \sum_n (-1)^n (\phi_n^\dagger)_a (\phi_n)_a + \frac{g^2}{2} \sum_{n,\alpha} (L_n^\alpha)^2 \quad (5.1)$$

where as we saw in chapter 3, L_n^α are the left generators and U_n is given by $U_n^j = \exp(\imath \theta_n \cdot \mathbf{T}^j)$ in some irreducible representation j of the gauge group with $\theta_n^\alpha = agA_1^\alpha(n)$ and the generators fulfill

$$[T^\alpha, T^\beta] = i f^{\alpha\beta\gamma} T^\gamma. \quad (5.2)$$

In order to erase the gauge field appearing in the hopping term of the Hamiltonian and after acquiring some intuition of the kind of transformation we applied in the $U(1)$ case, we look for a unitary transformation given by a fermionic operator that we will call Θ.

Moreover, we need to know how the Hamiltonian transforms under charge-generated unitary transformations. Let's apply $\Theta^Q = \prod_n \Theta^Q_{g_n} = \prod_n \exp(\imath\alpha_n \cdot \phi_n^\dagger \mathbf{T}^j \phi_n)$ with $g_n \in G$ to the hopping term in H. Before to do so, let me recall (3.35), how ϕ and $\phi^\dagger$ transform under Θ^Q

$$\Theta^{Q,j}_g \phi_a \Theta^{Q,j\dagger}_g = D^{j,\dagger}_{ab}(g)\phi_b, \qquad \Theta^{Q,j}_g \phi^\dagger_a \Theta^{Q,j\dagger}_g = \phi^\dagger_b D^j_{ba}(g), \tag{5.3}$$

where as we saw in (3.2.1) $D^j(g)$ is the representation given by

$$D^j_{ba}(g) = \left(e^{i\theta_g \cdot \mathbf{T}^j}\right)_{ba}. \tag{5.4}$$

From now on j will be omitted when there is no need for a particular representation. Given these transformation laws, the hopping term changes as follows

$$H_{hop} \mapsto \Theta^Q H_{hop} \Theta^{Q\dagger} = \varepsilon \sum_n \{(\phi_n^\dagger)_c D_{ca}(g_n)(U_n)_{ab} D_{bd}(g_{n+1}^{-1})(\phi_{n+1})_d + h.c.\}, \tag{5.5}$$

where we have denoted by $D(g_n)$ the gauge transformation applied to the fermionic field living on the site n.

Therefore, in order to erase the gauge field in the hopping term we need to solve

$$D(g_n)U_n D(g_{n+1}^{-1}) = \mathbb{1} \Longrightarrow D(g_{n+1}) = D(g_n)U_n \qquad \forall\, n. \tag{5.6}$$

With the analogous picture of Figure 4.2 in the non-Abelian case, let's fix boundary conditions on the chain by choosing $U_0 = \mathbb{1}$ and $D(g_0) = \mathbb{1}$, namely we have chosen **open boundary conditions** for both the gauge and the fermionic fields, giving as a result $D(g_1) = \mathbb{1}$. Solving for all links n is easy to see that

$$D(g_n) = U_1 U_2 \cdots U_{n-1} \qquad \forall\, n \tag{5.7}$$

where we didn't make reference to any specific representation and the index j has been omitted.

Therefore we need to find a Θ^n which generates (5.7) on each site n. One can check that such a transformation is given by

$$\Theta^n = \exp\left[i \sum_{k=1}^{n-1} \theta_k \cdot \phi_n^\dagger \mathbf{T} \phi_n\right] = e^{\imath\theta_1 \cdot \phi_n^\dagger \mathbf{T}\phi_n} e^{\imath\theta_2 \cdot \phi_n^\dagger \mathbf{T}\phi_n} \cdots e^{\imath\theta_{n-1} \cdot \phi_n^\dagger \mathbf{T}\phi_n}, \tag{5.8}$$

just recalling the transformation laws (5.3)[1].

Let's check that in fact this is true computing some terms. From the transformation laws of ϕ_a we know that

$$\begin{aligned} &e^{\imath\theta_2 \cdot \phi_n^\dagger \mathbf{T}\phi_n} (\phi_n)_a e^{-\imath\theta_2 \cdot \phi_n^\dagger \mathbf{T}\phi_n} = (\phi_n^\dagger)_b (U_2)_{ba} \\ &\Rightarrow e^{\imath\theta_1 \cdot \phi_n^\dagger \mathbf{T}\phi_n} e^{\imath\theta_2 \cdot \phi_n^\dagger \mathbf{T}\phi_n} (\phi_n^\dagger)_a e^{-\imath\theta_2 \cdot \phi_n^\dagger \mathbf{T}\phi_n} e^{\imath\theta_1 \cdot \phi_n^\dagger \mathbf{T}\phi_n} = (\phi_n^\dagger)_c (U_1)_{cb} (U_2)_{ba}. \end{aligned}$$

[1] For periodic boundary conditions one can obtain a similar transformation as it is done in Ref. [64]. Nevertheless it is easier for us to fix open boundary conditions in order to compare with MPS calculations.

The global transformation Θ we look for, acting on all sites, is given by

$$\boxed{\Theta = \prod_{k=1}^{\rightarrow} \exp\Big(\imath\theta_k \cdot \sum_{m>k} \mathbf{Q}_m\Big) \equiv \prod_{k=1}^{\rightarrow} W_k}, \tag{5.9}$$

where the arrow over $\prod$ means that the operators W_k must be ordered from left to right with increasing index k.

5.2.1. Rotated Hamiltonian

Once we have erased the gauge fields living on the links we would like to know how the other terms in the Hamiltonian change. It's easy to see that the mass term is invariant, i.e., it's a scalar under this transformation. However the electric term will change. Let's first of all analyze the structure of the electric part. We know that the left and right generators hold the following commutation relations on each link of the lattice

$$[L_\alpha, L_\beta] = -\imath f^{\alpha\beta\gamma} L_\gamma \qquad [R_\alpha, R_\beta] = \imath f^{\alpha\beta\gamma} R_\gamma, \tag{5.10}$$

where $f^{\alpha\beta\gamma}$ are the structure constants of the gauge algebra (5.2).

Now we would like to analyze how the electric term of the Hamiltonian changes under the transformation (5.7). Let's remember that H_E is expressed by

$$\frac{2}{g^2} H_E = \sum_{n,\alpha} (L_n^\alpha)^2 = \sum_n \mathbf{L}_n^T \cdot \mathbf{L}_n. \tag{5.11}$$

where we have denoted by $\mathbf{L}^T$ the row vector $\mathbf{L}^T = (L^\alpha)_\alpha$.

From (3.48) we know that given a representation U_k^j of the gauge field living on a given link k then

$$[L_k^\alpha, (U_k^j)_{mn}] = (T_\alpha^j)_{mp} (U_k^j)_{pn} \tag{5.12}$$

therefore since $W_k^j = \exp\Big(\imath\theta_k \cdot \sum_{m>k} \phi_m^\dagger \mathbf{T}^j \phi_m\Big)$, we see that W_k^j has the same matrix structure as $(U_k^j)_{mn}$ since the fermionic charge density $Q_m^{\alpha,j} = \phi_m^\dagger T_\alpha^j \phi_m$ is just a complex number on the bosonic Hilbert space and W_k^j has not matrix structure. Therefore we obtain

$$[L_k^\alpha, W_k^j] = \Big(\sum_{m>k} Q_m^{\alpha,j}\Big) W_k^j \Rightarrow L_k^\alpha W_k^j - W_k^j L_k^\alpha = \Big(\sum_{m>k} Q_m^{\alpha,j}\Big) W_k^j \tag{5.13}$$

$$\Rightarrow L_k^\alpha - W_k^j L_k^\alpha W_k^{j\dagger} = \sum_{m>k} Q_m^{\alpha,j} \Rightarrow \boxed{W_k^j L_k^\alpha W_k^{j\dagger} = L_k^\alpha - \sum_{m>k} Q_m^{\alpha,j}}$$

Thus, omitting the j index, L_n^α transforms under Θ

$$\Theta L_n^\alpha \Theta^\dagger = W_1 \dots W_N L_n^\alpha W_N^\dagger \dots W_1^\dagger = W_1 \dots W_n L_n^\alpha W_n^\dagger \dots W_1^\dagger \tag{5.14}$$

$$= W_1 \dots W_{n-1} \Big(L_n^\alpha - \sum_{m>n} Q_m^\beta\Big) W_{n-1}^\dagger \dots W_1^\dagger \tag{5.15}$$

$$= L_n^\alpha - \sum_{m>n} W_1 \dots W_{n-1} Q_m^\alpha W_{n-1}^\dagger \dots W_1^\dagger = L_n^\alpha - \sum_{m>n} \Big(U_{n-1}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \mathbf{Q}_m\Big)^\alpha, \tag{5.16}$$

where we have applied the transformation law given by

$$W_k Q_m^\alpha W_k^\dagger = (U_k^{\text{Adj.}})_{\alpha,\beta} Q_m^\beta \tag{5.17}$$

if $m > k$ and 0 otherwise, i.e., $\mathbf{Q}_m$ transforms as a 3-vector under color rotations.

Now we would like to know how Gauss' law transforms, since if we are able to erase the fermionic charge density then the solution to our problem becomes much easier. In order to do so we need first of all to know how R_n^α and Q_n^α change under Θ. Let's recall the important relations

$$[Q_n^\alpha, Q_m^\beta] = \imath\delta_{n,m} f^{\alpha\beta\gamma} Q_n^\gamma, \qquad R_n^\alpha = (U_n^{\text{Adj.}})_{\alpha\beta} L_n^\beta. \tag{5.18}$$

Gauss' law

1. Transformation of charge density: Since we know how Q_m^α transforms under W_k is easy to deduce how it does under Θ

$$\Theta Q_n^\alpha \Theta^\dagger = \left(U_{n-1}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \mathbf{Q}_n\right)^\alpha \tag{5.19}$$

2. Transformation of right generator: On the other hand the transformation of the right generator takes the form

$$\Theta R_n^\alpha \Theta^\dagger = \Theta (U_n^{\text{Adj.}})^{\alpha\beta} L_n^\beta \Theta^\dagger = (U_n^{\text{Adj.}})^{\alpha\beta} \left(L_n^\beta - \left(U_{n-1}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \sum_{m>n} \mathbf{Q}_m\right)^\beta\right) \tag{5.20}$$

$$= R_n^\alpha - \left(U_n^{\text{Adj.}} \left[U_{n-1}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \sum_{m>n} \mathbf{Q}_m\right]\right)^\alpha \tag{5.21}$$

Remark. Note that because of the way we have fixed the boundary conditions, the left and right electric fields L_0^α and R_0^α respectively, are invariant under Θ

$$\Theta R_0^\alpha \Theta^\dagger = R_0^\alpha \qquad \Theta L_0^\alpha \Theta^\dagger = L_0^\alpha, \tag{5.22}$$

since Θ does not depend on the gauge field θ_0. This will become an important fact when the total charge of the system is non-zero e.g., inserting one external charge.

From here we know all the ingredients which enter in Gauss' law, so applying the transformation Θ to

$$L_n^\alpha - R_{n-1}^\alpha = Q_n^\alpha \qquad \forall \alpha,\, n \neq 1 \tag{5.23}$$

we find that in the new picture (5.23) takes the form

$$L_n^\alpha - \sum_{m>n} \left(U_{n-1}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \mathbf{Q}_m\right)^\alpha - R_{n-1}^\alpha + \left(U_{n-1}^{\text{Adj.}} \left[U_{n-2}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \sum_{m>n-1} \mathbf{Q}_m\right]\right)^\alpha$$
$$= \left(U_{n-1}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \mathbf{Q}_n\right)^\alpha \tag{5.24}$$

and then

$$\boxed{L_n^\alpha = R_{n-1}^\alpha} \qquad \forall \alpha,\, n \neq 1 \tag{5.25}$$

We see that in the new rotated frame, after the transformation Θ has been applied, left and right generators on a site n are the same due to the "disappearance" of the fermionic charge density in (5.23). As noted before, the link $n = 1$ is special in this sense since in this case Gauss' law transforms to

$$L_1^\alpha - \sum_{m>1} Q_m^\alpha - R_0^\alpha = Q_1^\alpha \Longrightarrow \boxed{L_1^\alpha = R_0^\alpha + \sum_{m\geq 1} Q_m^\alpha}, \tag{5.26}$$

i.e., the sum of the right electric field on the link $n = 0$ plus the **total charge of the system** that in general will be zero.

Therefore the only thing that is left is to relate the different reference frames on each link of the lattice. However using equations (5.18),(5.25) and (5.26) we find that

$$L_n^\alpha = \left[U_{n-1}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \left(\mathbf{R}_0 + \sum_{m\geq 1} \mathbf{Q}_m\right)\right]^\alpha, \tag{5.27}$$

where $\mathbf{R}_0$ are the right generators of the electric field on the left extreme of the chain as in the Abelian case, due to the fact that we fixed open boundary conditions. Again these free parameters are background electric fields which also fulfill the commutation relations $[R_0^\alpha, R_0^\beta] = if^{\alpha\beta\gamma}R_0^\gamma$. We see that the electric field in a given link n is a linear combination of the electric fields in the previous ones.

Rotated Hamiltonian Now we would like to know how the Hamiltonian in the Θ-rotated picture looks like, so we just need to know how the electric part transforms. First, let's write (5.14) in a different way using (5.27)

$$\begin{aligned}\Theta \mathbf{L}_n \Theta^\dagger &= U_{n-1}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \left(\mathbf{R_0} + \sum_{m\geq 1} \mathbf{Q}_m - \sum_{m>n} \mathbf{Q}_m\right) \\ &= U_{n-1}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \left(\mathbf{R_0} + \sum_{m\leq n} \mathbf{Q}_m\right) \equiv \mathcal{U}_n \mathbf{J}_n\end{aligned} \tag{5.28}$$

where $\mathcal{U}$ is an orthogonal matrix.

Remark. The transformation $\mathcal{U}_n$ given by

$$\mathcal{U}_n = U_{n-1}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \tag{5.29}$$

is an orthogonal one since $U_m^{\text{Adj.}} \in \mathcal{O}(N^2-1)$ and the product of orthogonal transformations is closed in $\mathcal{O}(N^2-1)$. Moreover it's also a Hermitian gauge operator $(U_m^{\text{Adj.}})_{ab} = ((U_m^{\text{Adj.}})_{ab})^\dagger$. The reason why $U_m^{\text{Adj.}} \in \mathcal{O}(N^2-1)$ comes from the fact that the adjoint representation is **real** as stated in subsection 3.2.1. This implies

$$\Theta \mathbf{L}_n^T \Theta^\dagger = \mathbf{J}_n^T \mathcal{U}_n^T, \tag{5.30}$$

where we used that $L_n^{\alpha,\dagger} = L_n^\alpha$ and $Q_n^{\alpha,\dagger} = Q_n^\alpha$.

Therefore we have been able to solve Gauss' law and express the conjugate momenta variables L_n^α in terms of the fermion color charges and the background field $\mathbf{L}_0^\alpha$. The fact that $\{\mathbf{L}_n\}$ become no-dynamical is another indication that in (1+1) dimensions the gauge fields can be removed from the Hamiltonian [64]. Then we can deduce that the electric term (5.11) transforms as

$$\frac{2}{g^2}\Theta H_E \Theta^\dagger = \sum_n \Theta \mathbf{L}_n^T \Theta^\dagger \Theta \mathbf{L}_n \Theta^\dagger = \sum_n \mathbf{J}_n^\dagger \mathcal{U}^T \mathcal{U} \mathbf{J}_n = \sum_n \mathbf{J}_n^T \mathbf{J}_n = \sum_{n,\alpha} \left(R_0^\alpha + \sum_{m \leq n} Q_m^\alpha \right)^2 \tag{5.31}$$

These results combined give rise to the closed form for the Hamiltonian

$$\boxed{H \mapsto \Theta H \Theta^\dagger = \varepsilon \sum_n \{\phi_n^\dagger \phi_{n+1} + h.c.\} + m \sum_n (-1)^n \phi_n^\dagger \phi_n + \frac{g^2}{2} \sum_{n,\alpha} \left(R_0^\alpha + \sum_{m \leq n} Q_m^\alpha \right)^2} \tag{5.32}$$

By applying the transformation (5.9), we have obtained a rotated Hamiltonian (equivalent to the initial one) with no non-Abelian gauge fields. In addition, as in the Abelian case, we have been able to include Gauss' law directly into the Hamiltonian, generating a long-range force where in fact, the form of the Hamiltonian is the same as in the Abelian case with the additional sum over group indices. The importance of this transformation is that it allows us to only deal with fermionic degrees of freedom without being necessary to truncate the infinite dimensional gauge Hilbert space. This would likely be more convenient for exact computations using Tensor Networks like the analysis of the finite-density phase diagram of (1+1)-dimensional non-Abelian theories done in [63].

In spite of the fact that this transformation was supposed to exist in the discretized formulation of non-Abelian gauge theories in two spacetime dimensions as it does in the continuum formulation, it was not proven till 2009 in [64]. The alternative proof presented here, being less general, presents a more constructive step by step proof and as we will see now, allows us to introduce the external charges into the Hamiltonian as well.

5.2.2. Insertion of external charges

As in the Abelian case, we would like to analyze the phases of a non-Abelian theory via the potential energy $V_Q(L)$. Then we should be able to fix some external color charges. In principle it looks like the same procedure as we used in the Abelian case should work. Being true, one should pay attention to the underlying Hilbert spaces we are dealing with and remembering that the color charge generators should fulfill (5.18). We need to add an external charge density $(Q^{ext})_n$ into Gauss' law that as we saw section 3.4, must be treated quantum mechanically.

$$L_n^\alpha - R_{n-1}^\alpha = Q_n^\alpha + Q_{ext,n}^\alpha. \tag{5.33}$$

However, Q_{ext}^α is not an operator acting on the fermionic Fock space $\mathcal{F}_n$ on a site but on a different "external" Hilbert space $\mathcal{H}_{ext}$ where $\{Q_{ext}^\alpha\}_\alpha$ fulfill the commutation relations

$$[Q_{ext}^\alpha, Q_{ext}^\beta] = i f^{\alpha\beta\gamma} Q_{ext}^\gamma. \tag{5.34}$$

Moreover as we will see in the practical example for a $SU(2)$ gauge theory, the $dim(\mathcal{H}_{ext})$ is related to the dimension of the representation of the gauge group. From now on the fermionic Hilbert space is given by $\mathcal{H}_F \otimes \mathcal{H}_{ext}$.

In order to introduce the external color charges let's modify the transformation (5.9) in the following form

$$\tilde{\Theta} = \vec{\prod}_k \exp\left(\imath\theta_k \cdot \sum_{m>k}\left(\mathbf{Q}_m + \mathbf{Q}_m^{ext}\right)\right) \equiv \vec{\prod}_k W_k. \tag{5.35}$$

Let's check whether this is the correct transformation, i.e., we are able to erase the external charge density in (5.33). Following the same reasoning like the one to derive (5.13), we obtain

$$W_k L_k^\alpha W_k^\dagger = L_k^\alpha - \sum_{m>k}\{Q_m^\alpha + Q_{ext,m}^\alpha\}, \tag{5.36}$$

since Q_{ext}^α acts as a c-number on both the fermionic and gauge Hilbert spaces. Using

$$W_k Q_{ext,m}^\alpha W_k^\dagger = (U_k^{\text{Adj.}})_{\alpha,\beta} Q_{ext,m}^\beta \Longrightarrow \tilde{\Theta} Q_{ext,m}^\alpha \tilde{\Theta}^\dagger = \left(U_{n-1}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \mathbf{Q}_{ext,m}\right)^\alpha, \tag{5.37}$$

we obtain the transformation law for L_n^α

$$\boxed{\tilde{\Theta} L_n^\alpha \tilde{\Theta}^\dagger = L_n^\alpha - \sum_{m>n}\left(U_{n-1}^{\text{Adj.}} \dots U_1^{\text{Adj.}} \{\mathbf{Q}_m + \mathbf{Q}_{ext,m}\}\right)^\alpha}. \tag{5.38}$$

Therefore Gauss' law (5.33) transforms to

$$L_n^\alpha = R_{n-1}^\alpha \qquad \forall\, n \neq 1, \tag{5.39}$$

as obtained before in the absence of external charges. Then the only relevant difference w.r.t the result obtained in the previous section is the insertion of the external charge density into the Hamiltonian through (5.38) giving as a result

$$\boxed{\tilde{\Theta} H \tilde{\Theta}^\dagger = \varepsilon \sum_n \{\phi_n^\dagger \phi_{n+1} + h.c.\} + m \sum_n (-1)^n \phi_n^\dagger \phi_n + \frac{g^2}{2} \sum_{n,\alpha}\left(R_0^\alpha + \sum_{m\leq n}\{Q_m^\alpha + Q_{ext,m}^\alpha\}\right)^2} \tag{5.40}$$

The non-Abelian rotated Hamiltonian with external charges (5.40), resembles the form obtained for the Abelian case (4.60) and therefore one would expect a good description via the Gaussian method. As we will see, things become difficult due to the group (gauge) index.

Remark. We should check that in fact transformation (5.35) erases the gauge fields in the hopping term of the Hamiltonian. In order to do so, let's consider

$$H_h = (\phi_n^\dagger)_a (U_n)_{ab} (\phi_{n+1})_b = \phi_n^\dagger U_n \phi_{n+1}, \tag{5.41}$$

where as always the matrix product is consider in the group indices.

Remember that $U_n = U_n(\theta^\alpha, T^{\alpha,j})$ where $T^{\alpha,j}$ are $j \times j$ matrices in some j-dimensional representation and since $\tilde{\Theta} = \tilde{\Theta}(\theta^\alpha, Q^\alpha, Q_{ext}^\alpha)$ both operators commute

$$[\tilde{\Theta}, U_n]_\otimes = 0. \tag{5.42}$$

Then

$$H_h \mapsto \tilde{\Theta} H_h \tilde{\Theta}^\dagger = \tilde{\Theta}\phi_n^\dagger \tilde{\Theta}^\dagger \cdot U_n \cdot \tilde{\Theta}\phi_{n+1}\tilde{\Theta}^\dagger = \Theta\phi_n^\dagger\Theta^\dagger \cdot U_n \cdot \Theta\phi_{n+1}\Theta^\dagger, \tag{5.43}$$

where we used the fact that $[(\phi_n)_a, Q^\alpha_{ext}] = 0$. Since Θ is given by (5.9), we recover the original transformation (5.9) that we applied to the Hamiltonian to get rid of the gauge fields.

5.3. Gaussian approach

In this part we present the state dependent form for the transformed Hamiltonian (5.40) computed in section B.2. In this case the fermionic Fock space $\mathcal{F}$ can be constructed with three different kind of modes: the Nambu index distinguishing creation operators from the annihilation ones expand the factor $\mathcal{F}_N$, the group index a which spans the space $\mathcal{F}_G$ of different colored excitations, and the mode index which in this case makes reference to the spatial degrees of freedom spanning $\mathcal{F}_S$. Therefore

$$\mathcal{F} = \mathcal{F}_N \otimes \mathcal{F}_G \otimes \mathcal{F}_S \Rightarrow \Phi = \begin{pmatrix} \left((\phi_n)^N_{a,n=1}\right)_a \\ \left((\phi^\dagger)^N_{a,n=1}\right)_a \end{pmatrix}. \tag{5.44}$$

From (5.40) one easily sees that the hopping and mass term are exactly the same as we derived in the Abealian case and that we just need to apply Wick's theorem to the last term. In any chosen representation j we find that the stated dependent single-particle Hamiltonian matrix $\mathcal{H}(\Gamma)$ for the non-Abelian case takes the form

$$\begin{aligned} \mathcal{H}(\Gamma) = &\begin{pmatrix} Id_G \otimes (\varepsilon T + mD) & 0 \\ 0 & -Id_G \otimes (\varepsilon T + mD) \end{pmatrix} \\ &+ g^2 \begin{pmatrix} -\mathcal{M} \otimes \tilde{P} + \frac{1}{2}H_{11} + \mathcal{M}^{ext} & H_2 \\ H_5 & \mathcal{M}^T \otimes \tilde{P}^T - \frac{1}{2}H_{11}^T - (\mathcal{M}^{ext})^T \end{pmatrix}, \end{aligned} \tag{5.45}$$

where T and D are symmetric matrices already defined in section 4.3.3 and the remaining blocked matrices are derived in section B.2.

5.4. Application: (1+1)-dimensional SU(2)

In order to apply the Gaussian approximation to a specific model, we will analyze the non-Abelian $SU(2)$ theory, that has been also discussed in the literature [7, 14]. In this section we want to test the Gaussian ansatz in describing the quantum phase transition of the ground state of the system between the two possible different phases that have been realized previously [14].

5.4.1. Color configuration

Then main difference with respect to the Abelian case, is the new group index as it was introduced in the Hamiltonian formulation of LGT in chapter 3. As in the Abelian case, we want to study the confinement of color charges, i.e., eigenvalues $q_{\hat{d}}$

of the conserved charge $\hat{d}\cdot\mathbf{Q}_{ext}$ for some direction $\hat{d}\in\mathbb{R}^3$. The value of these charges $q_{\hat{d}}$ depends on the chosen representation j. However we know that in particle physics, particles are described in the fundamental representation of the gauge group and this happens to be $j=1/2$ in our case. Therefore the external Hilbert space is given by $\mathcal{H}_{ext}\cong\mathbb{C}^2$. As it's well known, the fundamental representation of $\mathfrak{su}(2)$ is given by $T^\alpha_{1/2}=1/2\sigma^\alpha$ with σ^α the Pauli matrices. Thus in the second quantized form of Q^α we can distinguish two different kinds "colors" or group indices $Q^\alpha_{ext}=\frac{1}{2}\sigma^\alpha$. Given this representation the color charges can take two different values $\pm1/2$. Moreover we choose to work in eigenstates of σ^z.

Since we would like to prove the screening or confinement of electric charges, we need to place two external static charges of opposite sign, quark-antiquark pair $\bar{q}q$, i.e., $\pm1/2$. Note the choice of the orientation of $\hat{d}$ is not relevant and the only requirement is $q\bar{q}$ configuration to form a color singlet. Since Q^z is chosen to be diagonal in this representation

$$Q^z=\frac{1}{2}(\phi^{r,\dagger}\phi^r-\phi^{g,\dagger}\phi^g), \tag{5.46}$$

we use the number eigenbasis of red and green fermionic quanta given by

$$|r,g\rangle \qquad r,g=0,1. \tag{5.47}$$

As an example, the non-interacting vacuum for fermions ($\varepsilon=0$) is expressed by

$$|\Omega\rangle_f=|2\rangle_1|0\rangle_2\dots|2\rangle_{N-1}|0\rangle_N, \tag{5.48}$$

where $|2\rangle_n$ is the number state with two fermions in the odd-site n given by

$$|2\rangle_n=\phi^{r\dagger}_n\phi^{g\dagger}_n|0\rangle \tag{5.49}$$

and $|0\rangle$ defined via $\phi^r|0\rangle=\phi^g|0\rangle=0$ such that

$$Q^\alpha_m|\Omega\rangle_f=0 \qquad \forall\,\alpha \text{ and } \forall\, m, \tag{5.50}$$

i.e., $|\Omega\rangle_f$ is the Dirac sea with zero net charge that in the original frame, with $|0\rangle_G$ the gauge vacuum for all links, fulfills Gauss' law.

5.5. Ground state with static charges is not Gaussian

Similar to the massive Schwinger model, the phenomena associated to string breaking has also been realized in the $SU(2)$ theory [14]. Therefore the description of such quantum phase transition establishes a good benchmark to test the Gaussian approximation.

However as we will see, the Gaussian approximation does not work correctly for this model neither in the confining nor in the string breaking phase. In this section we deduce the approximated form of the ground state of the system with two external static charges and show that such a state is not Gaussian. In order to do so we can work in the Original frame where Gauss' law is given by

$$L^{\alpha,1/2}_n-R^{\alpha,1/2}_{n-1}=Q^{\alpha,1/2}_n+Q^{\alpha,1/2}_{ext,\,n}, \tag{5.51}$$

where 1/2 reminds us the fact we are using the fundamental representation of $SU(2)$ and therefore the 4-dimensional Hilbert space on the link is expanded as we saw in subsection 3.5.2 by the states $|j, m_1, m_2\rangle$ on which the operators L^α and R^α act.

Let's consider a configuration with two external charges $\pm 1/2$ at positions i and k in strong-coupling limit $g >> 1$. Due to Gauss' law a line of electric flux of magnitude $1/2(1/2+1) = 3/4$ joining the charges appears being the *string* surrounded by the vacuum state for both gauge and fermionic fields. In this configuration the system would show a confining behavior as plotted in Figure 5.1.

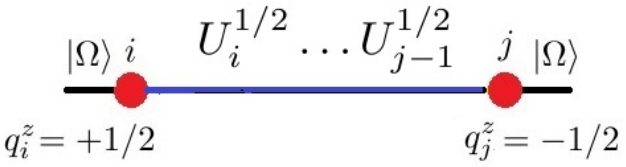


Figure 5.1.: Ground state configuration with two external charges joined by a flux tube (blue) of magnitude 3/4.

Since $\mathcal{H}_{ext} \cong \mathbb{C}^2$ we will use the spin notation for the sites i and k. Moreover we denote the gauge-fermionic vacuum on the lattice via $|\Omega\rangle = |\Omega\rangle_f \otimes |\Omega\rangle_G$ where $|\Omega\rangle_f$ is the Dirac sea and $|\Omega\rangle_G = \prod |0\rangle_G$ the vacuum state of the gauge field, i.e., with zero flux on every link. Therefore the considered state has the form

$$|\Psi\rangle = |\psi\rangle_{i,k} \otimes |\Omega\rangle \,. \tag{5.52}$$

We know that such a state should fulfill Gauss' law (5.51) in order to be considered physical. Let's rewrite (5.51) in the following way acting on $|\Psi\rangle$

$$L_n^{\alpha,1/2} |\Psi\rangle = R_{n-1}^{\alpha,1/2} |\Psi\rangle + Q_{ext,\,n}^{\alpha,1/2} |\Psi\rangle \qquad \alpha = x,\, y,\, z. \tag{5.53}$$

The equation (5.53) imposes three conditions for three non-commuting observables and therefore its solution is far from trivial. However let's think about (5.53) in terms of addition of angular momenta $\vec{S} = \vec{S}_1 + \vec{S}_2$ with $\vec{S}_1 = \mathbf{R}$ and $\vec{S}_2 = \mathbf{Q}_{ext}$ using Clebsch-Gordan coefficients. We know that on the left of the i site and on the right of k, the links are on the vacuum gauge state $|0\rangle_G$ and therefore in the 0-representation of $SU(2)$ as it was explained in chapter 3. Since the external charge on i is on $j = 1/2$-representation, applying (5.53) to the site i we find that the representation on the intermediate links must be

$$0_{i-1,\text{link}} \otimes \frac{1}{2} i = \frac{1}{2} i, \text{link}. \tag{5.54}$$

Now applying once more Gauss' law to the site k we find

$$\frac{1}{2} k - 1, \text{link} \otimes \frac{1}{2} k = \Big(0 \oplus 1\Big)_{k,\text{link}}, \tag{5.55}$$

therefore in order to be consistent this multiplication should give $j = 0$ for the links to the right of k. But this implies that the product

$$\frac{1}{2} i \otimes \frac{1}{2} k = 0, \tag{5.56}$$

i.e., the static charges at i and k should form a spin singlet, i.e.,

$$|\psi\rangle_{ik} = \frac{1}{\sqrt{2}}\Big(|\uparrow\downarrow\rangle_{i,k} - |\downarrow\uparrow\rangle_{i,k} \Big). \tag{5.57}$$

In spite of the fact we have worked with a configuration in the confining phase, this result is also true for the string breaking case. In this phase we should deal with a configuration like the one plotted in Figure 5.2.

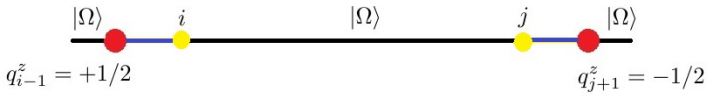


Figure 5.2.: Ground state configuration with two external charges joined by a flux tube (blue) of magnitude 3/4.

Now Gauss' law takes the form

$$L^\alpha_n = R^\alpha_{n-1} + Q^{\alpha,1/2}_{ext,\,n} + Q^{\alpha,1/2}_n \qquad \alpha = x,\, y,\, z, \tag{5.58}$$

and depending on the site we would have to consider either Q^α_n or $Q^\alpha_{ext,\,n}$ obtaining the result that the pair of particles at $i-1$, i and k, $k+1$ should form color singlets respectively. The only difference is that in this case, the color singlet is formed by a dynamical and a static fermion.

Once we have seen the relevant state configurations that must be considered in the Gaussian evolution in order to realize the quantum phase transition, the question is whether these states are Gaussian or could be approximated by a Gaussian. With out lost of generality let's consider the state in the confining phase and write the (fermionic) spin singlet in the second quantized form

$$|\psi\rangle_{ij} = \frac{1}{\sqrt{2}}\Big(c^\dagger_{i,\uparrow} c^\dagger_{k,\downarrow} - c^\dagger_{i,\downarrow} c^\dagger_{k,\uparrow} \Big) |0\rangle\,, \tag{5.59}$$

where $c_\uparrow$, $c_\downarrow$ are fermionic operators. Then

$$|\Psi\rangle = |\psi\rangle_{ik} \otimes |\Omega\rangle\,. \tag{5.60}$$

As in the Abelian case, the vacuum state $|\Omega\rangle$ is a Gaussian state however the singlet state is not. We could try to prove that a canonical transformation which transforms $|\psi\rangle_{ik}$ into the standard BCS form given by the equation 2.26 does not exist. However it is easier to prove it in the following way. In Equation 2.19 we defined a state as Gaussian if it can be written in the form

$$|G.S\rangle = \exp\Big[i\Big(C^\dagger \xi_f C \Big) \Big] |0\rangle = |0\rangle + i C^\dagger \xi_f C\, |0\rangle - \frac{1}{2}\Big(C^\dagger \xi_f C \Big)^2 |0\rangle + \ldots, \tag{5.61}$$

where now $C = (c_{i,\uparrow}, c_{i,\downarrow}, c_{k,\uparrow}, c_{k,\downarrow}, c^\dagger_{i,\uparrow}, c^\dagger_{i,\downarrow}, c^\dagger_{k,\uparrow}, c^\dagger_{k,\downarrow})^T$.

Therefore in order to obtain the state (5.59) from an expansion like (5.61), the quadratic term $c^\dagger_{i,\uparrow} c^\dagger_{k,\downarrow} - c^\dagger_{i,\downarrow} c^\dagger_{k,\uparrow}$ must appear in the exponent since we are considering even FGS. But if this is the case, expansion (5.61) should generate a vacuum state $|0\rangle$

and a four particles state $c^{\dagger}_{i,\uparrow}c^{\dagger}_{k,\downarrow}c^{\dagger}_{i,\downarrow}c^{\dagger}_{k,\uparrow}|0\rangle$. Since this is not the case for the singlet state $|\psi\rangle_{ik}$ given by (5.59), we can then conclude that $|\Psi\rangle$ is not an even fermionic Gaussian state.

In spite of the fact the proof has been given in the original non-transformed frame, the result is also true in the rotated frame (where the gauge Hilbert space does not appear anymore) due to the fact both are connected via the Bogoliubov transformation $\tilde{\Theta}$, generated by a quadratic polynomial on the fermionic operators, and therefore $|\psi\rangle_{ik}$ keeps its "non-Gaussianity" when the $\tilde{\Theta}$ is applied to it[2].

5.6. Conclusion

The unitary transformation given by (5.35) allows us to get rid of the unitary matrices appearing in the hopping term and insert Gauss' law in the Hamiltonian, easing the description of these systems. However, not only the quantum phase transition but both confining and string breaking phases **cannot be described by the Gaussian ansatz**. Since Gauss' law is fulfilled at all times, one could try to give an approximation for an acceptable initial Gaussian seed with two external charges. However due to the problem described in section 5.5, the insertion of external charges in the Gaussian setting to realize the phenomenon of confinement, cannot be worked out[3]. Even if we wouldn't consider external charges, this approximation would not be suitable to describe real-dynamics form example, where one would expect to realize the string breaking mechanism at some point of the evolution. Some ideas on how to proceed will be presented in the Outlook 6.2.

[2]Remember that the gauge fields θ^{α} act as identity operators on the fermionic sector.
[3] Some trials have been tested with no good results.

6. Outlook

6.1. Abelian (2+1)-dimensions: exact and numerical approach

So far we only work with (1+1)-dimensional systems. However, the idea is to apply the Gaussian method to more "realistic" systems that imitate Quantum Field Theories in more than 2 dimensions. Unlike the (1+1) dimensional case, there does not exist a unitary transformation which erases the gauge field in higher dimensional systems. Therefore one needs to proceed in a completely different way as before, describing both the gauge and fermionic degrees of freedom.

In this section, we suppose for simplicity we are dealing with a purely Abelian $U(1)$ gauge theory, where the fermionic degrees of freedom only appear as external charges and therefore the only dynamical degrees of freedom are the gauge ones. In this section we will follow the exposition given in [9]. The Hamiltonian is given by

$$\begin{aligned} H &= \underbrace{\frac{g^2}{2}\sum_{x,k} E^2_{(x,k)}}_{H_E} \underbrace{- \frac{1}{2g^2}\sum_{p} U_1 U_2 U_3^\dagger U_4^\dagger + h.c.}_{H_B} \\ &= \frac{g^2}{2}\sum_{x,k} E^2_{(x,k)} - \frac{1}{2g^2}\sum_{x} \cos(\theta_{x,1} + \theta_{x,2} - \theta_{x,3} - \theta_{x,4}), \end{aligned} \tag{6.1}$$

where we have set $a = 1$ since we are not yet interested in the continuum limit.

Moreover Gauss' law takes the form

$$G_x \equiv \sum_k \{E_{(x,k)} - E_{(x-\hat{k},k)}\} = Q_{ext,x}, \tag{6.2}$$

since as explained before no fermionic terms are consider in this first attempt. In this first part we consider the strong coupling limit ($g \to \infty$), where only the electric term H_E contributes to the Hamiltonian. In this limit, we can avoid one of the enumerated problems in chapter 4 related to fixing the dimension of the truncated gauge theory. In order to apply the Gaussian method, we need to write H_E in its second quantized form. To do so we use the Schwinger bosons representation already introduced in (4.3.1) , where we considered two kind of bosons on each link, namely a and b. In this representation the considered Hamiltonian takes the form

$$H_E = \frac{g^2}{2}\frac{1}{4}\sum_{x,k}\left(\hat{N}_a - \hat{N}_b\right)^2_{x,k} = \frac{g^2}{2}\frac{1}{8^2}\sum_{x,k}\left(R^T \cdot D \cdot RR^T \cdot D \cdot R\right)_{x,k}, \tag{6.3}$$

with $D = diag(1, -1, 1, -1)$ and where we have mapped $\hat{a}$ and $\hat{b}$ creation and annihilation operators to the quadratures $R_{(x,k)} = (X_a, X_b, P_a, P_b)^T_{(x,k)}$ given by the map

$$\hat{a} = \frac{1}{2}(X_a + iP_a) \qquad \hat{b} = \frac{1}{2}(X_b + iP_b), \tag{6.4}$$

for each link (x, k). Note that (6.3) is a quartic Hamiltonian and therefore the Gaussian method is an approximation.

In order to get the Mean-Field form of (6.3) we use the alternative method of taking derivatives of the averaged energy with respect Γ and $\langle R \rangle$ as introduced in subsection 2.6.1. Therefore we need to compute $\langle H_E \rangle_{G.S}$ on the Gaussian state ansatz, i.e., applying Wick's theorem. The result of this energy is given by

$$\begin{aligned}\langle H_E \rangle_{G.S} = \frac{g^2}{2}\Big(\frac{1}{8}\Big)^2 \sum_{x,k} \Big[8 + (\langle R \rangle^T \cdot D \cdot \langle R \rangle)^2 + 2 \langle R \rangle^T \cdot D \cdot \langle R \rangle Tr(\Gamma \cdot D) \\ + 4 \langle R \rangle^T \cdot D\Gamma D \cdot \langle R \rangle + \Big(Tr(\Gamma D)\Big)^2 + 2Tr(\Gamma D \Gamma D)\Big]_{(x,k)},\end{aligned} \tag{6.5}$$

where we have used the result that if $A = A^T$ then $Tr(\sigma_y A) = 0$. Now using the fact that

$$\langle E \rangle_{(x,k)} = \frac{1}{8}\Big(\langle R \rangle^T \cdot D \cdot \langle R \rangle + Tr(\Gamma D)\Big)_{(x,k)}, \tag{6.6}$$

the average of the generator of the gauge transformations G_x takes the form

$$\langle G_x \rangle = \frac{1}{8} \sum_k \Big[\Big(\langle R \rangle^T \cdot D \cdot \langle R \rangle + Tr(\Gamma D)\Big)_{(x,k)} - \Big(\langle R \rangle^T \cdot D \cdot \langle R \rangle + Tr(\Gamma D)\Big)_{(x-\hat{k},k)}\Big]. \tag{6.7}$$

Now we should think the implementation of this system, where the dynamics are governed by (6.3) but the states must fulfill Gauss' law (6.2). Such implementation will follow the same line of reasoning as introduced in subsection 4.3.1. In principle, in the absence of external charges we should impose

$$G_x \, |G.S\rangle = 0 \qquad \forall \, x, \tag{6.8}$$

and since $G_x^\dagger = G_x$, consider to minimize the energy

$$\langle H \rangle = \langle H_E \rangle + \mu \sum_x \langle G_x^2 \rangle, \tag{6.9}$$

since $G_x^2 \geq 0$. However imposing (6.8) on Gaussian states is too restrictive since the state must be an eigenstate of the generator of gauge transformations on every site and link with eigenvalue zero. In order to relax this constraint we use the fact that

$$\mathbb{E}\Big[\Big(G_x^2 - \langle G_x \rangle\Big)^2\Big] \geq 0 \Longrightarrow \langle G_x^2 \rangle \geq \langle G_x \rangle^2 \geq 0, \tag{6.10}$$

i.e., $\langle G_x \rangle^2$ is a lower bound of $\langle G_x^2 \rangle$, and consider instead the weaker minimization problem

$$\min_{\text{Gauss.}} \langle H \rangle = \min_{\text{Gauss.}} \langle H_E \rangle + \mu \sum_x \langle G_x \rangle^2 \tag{6.11}$$

with $\mu >> 1$. Nevertheless since $\langle G_x \rangle^2$ is quadratic, the Hamiltonian whose average is (6.11) is given by

$$H' = \frac{1}{2}\Big(H_E \otimes \mathbb{1} + \mathbb{1} \otimes H_E\Big) + \mu \sum_x G_x \otimes G_x, \tag{6.12}$$

i.e., we need to consider two copies of the same bosonic Fock space $\mathcal{F} \otimes \mathcal{F}$.

Applying the results obtained in chapter 2 about Gaussian states to two non-interacting copies approximated via a Gaussian state, we find the evolution equations

$$\frac{d}{d\tau}\Gamma = -\frac{1}{2}\Gamma\Omega\Gamma + \frac{1}{2}\sigma_y\Omega\sigma_y \quad \text{with} \quad \Omega = \Omega_H + 2\mu \sum_x \langle G_x \rangle \, \Omega_G(x) \tag{6.13}$$

$$\frac{d}{d\tau}\langle R \rangle = -\frac{1}{2}\Gamma\Big(\eta_H + 2\mu \sum_x \langle G_x \rangle \, \eta_G(x)\Big), \tag{6.14}$$

where Ω_H, $\Omega_G(x)$, η_H and $\eta_G(x)$ are given by

$$\eta_H = 2\frac{\delta \langle H_E \rangle}{\delta \langle R \rangle}, \quad \Omega_H = 4\frac{\delta \langle H_E \rangle}{\delta \Gamma} \quad \eta_G(x) = 2\frac{\delta \langle G_x \rangle}{\delta \langle R \rangle}, \quad \Omega_G(x) = 4\frac{\delta \langle G_x \rangle}{\delta \Gamma}. \tag{6.15}$$

The numerical implementation of this Hamiltonian has allowed us to check how well Gauss' law is fulfilled in the Gaussian approach. In order to do so, μ usually should be, at least, one order of magnitude bigger than other parameters of the theory. In Figure 6.1 we have plotted the electric flux distribution when the system is closed to the ground state of the system for the given configuration of static charges under the imaginary time evolution. This is one of the difficult configurations since the ground state is degenerated, there are multiple open strings contributing to the confining of static charges. In this limit ($g \to \infty$) we have also observed a confining (linear increasing w.r.t. distance) potential.

Magnetic term More difficulties appear when one wants to consider the magnetic term H_B. In this case apart from the truncation problem we encountered in subsection 4.3.1 which means an additional term to the Hamiltonian fixing the dimension of the truncation l in average

$$\min_{\text{Gauss.}} \sum_{(x,k)} \Big(\Big\langle \hat{N} \Big\rangle_{(x,k)} - 2l \Big)^2, \tag{6.16}$$

we also have to deal with the fact that the Schwinger representation of H_B consists on a eighth-order polynomial in creation and annihilation operators. Using the map (4.33) and (4.38), we obtain

$$H_B = \frac{1}{g^2[l(l+1)]^2} \sum_x \{\Big(a_1^\dagger b_1 a_2^\dagger b_2 b_3^\dagger a_3 b_4^\dagger a_4\Big)_x + h.c.\}. \tag{6.17}$$

At this point we need to find a method which allows us to compute the Mean Field Hamiltonian of this theory. The fastest way to compute Ω_H and η_H is via the computation of $\langle H_B \rangle$ applying Wick's theorem (which means 128 contractions via Wick's theorem) and subsequent computation of derivatives with respect to Γ and $\langle R \rangle$. This computation being simple is quite intractable analytically and therefore we have two possible ideas:

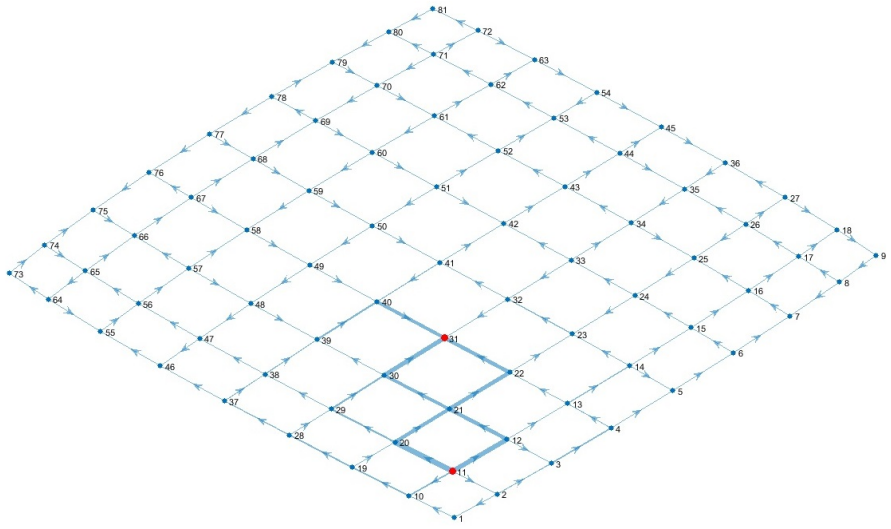


Figure 6.1.: Electric flux distribution with a pair of static particle-antiparticle (red points) in the strong coupling limit with open boundary conditions. The direction of the arrows points the direction of the electric field and their width the amplitude.

1. Numerical implementation of an algorithm which computes $\langle H_B \rangle$ and after that takes (numerical) derivatives.

2. Use the Weyl representation for Gaussian states introduced in the chapter 2 to compute

$$\left\langle a_1^\dagger b_1 a_2^\dagger b_2 b_3^\dagger a_3 b_4^\dagger a_4 \right\rangle_{G.S}, \tag{6.18}$$

via

$$\left\langle \exp\Big(- \lambda_1 a_1^\dagger b_1 - \lambda_2 a_2^\dagger b_2 - \lambda_3 b_3^\dagger a_3 - \lambda_4 b_4^\dagger a_4 + h.c. \Big) \right\rangle_{G.S}, \tag{6.19}$$

by taking derivatives w.r.t. $\{\lambda_i\}$. The integral one has to do is a Gaussian integral in phase space that can be computed with coherent state path integral formulation [24][1] and computing Matsubara sums. Nevertheless, the difficulty again appears when taking derivatives w.r.t. Γ and $\langle R \rangle$. A different approach which has been investigated is the use of a fermionic representation for the Schwinger algebra. However it has been noticed the fact that in this representation, the Gaussian method is not able to reproduce superposition of different open strings (it's the case for degenerated configurations) as the ones showed in Figure 6.1. The idea here it would be to introduce a non-Gaussian transformation via a Gutzwiller projector [65].

   Once this problem is solved, the next ingredient we would like to add are dynamical fermions, where we would have to deal with the hopping term. In this

[1] A similar integral it has been computed in [24].

case the hopping term is a interacting term of boson-boson, fermion-fermion and boson-fermion of order four. However we are considering pure Gaussian states ansatz that are product states in bosonic and fermionic degrees of freedom separately. Thus one would expect that the insertion of a non-Gaussian transformation is necessary.

6.2. Non-Abelian in (1+1)-dimensions.

In chapter 4 we firstly decoupled the matter field from the gauge field. However we found that a Gaussian ansatz cannot describe non-Abelian LGT in two dimensions, at least for $SU(2)$ gauge group. Therefore one option is to consider a larger parameter space via a non-Gaussian transformation as explained in 2.6.2 . However one needs to figure out the appropriate the transformation U_{NG}.

Since we are interested in the study of confinement, one possible idea it's to look for a transformation which could decouple the external charges from the rest of the system considered as a bath[2]. In this way the external charge could be treated as a classical variable. While this transformation for two impurities has not been found yet, it has been found for one. Therefore this would allow to study the behavior of $SU(2)$ and test whether there is also screening as it happens in the massless Schwinger model.

6.3. Study of vacuum structure

As we have seen in section 4.4.2, the massive Schwinger model shows a non-trivial structure of the vacuum. The system is periodic in a field θ that it's related to the chiral symmetry [54]. As we discussed in section 4.2.2, one can understand this periodicity from the bosonized version of the theory [54], but it has been also studied in the fermionic picture via the Pontryagin index [66] and the Density Matrix Renormalization Group method considering the lattice formulation we have used [59]. We would like to test whether we can describe or at least realize some of the features related to the θ-vacuum. In principle since the background field L_0 couples to a quadratic operator

$$\sum_n L_0^2 + g^2 L_0 \sum_n \sum_{k\leq n} \left\{ Q_k + Q_k^{ext} \right\}, \tag{6.20}$$

the Gaussian method should be able to realize some related phenomena. However, while the transformation connecting different θ-vacuum in the bosonic picture is a Gaussian (displacement) transformation, this does not appear to be the case in the fermionic picture. However it could happens that the Gaussian approach can shed some light on the study of the θ-vacuum structure since an interesting periodic pattern has been observed when considering the potential V_Q between two fixed static charges as a function of L_0. Nevertheless this has not been properly worked out during the writing of this thesis and it's left opened.

[2]This idea was given by my supervisor Dr. Tao Shi.

Appendices

A. Systematic derivation of $H_Q(\Gamma)$

In this appendix we explain how to obtain the mean field state dependent Hamiltonian $H_Q(\Gamma)$ in a systematic way. We want to obtain a quadratic Hamiltonian such that if $|G.S\rangle = \mathcal{U}|0\rangle$ is the minimizer of H then

$$\langle H\rangle_{G.S} = \langle H_Q(\Gamma)\rangle_{G.S}\,. \tag{A.1}$$

In order to do so we would like to expand H to second order polynomials in powers of Φ and $\Phi^\dagger$ like in (2.57) by means of Wick's theorem product expansion that we prove in the following using Ref. [31].

As we saw in Lemma 2.4.1, the FGS minimizer of $\langle H\rangle_{G.S}$ is the real ground state of $H_Q(\Gamma)$ that is a quadratic Hamiltonian. $H_Q(\Gamma)$ can be diagonalized (like in subsection 2.3.2) and expressed in terms of quasi-particles excitations γ_k and $\gamma_k^\dagger$ whose vacuum is given by $\mathcal{U}|0\rangle$. Operators ϕ_j and $\phi_j^\dagger$, which will be denoted indistinctly by A_i, are then linear combinations of γ_k and $\gamma_k^\dagger$ and therefore can be splitted as

$$A_i = A_i^+ + A_i^- \tag{A.2}$$

such that

$$A_i^-|G.S\rangle = 0 \qquad \langle G.S|A_i^+ = 0 \qquad \text{and } [A_i^-, A_j^+]_\mp \in \mathbb{C}, \tag{A.3}$$

with $[A,B]_\mp = AB \mp BA$ the commutation relations for bosons and fermions respectively, since the method can be applied to both.

A product of operators $A_i^\pm$ is **normally ordered** if all factors A_i^- are at the right of the factors A_j^+. In particular a product of operators of the same type, like for example $A_1^+\cdots A_k^+$ is normally ordered. This operation will be denoted via $:\cdot:$.

As an example consider a product that contains k factors A_i^+ mixed with $n-k$ factors A_i^-. The normal order of those is given by

$$:A_1^\pm \dots A_n^\pm: = (\pm 1)^\pi A_{i_1}^+\cdots A_{i_k}^+\cdots A_{i_n}^- \tag{A.4}$$

where for bosons $(+1)^\pi = 1$, while for fermions $(-)^\pi$ is the parity of the permutation that brings the sequence $1\dots n$ to $i_1\dots i_n$. Note that the $G.S$-average of normally ordered operators vanishes

$$\langle :A_1\cdots A_n:\rangle_{G.S} = 0. \tag{A.5}$$

The important result here is that a product $A_1\dots A_n$ can be written as a sum of normally ordered product. For two operators that it's the case

$$A_1A_2 = :A_1A_2: + [A_1^-, A_2^+]_\mp \tag{A.6}$$

where as we already noted $[A_1^-, A_2^+]_\mp \in \mathbb{C}$. On the other hand one usually defines the **contraction** of two operators by

$$\overbrace{A_1A_2} \equiv A_1A_2 - :A_1A_2: \tag{A.7}$$

that from (A.6) is found to be the complex number

$$\overbrace{A_1 A_2} = [A_1^-, A_2^+]_\mp. \tag{A.8}$$

Because of this important relation and the fact that $G.S$-expectation value of a normal ordered operator is zero, it follows that

$$\overbrace{A_1 A_2} = \left\langle \overbrace{A_1 A_2} \right\rangle_{G.S} = \langle A_1 A_2 \rangle_{G.S}\,. \tag{A.9}$$

When there is a product of n operators in between, the contraction is defined by

$$\overbrace{A(A_1 \cdots A_n)A'} = (\pm)^\pi \overbrace{AA'}(A_1 \cdots A_n). \tag{A.10}$$

Theorem A.0.1 (Wick's product identity)**.**

$$\begin{aligned} A_1 A_2 \cdots A_n =& : A_1 \cdots A_n : + \sum_{(ij)} : A_1 \cdots \overbrace{A_i \cdots A_j} \cdots A_n : \\ &+ \sum_{(ij)(rs)} : A_1 \cdots \overbrace{A_i \cdots \overbrace{A_r \cdots A_j} \cdots A_s} \cdots A_n : + \cdots \end{aligned} \tag{A.11}$$

The first sum runs on single contraction of pairs, the second sum runs on double contractions and so on. If n is even, the last sum contains terms which are products of contractions. This will be the case for fermionic Hamiltonians. If n is odd, the last sum has terms with single unpaired operators.

Proof. A proof of this theorem is given by induction over n and can be found in [31]. □

One of the consequences of Wick's product identity is Wick's theorem as we saw it in chapter 2 Theorem 2.3.1 in the case of pure FGS

Corollary.

$$\langle A_1 \cdots A_{2l} \rangle_{G.S} = {\sum_\pi}' (\pm)^\pi \left\langle A_{\pi(1)} A_{\pi(2)} \right\rangle_{G.S} \cdots \left\langle A_{\pi(2l-1)} A_{\pi(2l)} \right\rangle_{G.S}, \tag{A.12}$$

with ${\sum_\pi}'$ as defined in (2.38). Moreover since $G.S$-average of normally ordered expansion vanishes

$$\langle A_1 \cdots A_{2l+1} \rangle_{G.S} = 0. \tag{A.13}$$

Therefore this expansion allows us to use a systematic rule to expand H to any order in creation and annihilation operators (or quadratures in the bosonic case). Applying the expansion (A.11) to the corresponding Hamiltonian and truncating in second order normal ordered operators we find

$$H = \underbrace{\langle H \rangle_{G.S} + \frac{1}{2} : \Phi^\dagger \mathcal{H}(\Gamma) \Phi :}_{=H_Q(\Gamma)} + \mathcal{O}(\phi^4), \tag{A.14}$$

where both sides of the equation have the same $G.S$-average and $\mathcal{H}(\Gamma)$ is given by contractions of operators, i.e., elements of the covariance matrix.

Now taking into account that $A_iA_j = \langle A_iA_j\rangle_{G.S} + :\ A_iA_j\ :$ we find the quadratic state dependent Hamiltonian

$$\mathcal{H}_Q(\Gamma) = \frac{1}{2}\Phi^\dagger\mathcal{H}(\Gamma)\Phi. \tag{A.15}$$

This method can be applied to any Hamiltonian polynomial in creation and annihilation for bosonic and fermionic systems or a combination of boths. Bosonic systems could include a linear term in the quadratures. In the most general case the quadratic Hamiltonian would take the form

$$H_Q(\Gamma) = \langle H\rangle_G + \frac{1}{2} :\Phi^\dagger\mathcal{H}(\Gamma)\Phi: + \frac{1}{2}\eta_H^T\delta R + \frac{1}{4} :\delta R^T(\Gamma_b, \langle R\rangle)\delta R:, \tag{A.16}$$

with $\delta R = R - \langle R\rangle_{G.S}$ as defined in subsection 2.6.1.

In fact, this is the method that has been applied in this thesis in order to obtain $H_Q(\Gamma)$ following the ideas from [24].

B. Computations: mean-field Hamiltonians

In this appendix one can find the computation of the mean field Hamiltonians for the Schwinger model in chapter 4 and $SU(2)$ non-Abelian case in (1+1)-dimensions in chapter 5.

B.1. Schwinger model

Since H_M and H_{int} in (4.70) are already quadratic in creation and annihilation operators[1] then they are already in mean field form. We just need to apply the normal order $:\,:$ w.r.t the fermionic Gaussian state ansatz.

1.
$$H_{int} = \langle H_{int}\rangle + \varepsilon : \sum_n \{\phi_n^\dagger \phi_{n+1} + \phi_{n+1}^\dagger \phi_n\} := \langle H_{int}\rangle + \varepsilon : \sum_n \begin{pmatrix} \phi_n^\dagger & \phi_{n+1}^\dagger \end{pmatrix} \sigma_x \begin{pmatrix} \phi_n \\ \phi_{n+1} \end{pmatrix} :$$
$$= \langle H_{int}\rangle + \varepsilon : \phi^\dagger T \phi := \langle H_{int}\rangle + \frac{1}{2}\varepsilon : \Phi^\dagger \begin{pmatrix} T & 0 \\ 0 & -T \end{pmatrix} \Phi :,$$
with T the tridiagonal matrix with 1's on the ± 1 diagonals and 0 on the main one.

2.
$$H_M = \langle H_M\rangle + m : \sum_n (-1)^n \phi_n^\dagger \phi_n := \langle H_M\rangle + m : \phi^\dagger D \phi := \langle H_M\rangle + \frac{1}{2} m : \Phi^\dagger \begin{pmatrix} D & 0 \\ 0 & -D^T \end{pmatrix} \Phi :,$$
with $D = diag((-1)^n)$.

3. H_E is the most interesting term since is the only non-quadratic and long-range term. Here we will apply Wick's theorem for the fermionic case w.r.t. the Gaussian state.
$$\frac{2}{ag^2} H_E = \sum_n \big(L_0 - \sum_{k\le n} \pi_k + \sum_{k\le n} \phi_k^\dagger \phi_k\big)^2 = \sum_n \{ \underbrace{L_0^2 - 2L_0 \sum_{k\le n} \pi_k + \big(\sum_{k\le n} \pi_k\big)^2}_{constant} \}$$
$$+ \sum_n \{2(L_0 - \sum_{k\le n} \pi_k) \sum_{k\le n} \phi_k^\dagger \phi_k + \big(\sum_{k\le n} \phi_k^\dagger \phi_k\big)^2\}$$
Therefore from H_E we have obtained one quadratic term that for most of the cases will be irrelevant, since we work with zero background field $L_0 = 0$; and

[1] It's on this point where the Unitary transformation $\tilde{U}$ took its most important role.

a quartic term where fermionic charge densities on spatially separated nodes of the lattice interact. Let's therefore obtain the Mean Field Hamiltonian for the electric term:

$$:\sum_{k\leq n}\phi_k^\dagger\phi_k:=:\phi^\dagger id_n\phi:=\frac{1}{2}:\Phi^\dagger\begin{pmatrix} id_n & 0\\ 0 & -id_n\end{pmatrix}\Phi:,$$

where $id_n = diag(\underbrace{1,...,1}_{n1\text{'s}},0,...,0)$.

$$\begin{aligned}
\big(\sum_{k\leq n}\phi_k^\dagger\phi_k\big)^2 &= \sum_{k,p}^{n}\phi_k^\dagger\phi_k\phi_p^\dagger\phi_p = \langle\big(\sum_{k\leq n}\phi_k^\dagger\phi_k\big)^2\rangle + \sum_{k,p}^{n}\Big\{:\phi_k^\dagger\left\langle\phi_p^\dagger\phi_p\right\rangle\phi_k: - :\phi_k^\dagger\langle\phi_k\phi_p\rangle\phi_p^\dagger:\Big\}+\\
&\sum_{k,p}^{n}\Big\{:\phi_k^\dagger\left\langle\phi_k\phi_p^\dagger\right\rangle\phi_p: + :\phi_k\left\langle\phi_k^\dagger\phi_p\right\rangle\phi_p^\dagger: - :\phi_k\left\langle\phi_k^\dagger\phi_p^\dagger\right\rangle\phi_p: + :\phi_p^\dagger\left\langle\phi_k^\dagger\phi_k\right\rangle\phi_p:\Big\}\\
&= \langle\big(\sum_{k\leq n}\phi_k^\dagger\phi_k\big)^2\rangle + Tr^n(\left\langle\phi^\dagger\phi\right\rangle):\phi^\dagger id_n\phi: - :\phi^\dagger\langle\phi\phi\rangle^n\phi^\dagger: + :\phi^\dagger\left\langle\phi\phi^\dagger\right\rangle^n\phi:\\
&- :\phi^\dagger(\left\langle\phi^\dagger\phi\right\rangle^n)^T\phi: - \phi\left\langle\phi^\dagger\phi^\dagger\right\rangle\phi: + Tr^n(\left\langle\phi^\dagger\phi\right\rangle):\phi^\dagger id_n\phi:\\
&= \langle\big(\sum_{k\leq n}\phi_k^\dagger\phi_k\big)^2\rangle + :\begin{pmatrix}\phi^\dagger & \phi\end{pmatrix}\begin{pmatrix} 2Tr^n(\langle\phi\phi^\dagger\rangle)+\left\langle\phi\phi^\dagger\right\rangle-\left\langle\phi^\dagger\phi\right\rangle^T & -\langle\phi\phi\rangle\\ -\left\langle\phi^\dagger\phi^\dagger\right\rangle & 0\end{pmatrix}\begin{pmatrix}\phi\\ \phi^\dagger\end{pmatrix}:\\
&= \langle\big(\sum_{k\leq n}\phi_k^\dagger\phi_k\big)^2\rangle\\
&+ \frac{1}{2}:\Phi_n^\dagger\underbrace{2\begin{pmatrix} Tr^n(\langle\phi\phi^\dagger\rangle)-\frac{1}{2}+\left\langle\phi\phi^\dagger\right\rangle & -\langle\phi\phi\rangle\\ -\left\langle\phi^\dagger\phi^\dagger\right\rangle & -Tr^n(\langle\phi\phi^\dagger\rangle)+\frac{1}{2}-\left\langle\phi\phi^\dagger\right\rangle^T\end{pmatrix}}_{=H_4(n)}\Phi_n:,
\end{aligned}$$

where Tr^n means the trace over the $n\times n$ first entries of the respective matrix and Φ_n makes reference to the first (n,n)-components of Φ.

Therefore the state dependent quadratic Hamiltonian reads

$$\boxed{H_Q(\Gamma) = \langle H\rangle + \frac{1}{2}:\Phi^\dagger\big[\sigma_z\otimes(mD+\varepsilon T)+\frac{ag^2}{2}\sum_n\Big\{2(L_0-\sum_k^n\pi_k)\sigma_z\otimes id_n + H_4(n)\Big\}\big]\Phi:} \tag{B.1}$$

Computation of the energy

As we saw in chapter 2, the average energy plays an important role in the Gaussian approach since it should decrease during the imaginary time evolution allowing us to know the rate at which the system tends to the ground state. Therefore its analytical computation it's an important calculation in this method.

$$\langle H\rangle = \langle H_M\rangle + \langle H_{int}\rangle + \langle H_E\rangle \tag{B.2}$$

$$\langle H_{int}\rangle = \varepsilon(Tr^{+1}(\left\langle \phi^\dagger\phi\right\rangle) + h.c.) \tag{B.3}$$

where Tr^{+1} is defined as the sum of the upper-first diagonal's elements.

$$\begin{aligned}\langle H_M\rangle &= mTr(D\left\langle \phi^\dagger\phi\right\rangle),\\ \frac{2}{ag^2}\langle H_E\rangle &= \sum_n\Big(L_0^2 - 2L_0\sum_k^n \pi_k + (\sum_k^n \pi_k)^2\Big)\\ &\quad + 2\sum_n\Big\{(L_0 - \sum_k^n \pi_k)Tr^n(\left\langle \phi^\dagger\phi\right\rangle)\Big\} + \sum_n\langle(\sum_k^n \phi_k^\dagger\phi_k)^2\rangle,\end{aligned}$$

but

$$\begin{aligned}\sum_n\langle(\sum_k^n \phi_k^\dagger\phi_k)^2\rangle &= \sum_n\sum_{k,p}^n\left\langle \phi_k^\dagger\phi_k\phi_p^\dagger\phi_p\right\rangle = \sum_n\sum_{k,p}^n\Big\{\left\langle \phi_k^\dagger\phi_k\right\rangle\left\langle \phi_p^\dagger\phi_p\right\rangle - \left\langle \phi_k^\dagger\phi_p^\dagger\right\rangle\langle\phi_k\phi_p\rangle\\ &\quad + \left\langle \phi_k^\dagger\phi_p\right\rangle\left\langle \phi_k\phi_p^\dagger\right\rangle\Big\} = \sum_n\Big\{Tr^n(\left\langle \phi^\dagger\phi\right\rangle)^2 + Tr^n(\left\langle \phi^\dagger\phi^\dagger\right\rangle\underbrace{\langle\phi\phi\rangle}_{-\langle\phi\phi\rangle^T})\\ &\quad + Tr^n(\left\langle \phi^\dagger\phi\right\rangle\left\langle \phi\phi^\dagger\right\rangle^T)\Big\},\end{aligned}$$

Therefore

$$\begin{aligned}\langle H\rangle &= mTr(D\left\langle \phi^\dagger\phi\right\rangle) + \varepsilon(Tr^{+1}(\left\langle \phi^\dagger\phi\right\rangle) + h.c) + \frac{ag^2}{2}\sum_n\Big(L_0^2 - 2L_0\sum_k^n\pi_k\\ &\quad + (\sum_k^n\pi_k)^2\Big) + ag^2\sum_n\Big\{(L_0 - \sum_k^n\pi_k)Tr^n(\left\langle \phi^\dagger\phi\right\rangle)\Big\}\\ &\quad + \frac{ag^2}{2}\sum_n\Big\{Tr^n(\left\langle \phi^\dagger\phi\right\rangle)^2 + Tr^n(\left\langle \phi^\dagger\phi^\dagger\right\rangle\underbrace{\langle\phi\phi\rangle}_{-\langle\phi\phi\rangle^T}) + Tr^n(\left\langle \phi^\dagger\phi\right\rangle\left\langle \phi\phi^\dagger\right\rangle^T)\Big\}.\end{aligned} \tag{B.4}$$

B.2. $SU(2)$ theory

In this part we present the state dependent form for the transformed Hamiltonian (5.40) computed in section B.2. In this case the fermionic Fock space $\mathcal{F}$ can be constructed with three different kind of modes: the Nambu index distinguishing creation operators from the annihilation ones expand the factor $\mathcal{F}_N$, the group index a which spans the space $\mathcal{F}_G$ of different colored excitations, and the mode index which in this case makes reference to the spatial degrees of freedom spanning $\mathcal{F}_S$. Therefore

$$\mathcal{F} = \mathcal{F}_N\otimes\mathcal{F}_G\otimes\mathcal{F}_S \Rightarrow \Phi = (\phi_{a,n}, \phi_{a,n}^\dagger)^T.$$

From this perspective and considering the Hamiltonian

$$H = \varepsilon\sum_n\{\phi_n^\dagger\phi_{n+1} + h.c.\} + m\sum_n(-1)^n\phi_n^\dagger\phi_n + \frac{g^2}{2}\sum_{n,\alpha}\Big(L_0^\alpha - \sum_{m>n}\{Q_m^\alpha + Q_{\text{ext},\,m}^\alpha\}\Big)^2 \tag{B.5}$$

one can easily sees that the hopping and the mass term are exactly the same as we derived for the $U(1)$ case (4.3.3), where they are already quadratic operators, apart from the fact that we have now an additional group index. Therefore

$$\begin{aligned} H_{int} &= \varepsilon \sum_{a,n} \{(\phi_n^\dagger)_a (\phi_{n+1})_a + h.c.\} = \langle H_{int} \rangle + \varepsilon : \phi^\dagger [Id_G \otimes T] \phi : \\ &= \langle H_{int} \rangle + \frac{1}{2} \varepsilon : \Phi^\dagger \begin{pmatrix} Id_G \otimes T & 0 \\ 0 & -Id_G \otimes T^T \end{pmatrix} \Phi : \end{aligned} \tag{B.6}$$

with again T the tridiagonal matrix with 1's on the ± 1 diagonals and 0 on the main one, i.e., $T^T = T$, and the mass term

$$\begin{aligned} H_M &= \langle H_M \rangle + m : \sum_n (-1)^n \phi_n^\dagger \phi_n := \langle H_M \rangle + m : \phi^\dagger [Id_G \otimes D] \phi : \\ &= \langle H_M \rangle + \frac{1}{2} m : \Phi^\dagger \begin{pmatrix} Id_G \otimes D & 0 \\ 0 & -Id_G \otimes D \end{pmatrix} \Phi :, \end{aligned} \tag{B.7}$$

with $D = diag((-1)^n)$. On the other hand, the electric term is not quadratic and therefore we will need to apply Wick's theorem. Expanding the square we get

$$\begin{aligned} \frac{2}{g^2} H_E &= \sum_{n,\alpha} \left(L_0^\alpha - \sum_{m>n} \{ Q_m^\alpha + Q_{\text{ext},\, m}^\alpha \} \right)^2 \\ &= \sum_{n,\alpha} (L_0^\alpha)^2 + \sum_{n,\alpha;m,p>n} Q_{\text{ext},\, m}^\alpha Q_{\text{ext},\, p}^\alpha - 2 \sum_{n,\alpha} L_0^\alpha \sum_{m>n} Q_{\text{ext},\, m}^\alpha - 2 \sum_{n,\alpha} L_0^\alpha \sum_{m>n} Q_m^\alpha \\ &+ 2 \sum_{n,\alpha;m,p>n} Q_{\text{ext},\, p}^\alpha Q_m^\alpha + \sum_{n,\alpha;m,p>n} Q_m^\alpha Q_p^\alpha \end{aligned} \tag{B.8}$$

where the first three terms are constant, the fourth and fifth ones quadratic and the only non-quadratic term is the interaction between charges on different sites. Let's analyze term by term:

$$H_{E1} = -2 \sum_{n,\alpha} L_0^\alpha \sum_{m>n} Q_m^\alpha = -2 \sum_{n;m>n} \underbrace{\sum_\alpha L_0^\alpha (T^\alpha)_{a,b}}_{=\mathcal{M}_{a,b}} \phi_m^{a\dagger} \phi_m^b = -2 \sum_{n;m>n} \mathcal{M}_{a,b} \phi_m^{a\dagger} \phi_m^b. \tag{B.9}$$

In this point we realize the sum is over $m > n$ so we need to take into account this fact. Let me define the matrix

$$P_{m,n} = \begin{pmatrix} 0 & 0 & 0 & \dots \\ 1 & 0 & 0 & \cdots \\ 1 & 1 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{B.10}$$

then H_{E1} can be written as,

$$H_{E1} = -2\sum_{m,n}\mathcal{M}_{a,b}\phi_m^{a\dagger}\phi_m^b P_{m,n} = -2\sum_m \mathcal{M}_{a,b}\phi_m^{a\dagger}\phi_m^b \underbrace{\sum_n P_{m,n}}_{\tilde{P}_{m,m}} \tag{B.11}$$

$$= \langle H_{E1}\rangle - 2 : \phi^\dagger[\mathcal{M}\otimes\tilde{P}]\phi := \langle H_{E1}\rangle + \frac{1}{2} : \Phi^\dagger \begin{pmatrix} -2\mathcal{M}\otimes\tilde{P} & 0 \\ 0 & 2\mathcal{M}^T\otimes\tilde{P}^T \end{pmatrix}\Phi :,$$

where $\tilde{P}$ is a diagonal matrix in the spatial index which allows us to extend the sum over m without the n-dependent boundary. This could also been applied in the $U(1)$ case and in fact it was done so in the numerical implementation.

$$H_{E1'} = 2\sum_{n,\alpha;m,p>n} Q^\alpha_{\text{ext},\,p}Q^\alpha_m = 2\sum_{n,\alpha,m,p}(T^\alpha)_{ab}\phi_m^{a\dagger}\phi_m^b P_{m,n}Q^\alpha_{\text{ext},\,m}P_{p,n} \tag{B.12}$$

$$= 2\sum_{\alpha,m,p}(T^\alpha)_{ab}\phi_m^{a\dagger}\phi_m^b Q^\alpha_{\text{ext},\,p}\underbrace{A_{m,p}}_{\sum_n P_{m,n}P^T_{n,p}} = \sum_m \phi_m^{a\dagger}\underbrace{\left[2\sum_\alpha(T^\alpha)_{ab}\sum_p A_{m,p}Q^\alpha_{\text{ext},\,p}\right]}_{=2(\mathcal{M}^{ext})^m_{a,b}}\phi_m^b$$

$$= \langle H_{E1'}\rangle + : \phi^\dagger H_{ext}\phi :$$

$$H_{E2} = \sum_{n,\alpha;m,p>n} Q^\alpha_m Q^\alpha_p = \sum_{n,\alpha;m,p>n}(T^\alpha)_{a,b}(T^\alpha)_{i,j}\phi_m^{a\dagger}\phi_m^b\phi_p^{i\dagger}\phi_p^j. \tag{B.13}$$

In this case and since we will usually work in the fundamental representation of $SU(N)$, we could use the normalization condition

$$\sum_{\alpha=1}^{N^2-1}(T^\alpha)_{a,b}(T^\alpha)_{i,j} = \frac{1}{2}\Big(\delta_{a,j}\delta_{i,b} - \frac{1}{N}\delta_{a,b}\delta_{i,j}\Big), \tag{B.14}$$

or simply expand H_{E2} following the same prescription as before

$$H_{E2} = \sum_{n,\alpha,m,k}(T^\alpha)_{a,b}(T^\alpha)_{i,j}\phi_m^{a\dagger}\phi_m^b\phi_k^{i\dagger}\phi_k^j P_{m,n}P_{k,n} = \sum_{\alpha,m,k}(T^\alpha)_{a,b}(T^\alpha)_{i,j}\phi_m^{a\dagger}\phi_m^b\phi_k^{i\dagger}\phi_k^j$$

$$\underbrace{\sum_n P_{m,n}(P^T)_{n,k}}_{A_{m,k}} = \sum_{\alpha,m,k}(T^\alpha)_{a,b}(T^\alpha)_{i,j}A_{m,k}\,\phi_m^{a\dagger}\phi_m^b\phi_k^{i\dagger}\phi_k^j$$

$$= \sum_{\alpha,m,k}(T^\alpha)_{a,b}(T^\alpha)_{i,j}A_{m,k}\Big(-\phi_m^{a\dagger}\phi_k^{i\dagger}\phi_m^b\phi_k^j + \delta^{b,i}\delta_{m,k}\,\phi_m^{a\dagger}\phi_k^j\Big).$$

Now to this term we apply Wick's theorem, where we will have six terms, five of them different to each other

$$H^{MF}_{E2} = \langle H_{E2}\rangle + \sum_{\alpha,m,k}(T^\alpha)_{a,b}(T^\alpha)_{i,j}A_{m,k}\Big(2 : \phi_m^{a\dagger}\left\langle\phi_k^{i\dagger}\phi_k^j\right\rangle\phi_m^b : - : \phi_m^{a\dagger}\left\langle\phi_m^b\phi_k^j\right\rangle\phi_k^{i\dagger}$$

$$- : \phi_m^{a\dagger}\left\langle\phi_k^{i\dagger}\phi_m^b\right\rangle\phi_k^j : - : \phi_k^{i\dagger}\left\langle\phi_m^{a\dagger}\phi_k^j\right\rangle\phi_m^b : - : \phi_m^b\left\langle\phi_m^{a\dagger}\phi_k^{i\dagger}\right\rangle\phi_k^j : + \delta^{b,i}\delta_{m,k} : \phi_m^{a\dagger}\phi_k^j :\Big).$$

B. Computations: mean-field Hamiltonians

1.

$$2\sum_{\alpha,m,k}(T^\alpha)_{a,b}(T^\alpha)_{i,j}A_{m,k}:\phi_m^{a\dagger}\left\langle\phi_k^{i\dagger}\phi_k^j\right\rangle\phi_m^b:=2\sum_{\alpha,m}:\phi_m^{a\dagger}(T^\alpha)_{a,b}\Big[(T^\alpha)_{i,j}\sum_k A_{m,k}\left\langle\phi_k^{i\dagger}\phi_k^j\right\rangle\Big]\phi_m^b:$$
$$=:\phi^\dagger H_1\phi:$$

2.

$$-\sum_{\alpha,m,k}(T^\alpha)_{a,b}(T^\alpha)_{i,j}A_{m,k}:\phi_m^{a\dagger}\left\langle\phi_m^b\phi_k^j\right\rangle\phi_k^{i\dagger}:=-\sum_{\alpha,m,k}:\phi_m^{a\dagger}\Big[(T^\alpha)_{a,b}A_{m,k}\left\langle\phi_m^b\phi_k^j\right\rangle(T^{\alpha,t})_{j,i}\Big]\phi_k^{i\dagger}:$$
$$=:\phi^\dagger H_2\phi^\dagger:$$

3.

$$-\sum_{\alpha,m,k}(T^\alpha)_{a,b}(T^\alpha)_{i,j}A_{m,k}:\phi_m^{a\dagger}\left\langle\phi_k^{i\dagger}\phi_m^b\right\rangle\phi_k^j:=-\sum_{\alpha,m,k}:\phi_m^{a\dagger}\Big[(T^\alpha)_{a,b}A_{m,k}\Big(\left\langle\phi^\dagger\phi\right\rangle^T\Big)_{m,k}^{b,i}(T^\alpha)_{i,j}\Big]\phi_k^j:$$
$$=:\phi^\dagger H_3\phi:$$

4.

$$-\sum_{\alpha,m,k}(T^\alpha)_{a,b}(T^\alpha)_{i,j}A_{m,k}:\phi_k^{i\dagger}\left\langle\phi_m^{a\dagger}\phi_k^j\right\rangle\phi_m^b:=-\sum_{\alpha,m,k}:\phi_k^{i\dagger}\Big[(T^\alpha)_{i,j}(A^T)_{k,m}\Big(\left\langle\phi^\dagger\phi\right\rangle^T\Big)_{k,m}^{j,a}(T^\alpha)_{a,b}\Big]\phi_m^b:$$
$$=:\phi^\dagger H_4\phi:$$

Since A is symmetric we find that $H_3=H_4$.

5.

$$-\sum_{\alpha,m,k}(T^\alpha)_{a,b}(T^\alpha)_{i,j}A_{m,k}:\phi_m^b\left\langle\phi_m^{a\dagger}\phi_k^{i\dagger}\right\rangle\phi_k^j:=-\sum_{\alpha,m,k}:\phi_m^b\Big[(T^{\alpha,t})_{b,a}\left\langle\phi_m^{a\dagger}\phi_k^{i\dagger}\right\rangle A_{m,k}(T^\alpha)_{i,j}\Big]\phi_k^j:$$
$$=:\phi H_5\phi:$$

6.

$$\sum_{\alpha,m,k}(T^\alpha)_{a,b}(T^\alpha)_{i,j}A_{m,k}\delta^{b,i}\delta_{m,k}:\phi_m^{a\dagger}\phi_k^j:=\sum_{\alpha,m}:\phi_m^{a\dagger}\Big[(T^\alpha\cdot T^\alpha)_{a,b}A_{m,m}\Big]\phi_m^b:=:\phi^\dagger H_6\phi:$$

Now, writing the result in a matrix form and defining $H_{11}=H_1+2H_3+H_6$ we find

$$:H_{E2}^{MF}:=:\begin{pmatrix}\phi^\dagger & \phi\end{pmatrix}\begin{pmatrix}H_{11} & H_2\\ H_5 & 0\end{pmatrix}\begin{pmatrix}\phi\\ \phi^\dagger\end{pmatrix}:=\frac{1}{2}:\Phi^\dagger\begin{pmatrix}H_{11} & 2H_2\\ 2H_5 & -H_{11}^T\end{pmatrix}\Phi: \quad \text{(B.15)}$$

In conclusion, the single-particle Hamiltonian matrix $\mathcal{H}(\Gamma)$ for the non-Abelian case takes the form

$$\mathcal{H}(\Gamma)=\begin{pmatrix}Id_G\otimes(\varepsilon T+mD) & 0\\ 0 & -Id_G\otimes(\varepsilon T^T+mD^T)\end{pmatrix} \quad \text{(B.16)}$$
$$+g^2\begin{pmatrix}-\mathcal{M}\otimes\tilde{P}+\frac{1}{2}H_{11}+\mathcal{M}^{ext} & H_2\\ H_5 & \mathcal{M}^T\otimes\tilde{P}^T-\frac{1}{2}H_{11}^T-(\mathcal{M}^{ext})^T\end{pmatrix}$$

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Declaration of Authorship

I hereby declare that this thesis has been composed by myself. The results presented in Chapter 4 (except the continuum formulation appearing in section 4.2.2), Chapter 5, Outlook 6.1 and Appendix B are based entirely on my own work unless clearly referenced or stated otherwise.

Munich, 22 September 2017

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Pablo Sala de Torres-Solanot