Exact solutions for strongly interacting electron systems in $D > 1$ dimensions

Ph.D. thesis

by

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Exact solutions for strongly interacting electron systems in $D > 1$ dimensions

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Tanúsítom, hogy Gurin Péter doktorjelölt 1997. és 2001. között a fent megnevezett doktori alprogram keretében irányításommal végezte munkáját. Az értekezésben foglaltak a jelölt önálló munkáján alapulnak, az eredményekhez önálló alkotó tevékenységével meghatározóan hozzájárult. Az értekezést elfogadásra javaslom.

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Dr. Gulácsi Zsolt
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Preface

This thesis contains the summary of my research work carried out as a Ph.D. student at the Theoretical Physics Department of the University of Debrecen, Hungary and partly at the Low Temperature Physics Laboratory of the Institute of Nuclear Research of the Hungarian Academy of Sciences. The new results underlying this thesis have already been presented at international scientific meetings and published in six papers appeared in the Proceedings of 21th International conference on Low Temperature Physics [1], in Philosophical Magazine B [2, 3, 4, 5] and in Physical Review B [6].

Here I would like to take the occasion and thank to everybody who helped me during the time I did my research and wrote my thesis.

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Chapter 1

Introduction

1.1 Approximations vs. exact results

The importance of approximative methods in physics a matter of fact that is unquestionable. Without them can not be treated any problem which is at least a little realistic. However, the task and the purpose of theoretical physics is *not* the solution of problems which are as realistic as possible. For example imagine for a moment that one can write down a Hamiltonian which is a very realistic model of the iron, taking into account almost all microscopic interactions between particles, and one can solve it. From the solution it can be seen that the material — namely the iron — is ferromagnetic, and the Néel temperature is also determined with high accuracy. And it is the result of a surely very complicated computation. Was it worth to do? Have we known something new? The ferromagnetic feature of the iron, including the precise value of its Néel temperature, is well known by *experimentally*. But why it is a ferromagnet? This is the adequate question for theoretical physics. For the answer we should point to the main microscopic features of the iron that makes it magnetic. Perhaps this is common with Ni and Co, too. The purpose is to construct a *model* of the ferromagnetism, or more precisely the ferromagnetism of transition metals; may be other way leading to ferromagnetism in very different materials. That means the *understanding* of this phenomenon.

From this point we have to make distinction between the features of the model and the features of the real material desired to describe by it. We should not beat about the model at any coast to get a result which is observed in the real world. We should deduce result related to the model only by controlled approaches. I mean "controlled approach" the methods, which are either exact, or — at least —

there is a reliable estimate about the error, e.g. exists a really small parameter for perturbation computation. In the field of strongly correlated systems unfortunately there are very few well-tried controlled approaches, and most of them work only in one dimension. My purpose in this thesis is to give higher dimensional exact results related to important models of many-body physics.

After this little bit philosophical introduction let's see some concrete models of strongly correlated systems and the interesting questions which motivate the physicists — among them me — to study these models.

1.2 Motivation

Strongly correlated electron systems have been studied considerably in the last decade. From the relatively new phenomenon about heavy fermions and oxide superconductors till the perhaps oldest one not well-understood cooperative electronic phenomena, the ferromagnetism provide attractive problems for researchers of solid state physics. The fundamental models to describe strongly correlated electrons are given by the Hubbard model and the periodic Anderson model (Anderson lattice).

The Hubbard model has a long history in describing the magnetism of materials since the works of Hubbard [7], Gutzwiller [8] and Kanamori [9]. The Hubbard model has evoked much attention after the discovery of high-T_c superconductors [10]. Thus the importance of the Hubbard model of itinerant electrons is increasingly being appreciated. One dimensional Hubbard model has been studied in a very elegant way by Bethe Ansatz [11] and conformal field theory [12]. The solutions revealed that the weak-coupling bosonisation theory [13] can well describe the ground state of the Hubbard model in one dimension, which established the concept of Luttinger liquid. In spite of the success for the one dimensional correlated models, such as the Hubbard model and $t-J$ model, correlated electrons in two or three dimension are still far from a complete understanding, due to the fact that there are no many controlled approaches which are usable under these circumstances. In the study of the Hubbard model, main topics are likely the following:

- Magnetism: ferromagnetism or antiferromagnetism?
- Possibility of metal-insulator (Mott) transition.
- Possibility of superconductivity.

Chapter 3 and 5 of this thesis are connected with the first topic. In Chapter 3 I study the effect of the non-on-site interactions to characterize their influence on the stability of ordered phases, among them ferromagnetic and antiferromagnetic orderings. We succeeded in determining different parameter regions where the exact ground state wave function describes fully saturated ferromagnetic, paramagnetic insulator, and several kinds of charge and spin density wave (antiferromagnetic) phases. In Chapter 5 I study the simple Hubbard model without non-on-site interactions. I try to shed light on the origin of Nagaoka's ferromagnetism and discuss the case with more than one hole.

The periodic Anderson model (beside the Kondo lattice Hamiltonian) is established as a model to describe heavy fermions that show very characteristic behaviour. In heavy-Fermion systems with 4f or 5f atoms (such as Ce or U), the proximity of the electronic orbital to the Fermi level confers a Kondo effect at low temperature, i.e. an on-site compensation of localized magnetic moment by conduction electrons. A direct consequence is the observation at low temperature of a very large effective electronic mass $m*$ derived from the huge linear specific heat coefficient $\gamma = C/T$ and a correspondingly large Pauli susceptibility. Simultaneously, the observation of the de Haas-van Alphen quantum oscillations [14] also concludes in favour of the existence of heavy quasiparticles.

In addition to the Kondo effect, those systems are characterized by long-range RKKY (Ruderman-Kittel-Kasuya-Yoshida) interactions between neighbouring local moments mediated by conduction electrons. The competition between the Kondo effect and the RKKY interactions leads to the possibility of either a non-magnetic or a long-range magnetically-ordered ground state [15]. These ground states are separated by a zero-temperature quantum phase transition point. This transition is governed by the value of the exchange coupling between the spin of the conduction electron and the local moment. One of the most striking properties of the heavy-Fermion compounds discovered during these last years is the experimental possibility to explore this quantum phase transition [16] by varying the composition change, or by applying a pressure or a magnetic field. The observed behavior at low temperature at this quantum critical point is at odds with that usually expected from a simple Fermi liquid. The specific heat C depends on T as $C/T \sim -Ln(T/T_0)$, the magnetic susceptibility as $\chi \sim 1 - \alpha\sqrt{T}$, and the T-dependent part of the resistivity as $\Delta\rho \sim T$ [18] (instead of $C/T \sim \chi \sim Const$ and $\Delta\rho \sim T^2$ in the Fermi liquid state). Pressure or large magnetic fields are found to restore the Fermi liquid behavior.

The origin of this non-Fermi liquid regime is a largely discussed problem. There are three main interpretations which rely on (i) a single impurity multichannel Kondo effect in which the internal degree of freedom is provided by the 4f or 5f quadrupolar moment [17], (ii) a distribution of the Kondo coupling due to the disorder leading to a distribution of the Kondo temperature $P(T_K)$ [19] and (iii) the proximity of a quantum phase transition [18, 20, 21].

As partially explained in the above the followings are the most interesting questions which are likely related to the periodic Anderson model:

- Fermi liquid state with heavy mass, and non-Fermi liquid state.

- Interplay between Kondo effect and the RKKY interaction.
- Magnetism: ferromagnetism or antiferromagnetism?
- Metal-insulator transition: Kondo insulator.

Chapter 4 is connected with the first topic. However, the model investigated by me is not an original periodic Anderson model. The difference is that I take into account hopping on the level of f-electrons. This leads to an effective band which is completely flat in a special region of parameter space, and this feature remains valid in the interacting case. Due to this feature we can give the exact ground state in which the occupation number $n_{\vec{k}}$ is continuous together with its derivatives of any order.

1.3 Outline

This thesis deals with exact results related to strongly interacting, therefore usually strongly correlated electron systems. It means mainly (except Chapter 5) zero temperature properties: ground state wave function and energy. In the first Section I illustrated why the exact solutions are so important in physics, especially in the field I have worked. I sketched the difficulties of this duty, in consideration the problem of $D > 1$. The previous Section exposed the models and questions which are related to the topic of this thesis.

Chapter 2 explains the mentioned models in details: the general concepts of the model building, the exact steps and the approximations that have to be done to obtain a treatable model. Firstly, on the example of the tight-binding description, I explained the general principle needed to get lattice models. Then, starting from a highly general Hamiltonian which describes interacting electrons in solids, I derive one and two band Hamiltonians. Truncating the interaction terms, — on the line of tight-binding approximation, — I get models with nearest and next-nearest neighbour interactions. Simple Hubbard model can be got as a final approximation. I construe the circumstances under which the approximation steps can be done and the features of the constructed models.

In Chapter 3 I deal with a Hubbard model extended with next-nearest neighbour interaction terms to ascertain the effect of these interactions to the stability of ordered phases. By a method used by several authors in the last decade I determined domains in the parameter space where the exact ground state is fully-saturated ferromagnetic state, different types of commensurate charge-density waves and spin-density waves, furthermore a phase separation region were found, when the band is half filled. I find that the next-nearest neighbour interactions have qualitative importance in the sense that they can stabilize different types of spin and charge orderings which could not be present in the phase diagram in the absence of these terms. Moreover they have quantitative importance, because they can strongly modify the stability domains of all phases, which depend also on the dimension of the system.

Results have been got by the same method are presented in Chapter 4. These are connected to an interacting two band model, which is essentially a periodic Anderson model. Every result of this Chapter is related to $D = 2$ dimension. I found an interesting solution for this model, which can describe two different physical situations depending on the filling and the values of the coupling constants: a Mott insulator and a non-Fermi liquid phase. In the ground state the Fermi surface can not be defined, because there is no discontinuity or any other non-analycity of the occupation number in the momentum space. However, there is a well-defined Fermi energy, where the density of states diverges. The ground state is paramagnetic with large spin degeneracy. The results are valid at three-quarter filling and above.

In Chapter 5 I analyze a simple one-band Hubbard model in $U = \infty$ limit in any dimensions. The purpose is to understand why the Nagaoka state is stable for one hole, and why not for more holes. For this purpose I developed a formalism which deal with the charge and spin degrees of freedom separately, and directly shows their interaction as well. I find that the rearrangement of particles (spins) with odd parity permutations while the single hole is moving is impossible. Therefore, the fermionic feature of electrons is not playing any role, and the system is equivalent with a system of hypothetical hard core ($U = \infty$) half-spin boson system whose ground state is trivially ferromagnetic. In the presence of more than one hole this is not true any more and the complete separation of charge and spin degrees of freedom is impossible. Based on our representation of the Hamiltonian, the trace over the spin degrees of freedom can be computed exactly. The presented procedure allows us to express the partition function, free energy, specific heat and the expectation value of the square of the total spin. This allows to study the case more than one hole.

A brief summary closes the main part of this thesis in English and Hungarian language. There are even two Appendices, the first for some computational details of Chapter 4, the other one for some well-known mathematical facts about the symmetric group and its representations, which is used in Chapter 5.

Chapter 2

Models of interacting electron systems

In this Chapter I derive the model Hamiltonians which I deal with in this thesis and explain some important related problems which can be described by them. I concentrate on questions which are in connection of the topic of next chapters, but I think it is high enough to exemplify the reasons of so much theoretical effort which are to find the "solutions" of these models.

In this thesis I deal with tight-binding Hamiltonians, like Hubbard model, periodic Anderson model, etc. First of all I explain the philosophy of tight-binding description, then I introduce the second quantized formalism, and present the general way, how can lattice models be got to describe some characteristic low energy features of the electron system in a solid. Among the one-band models I present the simple and extended Hubbard Hamiltonians, and the physics which is hoped to be captured by them. In the frame of a detailed discussion of the ferromagnetism, which is one of the longest-standing yet unresolved problems in the physics of strongly correlated electron systems, I discuss Nagaoka's theorem and related works. Then I shed light on the reason why we introduce even further terms with increased interaction range. After it I write about the periodic Anderson models in a broader sense: models with two bands in one of which a Hubbard interaction. Finally I discuss the non-Fermi liquid behaviour which is often based on multi-band models (see e.g. Ref. [21]).

2.1 Tight-binding description

Before introducing interacting many-electron Hamiltonians, we describe the corresponding single-electron problem. A single atom has multiple electrons in different orbits. When atoms come together to form a solid, electrons in the outermost orbits become itinerant, while those in the inner orbits are still localized at the original atomic sites. However, between these two situations, electrons in outer but not the most outer orbits are mostly localized around the atomic sites, but tunnel to nearby similar orbits with non-negligible probabilities. As an approximation, we only consider the electrons in these orbits, which are expected to play essential roles in determining various aspects of low-energy physics of the system. In this way we get a lattice model in which electrons live on lattice sites and hop from one site to another. This is the idea of the tight-binding description, which is a kind of low-energy effective theory: we declare that electrons can live only on lattice sites, leaving the possibility of the hopping between sites by tunneling process.

The question that how many atomic orbits play important role remains. For simplicity it is often assumed that the essential physics can be captured by a single non-degenerate (s) orbital, whereby all other orbits are neglected.[1] Of course, actual atoms can have more than one orbits, and these orbits can be degenerated, however, in some solids, the degeneracy in the original atomic orbit is lifted by crystalline anisotropy. The philosophy behind the model building is that those electrons in other states do not play significant roles in determining the low-energy physics in which we are interested, and can be "forgotten" for the moment.

2.2 General lattice model of interacting electrons

Remaining the important ideas from the above philosophy we can proceed more precisely to describe the electrons in solids. Instead of the atomic orbits, which are not well-defined in a crystal, we can use more convenient one-particle states: the Bloch states and the Wannier states. For our purpose a crystal is medium having translational periodicity with L_j periods in the j-th direction. Here $j = 1, \dots D$, where D is the dimension of the system. We take into account periodic boundary conditions, therefore it is convenient to label the lattice vectors by the elements of the factor group $\Lambda := \mathbb{Z}^D/(L_1, \dots, L_D)$. This medium has D linearly independent vector $\vec{d}_i$, so called primitive lattice vectors. All points related to each other by a lattice vector $\vec{R}_{\mathbf{i}}$ so that $\vec{R}_{\mathbf{i}} = \sum_{j=1}^{D} \mathbf{i}_j \vec{d}_j$ where $\mathbf{i} = (\mathbf{i}_1, \dots, \mathbf{i}_D) \in \Lambda$ have identical properties as a medium for electron motion. Assuming that $\vec{R}_{\mathbf{0}}$ is the coordinate

[1] More precisely, in the band theory of electrons in solids, all other bands can be projected onto one effective band. The single band approximation requires the existence of a band gap above the effective band. Then the deviation of the coupling constants from their multi-band values can be determined, in principle, by perturbation theory.

of a fixed atom, the vectors $\vec{R}_{\mathbf{i}}$ are the coordinates of atoms. Hereafter we refer the set $\{\vec{R}_{\mathbf{i}} : \mathbf{i} \in \Lambda\}$ as the lattice and $\vec{R}_{\mathbf{i}}$ — or simplifying, shortly $\mathbf{i}$ — as the sites. We denote the number of the sites by $N_\Lambda = \prod_{j=1}^{D} L_j$, and the sum over all the sites by $\sum_{\mathbf{i}}$ instead of $\sum_{\mathbf{i}\in\Lambda}$.

From the above mentioned translational periodicity follows that the one particle Hamiltonian, which contains kinetic energy and the ionic potential, have a translational symmetry considering the lattice translations, therefore it commutes with the lattice translation operators defined by

$$\hat{T}_{\mathbf{i}}\psi(\vec{r}) = \psi(\vec{r} + \vec{R}_{\mathbf{i}}), \tag{2.1}$$

where ψ is an arbitrary one-particle wave function. Every $\hat{T}_{\mathbf{i}}$ are unitary operators, therefore their eigenvalues are in the complex unit circle. It is the custom to represent these eigenvalues in terms of wave vector $\vec{k}$, that is, to write

$$\hat{T}_{\mathbf{i}}\psi_{\vec{k}} = e^{i\vec{k}\vec{R}_{\mathbf{i}}}\psi_{\vec{k}}\ , \tag{2.2}$$

where $\vec{k}$ is an element of the reciprocal space, i.e., $\vec{k} = 2\pi\sum_{i=1}^{d}\lambda_i\vec{d}_i^*$, where $\vec{d}_i^*$ is the dual basis of $\vec{d}_i$, i.e., $\vec{d}_i\vec{d}_j^* = \delta_{i,j}$. Since all distinct eigenvalues of the lattice translational operators arise choosing the values of λ_i from an interval of length unity, we see that all significant values of $\vec{k}$ are reached if $\vec{k}$ varies within one primitive cell of the reciprocal lattice expanded by 2π, i.e., within the first Brillouin zone. Hereafter the set of these $\vec{k}$ vectors from the first Brillouin zone is denoted by $\hat{\Lambda}$. Outside the first Brillouin zone we reach $\vec{k}$ values which are equivalent. With this end in view, the $\sum_{\vec{k}}$ is a shorthand notation instead of $\sum_{\vec{k}\in\hat{\Lambda}}$.

As a short by-path, here we fix some conventions which will be convenient in the following Chapters. Both Λ and $\hat{\Lambda}$ are handled as ordered sets, i.e., they are endowed with a greater than relation. These orders are fixed but otherwise arbitrary. If we do not say others, by definition, the multipliers of every non-commutative product over Λ, $\hat{\Lambda}$, or some subsets of them stand in increasing order. The products of which multipliers stand in decreasing order is denoted by prime over the $\prod$, such as in equation (A.8). Finally, the following convention will be used: the boldface lattice indices refer to the order of Λ, i.e., the first, second, i-th and the last elements of Λ are denoted by **1, 2, i** and $\mathbf{N}_\Lambda$, respectively. When a normal type letter denotes a natural number between 1 and N_Λ then the boldface letter denotes the appropriate lattice site respect to the order of Λ.

Bloch functions $\varphi_{\vec{k},s}$ are the eigenfunctions of the Hamiltonian having lattice translational symmetry, which are simultaneously eigenfunctions of the lattice translation operators (2.1) with eigenvalues $e^{i\vec{k}\vec{R}}$. The corresponding eigenvalues of the Hamiltonian is denoted by $\epsilon_{\vec{k},s}$. Due to the using of periodic (Born – von Karman) boundary conditions there are not any technical difficulty to normalize the Bloch functions, which thus form an orthonormal system,

$$\int d\vec{r}\, \varphi^*_{\vec{k},s}(\vec{r})\, \varphi_{\vec{k}',s'}(\vec{r}) = \delta_{\vec{k},\vec{k}'}\, \delta_{s,s'}. \tag{2.3}$$

These functions, like any physically meaningful function of $\vec{k}$, must be periodic in reciprocal space. This means, in general, that the Bloch functions can be written as Fourier series of the form

$$\varphi_{\vec{k},s}(\vec{r}) = \frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{i}} e^{-i\vec{k}\vec{R}_{\mathbf{i}}} \chi_s(\vec{r} - \vec{R}_{\mathbf{i}}) \tag{2.4}$$

because the functions χ have the property that they depend only on the difference of $\vec{R}_{\mathbf{i}}$ and $\vec{r}$. The function $\chi_{\mathbf{i},s}(\vec{r}) := \chi_s(\vec{r} - \vec{R}_{\mathbf{i}})$ is the Wannier function localized at site $\mathbf{i}$, because the probability density of an electron described by the wave function $\chi_{\mathbf{i},s}(\vec{r})$ is concentrated near the site $\mathbf{i}$. It can be expressed explicitly through the inverse of equation (2.4) as

$$\chi_{\mathbf{i},s}(\vec{r}) = \frac{1}{\sqrt{N_\Lambda}} \sum_{\vec{k}} e^{i\vec{k}\vec{R}_{\mathbf{i}}} \varphi_{\vec{k},s}(\vec{r}). \tag{2.5}$$

Dealing with many-particle systems we can introduce the more convenient occupation number (in other word "second quantized") formalism. Within this formalism the Hamiltonian for electrons with spin σ interacting via a spin-independent interaction $V^{ee}(\vec{r}_1 - \vec{r}_2)$ in the presence of an ionic potential $V^{ion}(\vec{r})$ has the form [7, 22] $\hat{H} = \hat{H}_0 + \hat{H}_{int}$, where

$$\hat{H}_0 = \sum_{\sigma} \int d\vec{r}\, \hat{\psi}^\dagger_\sigma(\vec{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V^{ion}(\vec{r}) \right] \hat{\psi}_\sigma(\vec{r}) \tag{2.6}$$

$$\hat{H}_{int} = \frac{1}{2} \sum_{\sigma,\sigma'} \int d\vec{r}_1 \int d\vec{r}_2\; V^{ee}(\vec{r}_1 - \vec{r}_2) \hat{n}_\sigma(\vec{r}_1) \hat{n}_{\sigma'}(\vec{r}_2). \tag{2.7}$$

Here $\hat{\psi}_\sigma(\vec{r})$ and $\hat{\psi}^\dagger_\sigma(\vec{r})$ are the usual field operators and $\hat{n}_\sigma(\vec{r}) = \hat{\psi}^\dagger_\sigma(\vec{r})\hat{\psi}_\sigma(\vec{r})$ is the local density. We note that the interaction term is diagonal in the space variables $\vec{r}_1$, $\vec{r}_2$, i.e. it depends only on the (operator valued) densities of the electrons at site $\vec{r}_1$, $\vec{r}_2$ which interact via $V^{ee}(\vec{r}_1 - \vec{r}_2)$. The lattice potential entering the non-interacting part (2.6) leads to a splitting of the parabolic dispersion into infinite many bands which we enumerate by the index s, and the eigenfunctions of the non-interacting problem — by the above definition — is the Bloch wave functions $\varphi_{\vec{k},s}(\vec{r})$ with the band energies $\epsilon_{\vec{k},s}$. Constructing creation and annihilation operators $\hat{c}^\dagger_{\vec{k},s,\sigma}$, $\hat{c}_{\vec{k},s,\sigma}$ for electrons with spin σ in the band s with wave vector $\vec{k}$ as

$$\hat{c}^\dagger_{\vec{k},s,\sigma} = \int d\vec{r}\, \varphi_{\vec{k},s}(\vec{r}) \hat{\psi}^\dagger_\sigma(\vec{r}), \tag{2.8}$$

the non-interacting Hamiltonian can be written as

$$\hat{H}_0 = \sum_{\vec{k},s,\sigma} \epsilon_{\vec{k},s} \hat{c}^\dagger_{\vec{k},s,\sigma} \hat{c}_{\vec{k},s,\sigma}. \tag{2.9}$$

For the lattice representation of the Hamiltonian we use the Wannier basis instead. We may introduce creation and annihilation operators $\hat{c}^\dagger_{\mathbf{i},s,\sigma}$, $\hat{c}_{\mathbf{i},s,\sigma}$ for electrons with spin σ in the band s at site $\mathbf{i}$ as

$$\hat{c}^\dagger_{\mathbf{i},s,\sigma} = \int d\vec{r}\, \chi_{\mathbf{i},s}(\vec{r}) \hat{\psi}^\dagger_\sigma(\vec{r}). \tag{2.10}$$

Due to the orthonormality of Bloch functions and the normalization constant of the definition of the Fourier serious expansion (see the prefactor $1/\sqrt{N_\Lambda}$ in equations (2.4) and (2.5)) the Wannier functions are orthonormal, too. As a consequence, the creation and annihilation operators — both in the direct and the reciprocal space, defined by the formulas (2.8) and (2.10), respectively — are satisfy the canonical anticommutation relations,

$$[\hat{c}_{\vec{k},s,\sigma}, \hat{c}_{\vec{k}',s',\sigma'}]_+ = [\hat{c}^\dagger_{\vec{k},s,\sigma}, \hat{c}^\dagger_{\vec{k}',s',\sigma'}]_+ = 0, \qquad [\hat{c}^\dagger_{\vec{k},s,\sigma}, \hat{c}_{\vec{k}',s',\sigma'}]_+ = \delta_{\vec{k},\vec{k}'}\, \delta_{s,s'}\, \delta_{\sigma,\sigma'},$$
$$[\hat{c}_{\mathbf{i},s,\sigma}, \hat{c}_{\mathbf{j},s',\sigma'}]_+ = [\hat{c}^\dagger_{\mathbf{i},s,\sigma}, \hat{c}^\dagger_{\mathbf{j},s',\sigma'}]_+ = 0, \qquad [\hat{c}^\dagger_{\mathbf{i},s,\sigma}, \hat{c}_{\mathbf{j},s',\sigma'}]_+ = \delta_{\mathbf{i},\mathbf{j}}\, \delta_{s,s'}\, \delta_{\sigma,\sigma'}. \tag{2.11}$$

It can be checked easily by direct computation based on the anticommutation relations of the field operators.

The inverse relation of (2.10) is

$$\hat{\psi}^\dagger_\sigma(\vec{r}) = \sum_{\mathbf{i},s} \chi^*_{\mathbf{i},s}(\vec{r}) \hat{c}^\dagger_{\mathbf{i},s,\sigma}. \tag{2.12}$$

Thereby the Hamiltonian may be written in lattice representation as [7]

$$\begin{aligned} \hat{H} = & \sum_s \sum_\sigma \sum_{\mathbf{i},\mathbf{j}} t_{s;\mathbf{i},\mathbf{j}} \hat{c}^\dagger_{\mathbf{i},s,\sigma} \hat{c}_{\mathbf{j},s,\sigma} + \\ & \frac{1}{2} \sum_{s_1,s_2,s_3,s_4} \sum_{\sigma,\sigma'} \sum_{\mathbf{i},\mathbf{j},\mathbf{m},\mathbf{n}} \mathcal{V}^{s_1,s_2,s_3,s_4}_{\mathbf{i},\mathbf{j},\mathbf{m},\mathbf{n}} \hat{c}^\dagger_{\mathbf{i},s_1,\sigma} \hat{c}^\dagger_{\mathbf{j},s_2,\sigma'} \hat{c}_{\mathbf{n},s_4,\sigma'} \hat{c}_{\mathbf{m},s_3,\sigma}, \end{aligned} \tag{2.13}$$

where the matrix elements are given by

$$t_{s;\mathbf{i},\mathbf{j}} = \int d\vec{r}\, \chi^*_{\mathbf{i},s}(\vec{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V^{ion}(\vec{r}) \right] \chi_{\mathbf{j},s}(\vec{r}) \tag{2.14}$$

$$\mathcal{V}^{s_1,s_2,s_3,s_4}_{\mathbf{i},\mathbf{j},\mathbf{m},\mathbf{n}} = \int d\vec{r}_1 \int d\vec{r}_2\, V^{ee}(\vec{r}_1 - \vec{r}_2) \chi^*_{\mathbf{i},s_1}(\vec{r}_1) \chi^*_{\mathbf{j},s_2}(\vec{r}_2) \chi_{\mathbf{n},s_4}(\vec{r}_2) \chi_{\mathbf{m},s_3}(\vec{r}_1). \tag{2.15}$$

We note that in contrast to the field-operator representation defined in the continuum, the Wannier function representation does not lead to a site-diagonal form of the electron interaction, i.e. the interaction does not only depend on the densities $\hat{n}_{\mathbf{i},s,\sigma} = \hat{c}^{\dagger}_{\mathbf{i},s,\sigma}\hat{c}_{\mathbf{i},s,\sigma}$, but contains explicit off-diagonal contributions which will be discussed later.

2.3 One-band models

The Hamiltonian (2.13) is too general to be tractable in dimensions $D > 1$. Hence it has to be simplified using physically motivated truncations [7]. In particular, if the Fermi surface lies within a single conduction band, and if this band is well separated from the other bands, and the interaction is not too strong it may be justified to restrict the discussion to a single band ($s_1 = s_2 = s_3 = s_4$). In this case the Hamiltonian (2.13) reduces to

$$\hat{H} = \sum_{\sigma}\sum_{\mathbf{i},\mathbf{j}} t_{\mathbf{i},\mathbf{j}}\hat{c}^{\dagger}_{\mathbf{i},\sigma}\hat{c}_{\mathbf{j},\sigma} + \frac{1}{2}\sum_{\sigma,\sigma'}\sum_{\mathbf{i},\mathbf{j},\mathbf{m},\mathbf{n}} \mathcal{V}_{\mathbf{i},\mathbf{j},\mathbf{m},\mathbf{n}}\hat{c}^{\dagger}_{\mathbf{i},\sigma}\hat{c}^{\dagger}_{\mathbf{j},\sigma'}\hat{c}_{\mathbf{n},\sigma'}\hat{c}_{\mathbf{m},\sigma}, \tag{2.16}$$

For the one and two-site terms we use special notations. The on-site interactions is the Hubbard U:

$$U = \mathcal{V}_{\mathbf{i},\mathbf{i},\mathbf{i},\mathbf{i}}, \qquad \hat{U} = U\sum_{\mathbf{i}}\hat{n}_{\mathbf{i},\uparrow}\hat{n}_{\mathbf{i},\downarrow} \tag{2.17}$$

Because of the translational invariance the two-site matrix elements depend only on the separation between sites. These matrix elements and the related interaction terms are the followings.

The density–density interaction:

$$V_{\mathbf{j}} = \mathcal{V}_{\mathbf{i},\mathbf{i}+\mathbf{j},\mathbf{i},\mathbf{i}+\mathbf{j}}, \qquad \hat{V}_{\mathbf{j}} = V_{\mathbf{j}}\sum_{\mathbf{i}}\hat{n}_{\mathbf{i}}\hat{n}_{\mathbf{i}+\mathbf{j}}, \tag{2.18}$$

where $\hat{n}_{\mathbf{i}} = \sum_{\sigma}\hat{n}_{\mathbf{i},\sigma}$. The bond-charge–site-charge interaction, which describes a density-dependent hopping

$$X_{\mathbf{j}} = \mathcal{V}_{\mathbf{i},\mathbf{i},\mathbf{i},\mathbf{i}+\mathbf{j}}, \qquad \hat{X}_{\mathbf{j}} = 2\sum_{\sigma}\sum_{\mathbf{i}}\left(X_{\mathbf{j}}\hat{c}^{\dagger}_{\mathbf{i},\sigma}\hat{c}_{\mathbf{i}+\mathbf{j},\sigma}\hat{n}_{\mathbf{i},-\sigma} + X^{*}_{\mathbf{j}}\hat{c}^{\dagger}_{\mathbf{i}+\mathbf{j},\sigma}\hat{c}_{\mathbf{i},\sigma}\hat{n}_{\mathbf{i},-\sigma}\right). \tag{2.19}$$

The next term corresponds to the direct quantum-mechanical exchange, the so-called Heisenberg interaction,

$$\begin{aligned} J'_{\mathbf{j}} = \mathcal{V}_{\mathbf{i},\mathbf{i}+\mathbf{j},\mathbf{i}+\mathbf{j},\mathbf{i}}, \qquad \hat{J}'_{\mathbf{j}} &= J'_{\mathbf{j}}\sum_{\sigma,\sigma'}\sum_{\mathbf{i}}\hat{c}^{\dagger}_{\mathbf{i},\sigma}\hat{c}^{\dagger}_{\mathbf{i}+\mathbf{j},\sigma'}\hat{c}_{\mathbf{i},\sigma'}\hat{c}_{\mathbf{i}+\mathbf{j},\sigma} \\ &= -J'_{\mathbf{j}}\sum_{\mathbf{i}}\left(\hat{\vec{S}}_{\mathbf{i}}\hat{\vec{S}}_{\mathbf{i}+\mathbf{j}} + \frac{1}{4}\hat{n}_{\mathbf{i}}\hat{n}_{\mathbf{i}+\mathbf{j}}\right) \end{aligned} \tag{2.20}$$

where $\hat{\vec{S}}_{\mathbf{i}} = \frac{1}{2}\sum_{\alpha\beta} \hat{c}_{\mathbf{i},\alpha}\vec{\sigma}_{\alpha\beta}\hat{c}_{\mathbf{i},\beta}$ is the spin operator and $\vec{\sigma}$ denotes the vector of Pauli matrices. We have assumed only spin independent interactions in a non-relativistic theory and this lead us to an isotropic Heisenberg interaction. However, neglected effects, e.g. spin-orbit coupling, can lead anisotropy. Permitting of this possibility we have the following terms

$$\hat{J}^z_{\mathbf{j}} = -J^z_{\mathbf{j}} \sum_{\mathbf{i}} \hat{S}^z_{\mathbf{i}} \hat{S}^z_{\mathbf{i+j}}, \qquad \hat{J}^{xy}_{\mathbf{j}} = -J^{xy}_{\mathbf{j}} \sum_{\mathbf{i}} \left(\hat{S}^x_{\mathbf{i}} \hat{S}^x_{\mathbf{i+j}} + \hat{S}^y_{\mathbf{i}} \hat{S}^y_{\mathbf{i+j}}\right). \tag{2.21}$$

In Chapter 3, for the generality, our model contains these terms instead of the isotropic interaction $\hat{J}'$. (The additional density-density term which occurs in equation (2.20) has no importance, we can combine it with the term (2.18) redefining the coupling constant V.)

Finally, the last term describes the hopping of local pairs consisting of an up and a down electron,

$$Y_{\mathbf{j}} = \mathcal{V}_{\mathbf{i},\mathbf{i},\mathbf{i+j},\mathbf{i+j}}, \qquad \hat{Y}_{\mathbf{j}} = Y_{\mathbf{j}} \sum_{\sigma} \sum_{\mathbf{i}} \hat{c}^\dagger_{\mathbf{i},\sigma} \hat{c}^\dagger_{\mathbf{i},-\sigma} \hat{c}_{\mathbf{i+j},-\sigma} \hat{c}_{\mathbf{i+j},\sigma}. \tag{2.22}$$

With the above definitions the two-site part of the Hamiltonian from equation (2.16) becomes

$$\hat{H} = \sum_{\mathbf{j}} [\hat{T}_{\mathbf{j}} + \frac{1}{2}(\hat{V}_{\mathbf{j}} + \hat{X}_{\mathbf{j}} + \hat{J}'_{\mathbf{j}} + \hat{Y}_{\mathbf{j}})] + \hat{U}, \tag{2.23}$$

where the operator of the hopping term and its coupling constant are defined as follows,

$$t_{\mathbf{j}} = t_{\mathbf{i},\mathbf{i+j}}, \qquad \hat{T}_{\mathbf{j}} = \sum_{\sigma} \sum_{\mathbf{i}} t_{\mathbf{j}} \hat{c}^\dagger_{\mathbf{i},\sigma} \hat{c}_{\mathbf{i+j},\sigma}. \tag{2.24}$$

When we assume that the matrix elements does not depend on the direction of the separation $\mathbf{j}$ of sites, only on the distance $|\mathbf{j}|$ then the sums over the two sites $\mathbf{i}$ and $\mathbf{i}+\mathbf{j}$ can be reduced to $\sum_{\langle \mathbf{n},\mathbf{m}\rangle_l}$ where $\langle \mathbf{n},\mathbf{m}\rangle_l$ means that the sites $\mathbf{n}$, $\mathbf{m}$ are lth neighbours, i.e., for $l = 1$ $\mathbf{n}$ and $\mathbf{m}$ are nearest neighbours, for $l = 2$ they are next-nearest neighbours, etc. Under this circumstances a general one-band Hamiltonian which contains only two-site terms — allowing anisotropic Heisenberg interaction — can be written as

$$\hat{H} = \sum_{l} (\hat{T}_l + \hat{V}_l + \hat{X}_l + \hat{J}^{xy}_l + \hat{J}^z_l + \hat{Y}_l) + \hat{U}, \tag{2.25}$$

where

$$\hat{T}_l = t_l \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l} \sum_{\sigma} (\hat{c}^\dagger_{\mathbf{i}\sigma}\hat{c}_{\mathbf{j}\sigma} + \hat{c}^\dagger_{\mathbf{j}\sigma}\hat{c}_{\mathbf{i}\sigma}), \quad \hat{X}_l = X_l \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l} \sum_{\sigma} (\hat{c}^\dagger_{\mathbf{i}\sigma}\hat{c}_{\mathbf{j}\sigma} + \hat{c}^\dagger_{\mathbf{j}\sigma}\hat{c}_{\mathbf{i}\sigma})(\hat{n}_{\mathbf{i}-\sigma} + \hat{n}_{\mathbf{j}-\sigma}),$$
$$\hat{V}_l = V_l \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l} \hat{n}_{\mathbf{i}}\hat{n}_{\mathbf{j}}, \qquad \hat{Y}_l = Y_l \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l} \sum_{\sigma} \hat{c}^\dagger_{\mathbf{i},\sigma}\hat{c}^\dagger_{\mathbf{i},-\sigma}\hat{c}_{\mathbf{i}+\mathbf{j},-\sigma}\hat{c}_{\mathbf{i}+\mathbf{j},\sigma},$$
$$\hat{J}^z_l = -J^z_l \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l} \hat{S}^z_{\mathbf{i}}\hat{S}^z_{\mathbf{j}}, \qquad \hat{J}^{xy}_l = -J^{xy}_l \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l} \left(\hat{S}^x_{\mathbf{i}}\hat{S}^x_{\mathbf{j}} + \hat{S}^y_{\mathbf{i}}\hat{S}^y_{\mathbf{j}}\right). \tag{2.26}$$

For most purposes the general single-band Hamiltonians (2.16) and even (2.25) are still too complicated. It is possible to make further simplifying approximation on the line of the philosophy of tight-binding description [7]. Dealing with a narrow energy band the Wannier functions will closely resemble the atomic functions. Furthermore, if the bandwidth is to be small these functions must form an atomic shell which has a small radius compared with the inter-atomic distances. Taking into account the weak overlap between neighbouring orbitals, one may expect that the overlap between close neighbours is the most important. Therefore the site indices in equation (2.16) are restricted to closely neighbour positions, which leads in equation (2.25) that l is restricted to small numbers, or in case of direction dependent couplings, in equation (2.23) $\mathbf{j}$ does not run over its all possible values Λ, only over a small set $\mathcal{N}$, where $\mathcal{N}$ determines the neighbours of sites with which they interact: $\{\mathbf{i}+\mathbf{j} : \mathbf{j} \in \mathcal{N}\}$ are the "important" close neighbours of a given site $\mathbf{i}$. In this line we get extended Hubbard models with only nearest-neighbour interactions, or nearest and next-nearest neighbour interactions. On bipartite lattice in the first case three and four-site terms from equation (2.16) does not remain, and usually these terms are neglected other cases, too.

Among all interactions (2.17–2.22) the Hubbard interaction is certainly the strongest. Hence, in a final truncation step one may try to neglect all the other interaction terms, leaving simultaneously the nearest-neighbour hopping only. This leave us to the (simple) Hubbard model, the simplest correlation model for lattice electrons.

2.4 Hubbard model

The Hubbard model describes a tight-binding electron model in which electrons hop around the lattice and interact with each other through short-range repulsive interactions. The full Hamiltonian of the single-band Hubbard model is simply

$$\hat{H} = \hat{T} + \hat{U} \tag{2.27}$$

(Further usual simplification to write only the nearest neighbour hopping $\hat{T}_1$ instead of the whole $\hat{T}$, but it is not essential.) Both $\hat{T}$ and $\hat{U}$ can be easily diagonalized. The difficulty is, however, that electrons behave as "waves" in $\hat{T}$, while they behave as "particles" in $\hat{U}$. How do they behave in a system whose Hamiltonian is a sum of these totally different Hamiltonians? This is indeed a fascinating problem which is deeply related to the wave-particle dualism in quantum physics. We might say that many of the important models in many-body problems are minimum models which take into account both the wave-like nature and the particle-like nature of matter.

From a technical point of view, the wave-particle dualism implies that the Hamiltonians $\hat{T}$ and $\hat{U}$ do not commute with each other. Even when each Hamiltonian is diagonalized, it is still highly nontrivial (or impossible) to find the properties of their sum. Of course, mathematical difficulty does not automatically guarantee that the model is worth studying. A truly exciting characteristic of the Hubbard model is that, though the Hamiltonians $\hat{T}$ and $\hat{U}$ do not favor any nontrivial order, their sum $H = \hat{T} + \hat{U}$ is believed to generate various types of nontrivial order including antiferromagnetism, ferromagnetism, and superconductivity. When we sum up the two innocent Hamiltonians $\hat{T}$ and $\hat{U}$, competition between their wave-like and particle-like characters takes place, and one gets various interesting "physics". To confirm this fascinating scenario is a challenging problem in theoretical and mathematical physics.

2.4.1 The question of ferromagnetism and the Hubbard model

The Hubbard model was originally introduced in an attempt to understand itinerant ferromagnetism in $3d$-transition metals [7, 8, 9]. The expectation was that in this model ferromagnetism would arise naturally since in a polarized state the electrons do not interact at all. However, it soon became clear that in a ferromagnetic state the kinetic energy is also reduced. This makes the stability of ferromagnetism in the Hubbard model a particularly delicate problem. Indeed, the kinetic energy with nearest neighbour hopping usually favors antiferromagnetism. Lieb's exact result [23] leads also to antiferromagnetism for all regular bipartite lattices, however it can lead to ferro- (or ferri-, instead) magnetism on decorated lattices. At half filling ($n = 1$) and on bipartite lattices antiferromagnetism is a generic effect since it appears both at weak coupling (Hartree-Fock mean-field theory) and strong coupling (Anderson's superexchange mechanism). Hence it arises naturally in any perturbational approach and is tractable by renormalization group methods [24]. In spite of this, ferromagnetism is a non-trivial strong coupling phenomenon which can not be investigated by any standard perturbation theory.

The above discussion shows that, to understand the microscopic origin of itinerant ferromagnetism, non-perturbative techniques are required. Unfortunately, there are not many controlled approaches (see footnote on page 3) of this type available. Rigorous mathematical methods (for recent review see Refs. [25, 26], numerical methods [27], and variational approaches [28, 29, 30, 31] are the ones most frequently used.

A well-known exact theorem is due to Nagaoka [32, 33] and Thouless [34]. It provides explicit, but highly idealized conditions under which ferromagnetism is stable in the Hubbard model. It proves that for infinitely large repulsive Hubbard U the macroscopic degeneracy of the ground state at half filling (when the number of electrons is exactly equal with the number of lattice points, hereafter denoted by N_Λ) is lifted by a single hole, i.e., when $N = N_\Lambda - 1$. In this case the saturated ferromagnetic ground state is stable for any value of the hopping t on square, simple cubic and bcc lattices, and for $t < 0$ on triangle, fcc and hcp lattices. A very elegant and fully general proof was given by Tasaki [35] based on the Perron–Frobenius theorem. For the Nagaoka mechanism to work the lattice needs to contain loops along which the hole can move. Once the hole moves, the maximal overlap between the initial and the final state clearly occurs in a ferromagnetic configuration. The problem is that Nagaoka's proof does not even extend to two holes, that a single hole is thermodynamically irrelevant, and that the limit of $U = \infty$ is highly unrealistic.

Several theoretical results state the instability of Nagaoka's ferromagnetism for two holes. [30, 31, 36] Most of these works are essentially based on variational arguments where one constructs sophisticated variational states with total spin $S = N_\Lambda/2 - 1$ which have lower energy than the ferromagnetic state ($S = N_\Lambda/2$). Sütő extended this result up to six holes for bcc lattice and up to for holes for triangular lattice. [30] These proofs are very sensitive to the boundary conditions. They can be chosen so, that those variational wave functions have no lower energy than Nagaoka's state. It is understandable considering the proximity of the highly degenerated half-filled point. Compared to this point the few hole means an $\mathcal{O}(1/N_\Lambda)$ perturbation, while the boundary conditions $\mathcal{O}(1/L)$ (L is the linear size of the system). It emphasizes again that these results — as well as Nagaoka's one — are hold for non-thermodynamic systems, and one need much daring to draw a conclusion about the magnetic properties of the system in thermodynamic limit.

We mention an other statement related to the two hole case. [37] In the cited reference the author states that the singlet ground state in the two hole case has lower energy than the energy of Nagaoka's state. We will return to this question in Chapter 5 and show that the argument which support this statement is completely wrong.

A step into the direction of thermodynamically relevant result was taken by Trugman [38] and Tian, Shen and Qui [39]. However, they still not study thermodynamic situation, but the number of holes N_h does not remain finite as the size of the lattice goes to infinity. The more general conditions is in Ref. [40]: when $N_h < (N_\Lambda)^\alpha$ with $0 < \alpha < 2/(D+2)$ then the gap between the energy of the Nagaoka state and the actual ground state vanishes as $N_\Lambda \to \infty$. We do not interpret, however, these results as proofs of stability of Nagaoka's ferromagnetism since they do not rule out the possibility of paramagnetism, because it can happen that states with zero spin became degenerated with the ground state, too. E.g., the trivial case with $t_{\mathbf{i},\mathbf{j}} = 0$ is not a ferromagnet, however there is no gap between the ground state energy and the fully polarized ferromagnatic state.

Finally a note about the sign of the hopping amplitude. It is usually assumed that $t_{\mathbf{i},\mathbf{j}} \leq 0$. However, there are neither theoretical consideration nor many examples which can verify it. Furthermore, in case of bipartite lattice this sign can be changed by a gauge transformation: redefining the annihilitaion and creation operators as $\hat{\tilde{c}}_{\mathbf{i},\sigma} = -\hat{c}_{\mathbf{i},\sigma}$ if $\mathbf{i} \in \Lambda_A$ and $\hat{\tilde{c}}_{\mathbf{i},\sigma} = \hat{c}_{\mathbf{i},\sigma}$ if $\mathbf{i} \in \Lambda_B$, where $\Lambda = \Lambda_A \cup \Lambda_B$ is the bipartite resolution. In case of $t_{\mathbf{i},\mathbf{j}} \leq 0$ the band-energy minimum is the single point $\vec{k} = 0$ while in the opposite case it is in the border of the Brillouin zone, and thus can be highly degenerate. The physical intuition can be different in the two cases. The assumption $t_{\mathbf{i},\mathbf{j}} \geq 0$ leads to ferromagnetism for more general lattice structures, and Tasaki's proof for Nagaoka's theorem shows that from mathematical point of view it is a more "natural" assumption. As Lieb wrote: "If this upsets anyone's physical proclivity, that is a pity." [41]

2.4.2 The importance of next-nearest neighbour interactions

Keeping only the Hubbard interaction is the result of an extreme truncation of the interaction in the general Hamiltonian (2.16). All interactions beyond the purely local part are totally neglected. The interaction in the simple Hubbard model is therefore very unspecific — it does not depend on the lattice at all and hence not on the spatial dimension. The lattice structure enters only via the kinetic energy. Therefore the stability of ordered phases, — ferromagnetism, antiferromagnetism, etc., — in the Hubbard model can be expected to depend in a sensitive way on the precise form of the kinetic energy. Keeping interactions with longer range the model contains more information about the lattice structure. From this point of view the importance of the next-nearest neighbour terms are non-negligible.

Considering the spin ordering, the Heisenberg interaction caused by direct quantum-mechanical exchange of electrons can easily lead to ferromagnetism or antiferromagnetism. However, since this interaction is rather weak (Hubbar in Ref. [7] estimated $J'_{\mathbf{1}} \sim \frac{1}{40}$ eV for 3d-metals, i.e., $J'_{\mathbf{1}} << U$) it cannot be the sole origin of itinerant ferromagnetism in systems like Fe, Co, Ni. Nevertheless it may be qualitatively important. It can stabilize magnetic orderings in a system with more or less ferromagnetic or antiferromagnetic tendencies; it may give the ultimate push. It is therefore unjustified to neglect the exchange interaction for merely quantitative reasons. In this context the importance of the nearest and next-nearest couplings are comparable. It can be seen also from exact stability criteria for ferromagnetism in systems described by extended Hubbard model which contains couplings between arbitrary sites deduced by Strack and Vollhardt [42]. The relation between the nearest and next-nearest Heisenberg couplings can determine the kind of the magnetic ordering.

Similar things can be told about the role of the density-density terms $\hat{V}_l$. They can stabilize different charge orderings. The pair-hopping terms $\hat{Y}_l$ can be important from the point of view of superconductivity. From theoretical side, at the level of exact results, this question was analyzed in Refs.[43, 44], however only nearest neighbour terms were considered. Nevertheless experimental results suggest that the next-nearest neighbour interactions play an important role in superconductivity.

Moreover, from quantitative point of view, direct experimental results support that the next-nearest neighbour interactions are not negligible. Their presence is clearly signaled in different experiments, for example in Auger core-valence line shapes experiments [45] that even allow the direct observation and measurement of interparticle interaction strength and its distance dependence in valence bands of solids [46], angle resolved photoemission data [47], interpretation of two magnon Raman scattering intensity peaks [78, 49], study of antiferromagnetic ordering [50], phonon-assisted superexchange interactions connecting second — and third — neighbours [51]. The importance of next to nearest neighbour contributions in the hopping term is also emphasized [52, 53].

2.5 The periodic Anderson model

However the Hamiltonian (2.16) are quite general, and very elegant to deduce models hoped to be relevant to describe some system directly from (2.16), but the model building is mainly based on experimental results and physical intuition which is more closer to the tight-binding picture. This is the reason why we do not deduce the periodic Anderson model from (2.16) which does not contain hybridization terms between the bands due to the definition of the Bloch states from Section 2.2. As a consequence, the Wannier states — whose definition based on the Bloch states, see equation (2.4) — do not necessary reflect the very well known features of the atomic orbits.

The periodic Anderson model is established as a model to describe heavy fermion systems. A suitable model of these systems must have the following basic ingredients: a broad band of (5d,6s) conduction electrons, 4f electrons strongly localized at sites, and a hybridization between conduction band and f-electron states to allow for transitions from the band into f-states and vice versa. Furthermore, the strong correlation of the f-level has to be taken into account; for because of their strong localization there exists a strong Coulomb repulsion between two f-electrons at the same site making multi-occupancy of the degenerated f-levels of each site highly unfavorable. This local correlation must be taken into account to assure that the filling of the f-shells and the formation of local magnetic moments follows Hund's rules. A common belief that to capture the essential physics it is enough to take into account one conduction band and only a spin degeneracy of the localized f-levels, though this is certainly not realistic[2]. So the model Hamiltonian reads

$$\hat{H} = \hat{H}_c + \hat{H}_f + \hat{H}_{hyb.} \tag{2.28}$$

where

$$\hat{H}_c = \hat{T}_c = \sum_{\mathbf{i},\mathbf{j},\sigma} t^c_{\mathbf{i},\mathbf{j}} \hat{c}^\dagger_{\mathbf{i},\sigma} \hat{c}_{\mathbf{j},\sigma} \tag{2.29}$$

describes the conduction band;

$$\hat{H}_f = E_f \sum_{\mathbf{i},\sigma} \hat{f}^\dagger_{\mathbf{i},\sigma} f_{\mathbf{i},\sigma} + U \sum_{\mathbf{i}} \hat{n}^f_{\mathbf{i},\uparrow} \hat{n}^f_{\mathbf{i},\downarrow}, \tag{2.30}$$

describes the f-levels localized at sites $\mathbf{i}$ with uniform site energy E_f and on-site repulsion U;

$$\hat{H}_{hyb.} \equiv \hat{V} = \sum_{\mathbf{i},\mathbf{j},\sigma} \left(V_{\mathbf{i},\mathbf{j}} \hat{c}^\dagger_{\mathbf{j},\sigma} \hat{f}_{\mathbf{i},\sigma} + V^*_{\mathbf{i},\mathbf{j}} \hat{f}^\dagger_{\mathbf{i},\sigma} \hat{c}_{\mathbf{j},\sigma} \right) \tag{2.31}$$

describes the hybridization between conduction band and f-electrons. As usual we denote the operator and the coupling of the hybridization by V as well like the density-density interaction in a given band (see equation (2.18)). This does not lead to confusion because in this thesis we do not deal with models which contains these two kinds of interaction simultaneously.

Equation (2.28) defines the Hamiltonian of the periodic Anderson model. We can generalize this model including a hopping on the f-level, and because of the reason drawn up at the end of Section 2.3 we may take into account only the interaction between closely neighbours. In this case the Hamiltonian is a sum of the following terms:

$$\begin{aligned}
\hat{T}_c &= \sum_{\mathbf{j}\in\mathcal{N}} \sum_{\mathbf{i},\sigma} t^c_{\mathbf{j}} \hat{c}^\dagger_{\mathbf{i},\sigma} \hat{c}_{\mathbf{i}+\mathbf{j},\sigma}, & \hat{T}_f &= \sum_{\mathbf{j}\in\mathcal{N}} \sum_{\mathbf{i},\sigma} t^f_{\mathbf{j}} \hat{f}^\dagger_{\mathbf{i},\sigma} \hat{f}_{\mathbf{i}+\mathbf{j},\sigma}, \\
\hat{V} &= \sum_{\mathbf{j}\in\mathcal{N}} \sum_{\mathbf{i},\sigma} (V_{\mathbf{j}} \hat{c}^\dagger_{\mathbf{i},\sigma} \hat{f}_{\mathbf{i}+\mathbf{j},\sigma} + V^*_{\mathbf{j}} \hat{f}^\dagger_{\mathbf{i}+\mathbf{j},\sigma} \hat{c}_{\mathbf{i},\sigma}), & \hat{V}_0 &= \sum_{\mathbf{i},\sigma} (V_0 \hat{c}^\dagger_{\mathbf{i},\sigma} \hat{f}_{\mathbf{i},\sigma} + V^*_0 \hat{f}^\dagger_{\mathbf{i},\sigma} \hat{c}_{\mathbf{i},\sigma}), \\
\hat{E}_f &= E_f \sum_{\mathbf{i},\sigma} \hat{n}^f_{\mathbf{i},\sigma}, & \hat{U} &= U \sum_{\mathbf{i}} \hat{n}^f_{\mathbf{i},\uparrow} \hat{n}^f_{\mathbf{i},\downarrow},
\end{aligned} \tag{2.32}$$

[2]However, the maximum angular momentum degeneracy is usually reduced because of the spin–orbit interaction and crystal field splitting.

where $\hat{n}^f_{\mathbf{i},\sigma} = f^\dagger_{\mathbf{i},\sigma} f_{\mathbf{i},\sigma}$ is the particle number on the f level and $\mathcal{N}$ determines the range of the interaction. For a given site $\mathbf{i}$ the hopping and hybridization is taken into account between $\mathbf{i}$ and its neighbouring sites $\mathbf{i}+\mathbf{j}$ where $\mathbf{j} \in \mathcal{N}$. The set $\mathcal{N}$ is symmetric in the sense that from $\mathbf{j} \in \mathcal{N}$ follows $-\mathbf{j} \in \mathcal{N}$, too, because the Hamiltonian have to be Hermitian. This implies also $t_{-\mathbf{j}} = t^*_{\mathbf{j}}$, but does not require similar relation for the hybridization couplings. Such a generalized model can be considered as a periodic Anderson model given in a direct space version, or a two-band Hubbard model containing the contribution of the Hubbard U only in one band, the other band being non-interacting. This type of model is analyzed in Chapter 4.

2.5.1 Some basic (exact) properties of the model

The above defined model has several exactly solvable, relatively trivial limits. These can serve as starting points of perturbative computations.

The limit $U = 0$ is exactly solvable. In this case there is no correlation between the electrons with different spin, i.e., there are simply 2 independent spinless one particle two-band systems. The one particle models can be diagonalized easily. When $t^f_{\mathbf{i},\mathbf{j}} = 0$ then the resulting f-electron spectral function consists of a peak around E_f of width proportional to $V^2\rho_0$ (ρ_0 is the unperturbed conduction band density of states).

In the limit of vanishing hybridization $V_{\mathbf{i},\mathbf{j}} = 0$ the conduction band is completely decoupled from the f-electron system, and we have a noninteracting band and a Hubbard model. In this situation the $t^f_{\mathbf{i},\mathbf{j}} = 0$ case is also exactly solvable, because the f-electron systems at different lattice sites are also decoupled. Each f-electron system can be diagonalized trivially, and the resulting f-electron spectrum is composed of delta peaks at energies E_f, $E_f + U$, and if the hybridization V is small compared to U, one can expect well separated f-peaks near to E_f, $E_{\alpha,n} + U$, also in the general case of finite hybridization V.

The limit of vanishing band widths $t^c_{\mathbf{i},\mathbf{j}} = t^f_{\mathbf{i},\mathbf{j}} = 0$ is also solvable, because it completely decouples the different sites, and at each site one has to diagonalize a finite matrix of dimension 16.

In the $U = \infty$ limit in $D = 1$ dimension the model is also exactly solvable with the special choice of the parameters. We have only nearest-neighbour hybridization (V) and hopping in both bands(t^c and t^f), the number of particles per site is two, furthermore the following conditions are hold: $t^f = V^2/t^f$ $E_f = 2t^c - 4V^2/t^c$. In this case the exact ground state is described by a non-magnetic and Gutzwiller type wave function with ground state energy $E_0 = -4V^2/t^c$ [54]. The method used in the cited reference is similar to ours used in Chapter 4.

However the number of exact results are very limited even in one dimension, there are many approximative results. In the following I mention a few of the properties the model is commonly expected to fulfill.

It is well-known that the single-impurity Anderson model can be mapped on the (single-impurity) Kondo model [55] if E_f lies far below and $E_f + U$ far above the chemical potential μ (Schrieffer–Wolff transformation [56]). Thus the single-impurity Anderson model should contain the Kondo effect for a certain parameter regime. It has been predicted by several approximation methods, such as the mean-field approximation [57] or the Gutzwiller approximation [58]. In these theories the single-impurity Kondo-like exponent in the energy survives also in the lattice case with slight modification.

When there are several magnetic ions or even a lattice of magnetic moments in the metal there should be an effective interaction between the moments mediated by a spin-polarization of the conduction electrons, namely the Rudeman–Kittel–Kasuya–Yoshida or RKKY interaction. Thus the periodic Anderson model should show magnetic order for certain parameters, a point not yet investigated except within the frame of a mean-field treatment [59].

2.6 Non-Fermi liquid behaviour

The topic of non-Fermi liquid behavior in $D > 1$ dimensions and normal (non-symmetry broken) phase is currently of great interest [60]. This is mainly due to the large amount of experimental results, obtained in the last decade, showing non-Fermi liquid behavior in the normal phase of a variety of materials, including $D > 1$ dimensional systems. Examples are: high T_c superconductors [61], heavy-fermions [62], layered systems [63], quasi-one dimensional conductors, doped semiconductors, systems with impurities, materials presenting proximity to metal-insulator transitions [64], etc. These results changed considerably our notion of interacting Fermi systems. Indeed, until recently, Fermi-liquid theory seemed universally applicable to all sufficiently pure interacting Fermi systems, and its main features even to dirty systems, provided that their normal phase is not destroyed by a symmetry breaking process [60]. This "dogma" has been based on high precision experimental verifications in liquid $He3$ and simple metals [65].

The concept of Fermi liquid itself has been introduced by Landau many decades ago [66] (for a thorough discussion see [67]), and in principle has the meaning that in spite of the interactions, the low energy behavior can be well described within a picture of almost noninteracting quasi-particles. Formulated in rigorous terms [64, 68], in a normal Fermi liquid we have a one-to-one correspondence between the non-interacting and interacting single-particle states (determined e.g., by a perturbation theory convergent up to infinite orders). Furthermore, a quasi-particle pole is present in the single-particle propagator that gives rise to a step-like discontinuity of the momentum distribution function $n_{\vec{k}}$ at the Fermi surface, whose position is specified by a sharp Fermi momentum value $\vec{k}_F$. The so called Luttinger theorem [69] is fulfilled for such a system. This means that the volume of the Fermi sphere is the same as that of the non-interacting system, that there is a well-defined Fermi surface with a discontinuity of the conduction electron occupation number at zero temperature, and that the quasi-particles at the Fermi energy have infinite lifetime, i.e., the selfenergy imaginary part must vanish at the Fermi energy.

The observation of non-Fermi liquid behavior in the materials presented above polarized a huge intellectual effort in the last decade [70] for the understanding of this new fermionic state. In this field the theoretical interpretations are often based on multi-band models [21], the presence of a some kind of gap in the normal phase being clearly established in many cases and subject of intensive experimental [71] and theoretical [21, 72] studies. However, despite the great number of papers published in the field (see for example the references cited in [60] or [68]), and the fact that the observed most interesting and important normal non-Fermi liquid properties emerge in two spatial dimensions, (for example the normal phase of the high T_c superconductors), on the theoretical side, for pure systems, the existence of a non-Fermi liquid state in a normal phase has been proved exactly only in one dimension (i.e. Luttinger liquid [73]). The extension possibility of non-Fermi liquid normal phase properties to 2D has not been demonstrated rigorously up today. In fact, a rigorous theory of a non-Fermi liquid normal state in higher than one dimensions is missing.

Driven by these facts, we were motivated to focus our attention on possible non-Fermi liquid states in models described in the previous Section. Chapter 4 contains our related results.

Chapter 3

Extended Hubbard models: the effect of the next-nearest neighbour interaction terms

In this chapter we study extended Hubbard models to characterize the influence of the next-nearest neighbour interactions on the stability of ordered phases. The behaviour of many body systems containing interparticle interactions with increased interaction range is under an extensive study in the last period. The multiple motivations originate from the extremely interesting behaviour of systems with long range interactions [80, 81]. Unusual properties arise in the presence of competing forces [87] especially when short- and long-range interactions are present [82]. The interpretation of material properties related to systems of grate theoretical and experimental interest suggests that besides short-range interactions also the longer range forces play important role in the development of the main physical properties [79]. Finally, an increasing number of experimental facts indicate the presence of longer-range couplings as well as short-range forces in different materials of interest (see Section 2.4.2).

Connected to lattice models in dimensions higher than one, from the theoretical viewpoint, the importance of the effects that could arise given by the presence of the next-nearest neighbour couplings is known and often used [88, 79, 86]. These couplings have qualitative importance even if they are weak. The Heisenberg interaction, i.e. the direct quantum mechanical exchange interaction between nearest neighbours should be able to lead to ferromagnetism in a rather straightforward way even in the case of itinerant electrons. [85, 25] The presence of next-nearest neighbour couplings can modify this result, and lead to different type of antiferromagnetic orderings.

All these considerations lead us to study an extended Hubbard model in $D > 1$ dimensions, presenting here exact results related to its phase diagram in the presence of an increased interaction range up to next-nearest neighbour coupling terms at zero temperature and half filling.

3.1 The model

Our Hamiltonian describes an extended Hubbard model supplemented with nearest-neighbour and next-nearest neighbour terms. The Hamiltonian follows the form of equation (2.25) but now we neglect the pair-hopping term, $\hat{Y}$.

$$\hat{H} = \sum_{l=1}^{2} \left[\hat{T}_l + \hat{X}_l + \hat{V}_l + \hat{J}_l^z + \hat{J}_l^{xy} \right] + \hat{U}. \tag{3.1}$$

The interaction terms and coupling constants are defined in equation (2.26).

The more restrictive assumption using in the following part of this chapter is that $X_1 = -t_1$ and $X_2 = -t_2$. (Let us remember the remark at the end of Section 2.4.1 about the sign of t.) In this case the number of doubly occupied sites is conserved, i.e., $[\hat{T} + \hat{X}, \hat{U}] = 0$, (but $[\hat{T} + \hat{X}, \hat{H}] \neq 0$). This assumption, which made possible the exact solution, seems to be a little artificial. However, since $-t$ is typically of the order of 0.2-2 eV the values of X and t seem to be quite comparable. This was explicitly shown for a square lattice of oxygen ions representing a CuO_2 plane [75].

During this chapter, only D-dimensional hypercubic lattices containing N_Λ lattice sites are considered at half filling, i.e. $n = \langle \hat{n} \rangle = (1/N_\Lambda) \langle \sum_{\mathbf{i},\sigma} \hat{n}_{\mathbf{i},\sigma} \rangle = 1$.

3.2 Procedure used

Concerning the procedure, we used a technique used by Brandt and Giesekus [77] and developed by others [84, 44]. It is often used in the literature [76, 25, 85, 42, 43] because it has the advantage to provide exact results in all dimensions related to the ground state energy, E_0. The main idea is to deduce exact upper and lower bounds for the ground state energy, — we denote them by E_0^u and E_0^l, respectively, — and to compare these two bound values within the parameter space. Denoting by λ_i the coupling constants ($i = 1, ..., p$), we have

$$E_0^l(\lambda_1, ..., \lambda_p) \leq E_0(\lambda_1, ..., \lambda_p) \leq E_0^u(\lambda_1, ..., \lambda_p). \tag{3.2}$$

From equation (3.2), with the condition $E_0^l = E_0^u$ one can find domains $\mathcal{D}_0(\lambda_1, ..., \lambda_p)$ of the $\{\lambda_i\}$ parameter space, inside which the ground state energy is exactly E_0. Using the variational method for the upper bound, the ground state ψ_0 is also known for the analyzed region.

We deduced the lower bounds E_0^l transforming the model Hamiltonian $\hat{H}$ into a $\hat{H}_0$ term with known ground state energy given by E_0^l and additional contributions expressed in terms of positive semidefinite operators:

$$\hat{H}(\lambda_1, ..., \lambda_p) = \hat{H}_0(\lambda_1, ..., \lambda_p) + \sum_i f_i(\lambda_1, ..., \lambda_p)\hat{P}_i, \tag{3.3}$$

where

$$\langle\psi|\hat{P}_i|\psi\rangle \geq 0$$

for all ψ vector of the Hilbert space. We can consider the ground state energy of $\hat{H}_0$ as a lower bound to the ground state energy of $\hat{H}$ under the conditions that the last terms in equation (3.3) are positive simidefinites. Exact ground states can be obtained in this manner by searching for such trial wave functions ψ whose eigenvalue given by every $\hat{P}_i$ is zero, because in this case the upper bound $E_0^u = \langle\psi|\hat{H}|\psi\rangle/\langle\psi|\psi\rangle$ given by the variational method is certainly coincide with the lower bound. Although $\hat{P}_i$ are positive semidefinite operators, the last term in equation (3.3) is positive only if the $f(\lambda_1, ..., \lambda_p)$ coefficients are non negative. These conditions lead to inequalities among the coupling constants that define the $\mathcal{D}_0(\lambda_1, ..., \lambda_p)$ domains of the parameter space where ψ is the ground state wave function with energy $E_0^l = E_0^u$. We note, that in this way one can derive, in general, sufficient but not necessary conditions. This is the reason why we can expand domains of some phases, due to a better resolution (3.3) for a particular case.

3.3 The upper bound values

First of all we define D subdomains of the starting D-dimensional hypercubic lattice denoted by $\mathcal{A}_{D,m}$, $(m = 0, 1, ..., D-1)$ with the following three conditions:

(a) The $\mathcal{A}_{D,m}$ domain contains $N_\Lambda/2$ lattice sites.

(b) $\mathcal{A}_{D,m}$ build up a Bravais-lattice (but it is not obligatory that this is of hypercubic type).

(c) If $\mathbf{i} \in \mathcal{A}_{D,m}$, then $\mathbf{i}$ has $2m$ nearest-neighbours that are also elements of $\mathcal{A}_{D,m}$.

We generalize this definition of $\mathcal{A}_{D,m}$ for the case $m = D$, however the three conditions above can not be satisfied exactly in that case. Furthermore, we look like slubberers, because our definition for this case is not unique, but this ununiquess does not lead to confusion. In connection with the wave functions which describe charge-density wave phases (marked by C below) we dispense with the exact satisfaction of condition (c), and we handle $\mathcal{A}_{D,D}$ as a macroscopically compact half of the lattice. In connection with the wave functions which describe spin-density wave phases (marked by S below) we dispense completely with the satisfaction of condition (a), and $\mathcal{A}_{D,D}$ is the whole lattice in this case, by definition.

Using this notation we define two types of wave functions:

$$\psi^C_{D,m} = \prod_{\mathbf{i}\in\mathcal{A}_{D,m}} \hat{c}^\dagger_{\mathbf{i},\uparrow}\hat{c}^\dagger_{\mathbf{i},\downarrow} \mid 0\rangle, \qquad (m = 0, 1, ..., D), \tag{3.4}$$

$$\psi^S_{D,m} = \prod_{\mathbf{i}\in\mathcal{A}_{D,m}} \hat{c}^\dagger_{\mathbf{i},\uparrow} \prod_{\mathbf{i}\notin\mathcal{A}_{D,m}} \hat{c}^\dagger_{\mathbf{i},\downarrow} \mid 0\rangle, \qquad (m = 0, 1, ..., D). \tag{3.5}$$

Let us make some remarks regarding these definitions. Because of (a) the above defined wave functions correspond to half filling. Furthermore, as a consequence of the definition of $\mathcal{A}_{D,m}$ the following statement holds: If $i \in \mathcal{A}_{D,m}$, then i has $Z_2 - 4m(D-m)$ next-nearest neighbours that are also elements of $\mathcal{A}_{D,m}$, where $Z_2 = 2D(D-1)$ represents the number of next-nearest neighbours. The number of nearest neighbours is denoted by $Z_1 = 2D$.

As a consequence of our different definitions for $\mathcal{A}_{D,D}$ for the spin and charge-density wave cases, $\psi^C_{D,D}$ describes a phase separation in charge, i.e. a macroscopic compact half of the lattice contains only doubly occupied sites, and the other half of the lattice is completely empty. Surface corrections at the separation between the empty and doubly occupied region of the lattice were neglected here, a fact that emphasizes that our results relating to $\psi^C_{D,D}$ are exact only in thermodynamic limit. In the same situation ($m = D$ and $N = N_\Lambda$), $\psi^S_{D,D}$ describes the fully saturated ferromagnetic phase, by definition. Otherwise, for $m < D$, $\psi^C_{D,m}$ and $\psi^S_{D,m}$ describe different type of commensurate charge-density waves and spin-density waves, respectively. They can be seen in Fig. 3.1 in $D = 2$ case.

The subdomain $\mathcal{A}_{D,m}$ indexed with $0 \leq m < D$ can be characterized as follows. It contains all sites of every second plane of the $(\alpha_1, ..., \alpha_D)$ Miller-indexed lattice planes family, and does not contain the sites that belong to the remaining intermediate planes. Here, among the α_i indices there are $D-m$ of which value is 1 and the value of the remaining m indices is zero. In fact, there are $2\binom{D}{m}$ subdomains of the lattice which satisfy the three defining conditions of $\mathcal{A}_{D,m}$. These can be obtained each from other by rotations with $\pi/2$ or by a shift with a lattice vector. (This shift interchanges the planes which are contained by $\mathcal{A}_{D,m}$ and which are not.) We use later on the notation $\{A_{D,m}\}$ denoting the set of these different subdomains mentioned above.

Using the wave functions defined in equations (3.4,3.5) as trial wave functions for the expectation value of $\hat{H}$, the following upper bounds E^u_0 can be given at

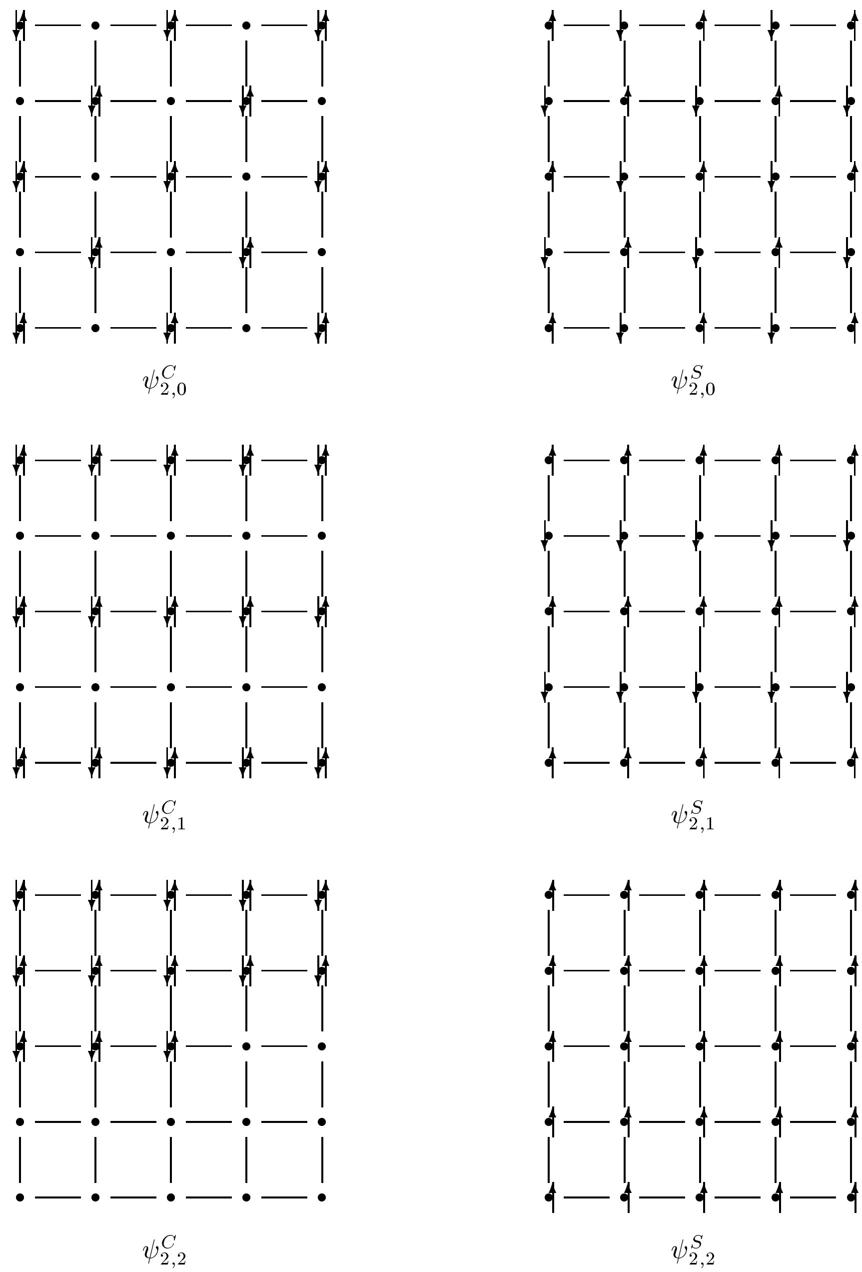

Figure 3.1: Exemplification of wave functions $\psi^C_{D,m}$ and $\psi^S_{D,m}$ in the $D = 2$ case.

$X_1 = -t_1$, $X_2 = -t_2$, $0 \leq m \leq D$:

$$E^S_{D,m} = \epsilon^S_{D,m} N_\Lambda = \Big(\frac{Z_1}{2}V_1 + \frac{Z_2}{2}V_2 + \frac{D-2m}{4}J^z_1 + \Big[m(D-m) - \frac{Z_2}{8}\Big]J^z_2\Big)N_\Lambda \ ,$$
$$E^C_{D,m} = \epsilon^C_{D,m} N_\Lambda = \Big(\frac{1}{2}U + 2mV_1 + [Z_2 - 4m(D-m)]V_2\Big)N_\Lambda \ . \qquad (3.6)$$

We mention that in the presented conditions the trial wave functions represent eigenfunctions as well.

3.4 The lower bound values

In order to describe simultaneously the studied cases we introduce the two-valued index $\mathcal{X} \in \{C, S\}$. In this manner, $\psi^{\mathcal{X}}_{D,m} := \psi^C_{D,m}$ or $\psi^S_{D,m}$ depending on the value of $\mathcal{X}$. The corresponding energies are denoted as $E^{\mathcal{X}}_{D,m}$ and the following parameterizations within $\hat{H}$ are used:

$$\lambda^{\mathcal{X}}_l := \begin{cases} V_l \\ J^z_l \end{cases} \quad \hat{h}^{\mathcal{X}}_{\mathbf{i}} := \begin{cases} \hat{n}_{\mathbf{i}} \\ \hat{S}^z_{\mathbf{i}} \end{cases} \quad \hat{H}^{\mathcal{X}}_l := \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l} \hat{h}^{\mathcal{X}}_{\mathbf{i}} \hat{h}^{\mathcal{X}}_{\mathbf{j}} \equiv \begin{cases} \hat{V}_l/V_l & \text{if } \mathcal{X} = C. \\ \hat{J}^z_l/J^x_l & \text{if } \mathcal{X} = S. \end{cases}$$

In this Section we show that the wave functions $\psi^{\mathcal{X}}_{D,m}$ defined in the previous Section are exact ground states of the starting Hamiltonian. For this reason, as mentioned in Section 3.2, the Hamiltonian is identically transcribed into the form presented in equation (3.3) in such a way that the lower bound is introduced via $\hat{H}_0 = E^{\mathcal{X}}_{D,m}\hat{n}$, where $E^{\mathcal{X}}_{D,m}$ are given in equation (3.6). This procedure is suitable because of the half filling condition.

Now we construct the $\hat{P}_i$ operators. For this reason, first of all we define the operators $\hat{Q}$ for $m = 0, \ldots, D$:

$$\hat{Q}^{\mathcal{X}}_{D,m} := \frac{1}{2}\sum_{\Box}\sum_{\{\mathcal{A}_{D,m}\}}\Big(\sum_{\mathbf{i}\in\mathcal{A}_{D,m}\cap\Box}\hat{h}^{\mathcal{X}}_{\mathbf{i}} - \sum_{\mathbf{j}\notin\mathcal{A}_{D,m}\cap\Box}\hat{h}^{\mathcal{X}}_{\mathbf{j}}\Big)^2 - \delta_{\mathcal{X},C}\delta_{D,m}2^D N_\Lambda \hat{n},$$

where $\sum_\Box$ means summation over the unit cells of the lattice and $\sum_{\{\mathcal{A}_{D,m}\}}$ means summation over the possible configurations which satisfy the definition of $\mathcal{A}_{D,m}$. Because of this summation, the presented $\hat{Q}^{\mathcal{X}}_{D,m}$ operators can be handled without specifying concrete coordinate axis. All $\hat{Q}^{\mathcal{X}}_{D,m}$ operators are positive semidefinite because they are sums of squared terms of self-adjoint operators. However $\hat{Q}^C_{D,D}$ is an exception. Its positive semidefinite character can be verified using the Schwarz inequality under the half filling condition.

The introduced operators are linear combinations of $\hat{H}^{\mathcal{X}}_{D,m}$ (except for the extra term of $\hat{Q}^{C}_{D,D}$):

$$\hat{Q}^{\mathcal{X}}_{D,m} + \delta_{\mathcal{X},C}\delta_{D,m}2^D N_\Lambda \hat{n} = \sum_{l=0}^{D} A^l_{D,m}\hat{H}^{\mathcal{X}}_l ,$$

where, provided that the lattice is hypercubic

$$A^l_{D,m} = 2^{D-l}\frac{2}{1+\delta_{l,0}}\sum_{i=0}^{l}(-1)^i\binom{D-l}{D-m-i}\binom{l}{i}. \tag{3.7}$$

We mention that, in equation (3.7), the $\binom{n}{k}=0$ was considered for $k<0$ or $k>n$.

The sum of the $\hat{Q}^{\mathcal{X}}_{D,m}$ operators multiplied by positive coefficients are also positive semidefinite. This give us the possibility of defining the required operators $\hat{P}_i$ as follows:

$$\begin{aligned}\hat{P}^{\mathcal{X}}_{D,q} &:= C^{\mathcal{X}}\sum_{m=0}^{D}\alpha^m_{D,q}\hat{Q}^{\mathcal{X}}_{D,m}\\ &= C^{\mathcal{X}}\sum_{l=0}^{D}\Big(\sum_{m=0}^{D}\alpha^m_{D,q}A^l_{D,m}\Big)\hat{H}^{\mathcal{X}}_l - \delta_{\mathcal{X},C}\frac{\alpha^D_{D,q}}{4}2^D N_\Lambda\hat{n} ,\end{aligned} \tag{3.8}$$

where the normalization constants are $C^C=\frac{1}{4}$, $C^S=1$ and $q=\frac{1}{2},\frac{3}{2},\ldots,\frac{2D+1}{2}$. These unusual non-integer indices are used for later convenience. Expressing $\hat{V}_l$ and $\hat{J}^z_l$ from the Hamiltonian in terms of $\hat{P}^{\mathcal{X}}_{D,q}$ we determine the coefficients $\alpha^m_{D,q}$ in equation (3.8). Considering vanishing coefficients for $\hat{H}^{\mathcal{X}}_l$ with $l>2$ we get a linear system of equations for $\alpha^m_{D,q}$ which gives

$$\alpha^m_{D,q} = \frac{(m-q-\frac{1}{2})(m-q+\frac{1}{2})}{2^{2D+1}},\ \text{if } q\neq D+\frac{1}{2}, \qquad \alpha^m_{D,D+\frac{1}{2}} = \frac{Dm(D-m)}{2^{2D+1}} ,$$

and we obtain

$$\hat{P}^{\mathcal{X}}_{D,q} = \begin{cases} -\frac{D}{2}\hat{H}^{\mathcal{X}}_2 + \frac{1}{2}D^2(D-1)\hat{H}^{\mathcal{X}}_0 & \text{if } q=\frac{2D+1}{2}\\ \frac{1}{2}\hat{H}^{\mathcal{X}}_2 + (D-2q)\hat{H}^{\mathcal{X}}_1 + \frac{1}{2}[(D-2q)^2+D-1]\hat{H}^{\mathcal{X}}_0 - & \\ \qquad - \delta_{\mathcal{X},C}\frac{(D-q-\frac{1}{2})(D-q+\frac{1}{2})}{2^{D+3}}N_\Lambda\hat{n} & \text{if } q=\frac{1}{2},\frac{3}{2},\ldots\frac{2D-1}{2}.\end{cases} \tag{3.9}$$

Noticeably, in one dimension this procedure can be applied only for a Hamiltonian which does not take into consideration next-nearest neighbour interactions. This is because $\hat{H}^{\mathcal{X}}_2$ cannot be expressed in terms of $\hat{P}^{\mathcal{X}}_{1,q}$. However, in this Chapter we are interested in the effect of the next-nearest neighbour terms. As a consequence, we restrict ourselves here to the cases $D \geq 2$.

Although the Hamiltonian (3.1) does not contain the $\hat{H}_0^{\mathcal{X}}$ term explicitly, its coefficient in equation (3.8) is not zero. This coefficient is connected to the transformation of the $\hat{U}, \hat{T}_l, \hat{X}_l$ and $\hat{J}_l^{xy}$ in positive semidefinite factors. For example, in order to express $\hat{U}$ in terms of $\hat{P}_i$ from equation (3.3) we use the following positive semidefinite operators:

$$\hat{P}_u^C := 4\hat{J}_0^z/J_0^z = N_\Lambda \hat{n} - 2\hat{U}/U, \qquad \hat{P}_u^S := 2\hat{U}/U = \hat{V}_0/V_0 - N_\Lambda \hat{n}. \tag{3.10}$$

In connection with the kinetic energy terms, we use a generalization of the operators introduced by Strack and Vollhardt in Ref.[84]:

$$\begin{aligned} \hat{P}_{kin.,l}^C &= \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l,\sigma} (\hat{Q}_{\mathbf{i},\mathbf{j},\sigma}^C)^\dagger \hat{Q}_{\mathbf{i},\mathbf{j},\sigma}^C + \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l,\sigma} (\hat{\xi}_{\mathbf{i},\sigma} - \hat{\xi}_{\mathbf{j},\sigma})(\hat{\xi}_{\mathbf{i},\sigma}^\dagger - \hat{\xi}_{\mathbf{j},\sigma}^\dagger), \\ \hat{P}_{kin.,l}^S &= \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l,\sigma} (\hat{Q}_{\mathbf{i},\mathbf{j},\sigma}^S)^\dagger \hat{Q}_{\mathbf{i},\mathbf{j},\sigma}^S + \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l,\sigma} (\hat{\xi}_{\mathbf{i},\sigma}^\dagger + \hat{\xi}_{\mathbf{j},\sigma}^\dagger)(\hat{\xi}_{\mathbf{i},\sigma} + \hat{\xi}_{\mathbf{j},\sigma}), \end{aligned} \tag{3.11}$$

where

$$\begin{aligned} \hat{Q}_{\mathbf{i},\mathbf{j},\sigma}^C &= \hat{c}_{\mathbf{i},\sigma} - \hat{c}_{\mathbf{j},\sigma} + \hat{\xi}_{\mathbf{j},\sigma} - \hat{\xi}_{\mathbf{i},\sigma}, \\ \hat{Q}_{\mathbf{i},\mathbf{j},\sigma}^S &= \hat{c}_{\mathbf{i},\sigma}^\dagger + \hat{c}_{\mathbf{j},\sigma}^\dagger - \hat{\xi}_{\mathbf{i},\sigma}^\dagger - \hat{\xi}_{\mathbf{j},\sigma}^\dagger, \\ \hat{\xi}_{\mathbf{i},\sigma} &= \hat{c}_{\mathbf{i},\sigma} \hat{n}_{\mathbf{i},-\sigma}. \end{aligned}$$

We mention that the $\hat{P}_{kin.,l}^{\mathcal{X}}$ operators introduced here are positive semidefinite by definition. The operators $\hat{T}_l$ and $\hat{X}_l$ can be expressed in terms of operators (3.11) and (3.10) provided that $-t_l = X_l$. We need this assumption to get the form of equation (3.3) for the Hamiltonian which implies that all our final results are valid in the restricted parameter region $-t_l = X_l$.

Finally we should express the contributions $\hat{J}_l^{xy}$ in terms of positive semidefinite operators. For this reason first of all we transform the isotropic Heisenberg interaction $\hat{J}_l := \hat{J}_l^{xy} + (J_l^{xy}/J_l^z)\hat{J}_l^z$ instead of $\hat{J}_l^{xy}$. After this step, the remaining anisotropic part $(1 - J^{xy}/J^z)\hat{J}_l^z$ can be expressed using $\hat{P}_{D,m}^S$. For convenience, the obtained results will be given in terms of $\varepsilon_{D,m}^{\mathcal{X}} := \epsilon_{D,m}^{\mathcal{X}}(U, V_1, V_2, J_1^z - J_1^{xy}, J_2^z - J_2^{xy})$. This means that the last two variables of $\epsilon_{D,m}^{\mathcal{X}}$ (which were originally J_1^z and J_2^z) have to be substituted for the anisotropic part of the Heisenberg couplings. We have $\varepsilon_{D,m}^C = \epsilon_{D,m}^C$ but $\varepsilon_{D,m}^S \neq \epsilon_{D,m}^S$.

For the isotropic part $\hat{J}_l$ we introduce the following operators:

$$\begin{aligned} \hat{P}_{F1}^l &= \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l} \sum_\sigma \frac{1}{2}\Big(\hat{n}_{\mathbf{i},\sigma}\hat{n}_{\mathbf{j},-\sigma}(1-\hat{n}_{\mathbf{i},-\sigma})(1-\hat{n}_{\mathbf{j},\sigma}) - \hat{c}_{\mathbf{i},\sigma}^\dagger \hat{c}_{\mathbf{j},-\sigma}^\dagger \hat{c}_{\mathbf{j},\sigma}\hat{c}_{\mathbf{i},-\sigma}\Big), \\ \hat{P}_{F2}^l &= \sum_{\langle \mathbf{i},\mathbf{j}\rangle_l} \sum_\sigma \Big((1-\hat{n}_{\mathbf{i},\sigma})(1-\hat{n}_{\mathbf{j},\sigma}) + \hat{n}_{\mathbf{i},\sigma}\hat{n}_{\mathbf{j},\sigma}\Big)(\hat{n}_{\mathbf{i},-\sigma} - \hat{n}_{\mathbf{j},-\sigma})^2, \end{aligned}$$

and define the following terms

$$\hat{P}^{+}_{Heis.,l} = \hat{P}^{l}_{F1} + \frac{1}{8}\hat{P}^{l}_{F2}, \quad \hat{P}^{-}_{Heis.,l} = \frac{1}{2}\sum_{\langle \mathbf{i},\mathbf{j}\rangle_l} \left(\hat{\vec{S}}_{\mathbf{i}} + \hat{\vec{S}}_{\mathbf{j}}\right)^2. \tag{3.12}$$

The operators $\hat{P}_{F1}$ and $\hat{P}_{F2}$ are self-adjoint projection operators, therefore $\hat{P}^{+}_{Heis.l}$ and $\hat{P}^{-}_{Heis.l}$ are positive semidefinite by definition.

Based on the operators defined in equations (3.8), (3.10), (3.11) and (3.12), in the case when $X_l = -t_l$ ($l = 1, 2$) we can write the Hamiltonian in the form of equation (3.3) as follows:

$$\begin{aligned} \hat{H} = {} & (E^{\mathcal{X}}_{D,m} + \delta_{\mathcal{X},S} N_\Lambda \tilde{J}^{xy})\hat{n} + \sum_{l=1}^{2} |J^{xy}_l| \hat{P}^{sgn(J^{xy}_l)}_{Heis.,l} + \sum_{l=1}^{2} -t_l \hat{P}^{\mathcal{X}}_{kin.,l} \\ & + \sum_{k=\pm\frac{1}{2}} (\varepsilon^{\mathcal{X}}_{D,m+2k} - \varepsilon^{\mathcal{X}}_{D,m})\beta_{D,m}\hat{P}^{\mathcal{X}}_{D,m-k} \\ & + \sum_{k'=\pm\frac{1}{2}} (\varepsilon^{\bar{\mathcal{X}}}_{D,\tilde{m}+2k'} - \varepsilon^{\bar{\mathcal{X}}}_{D,\tilde{m}})\beta_{D,m}\hat{P}^{\bar{\mathcal{X}}}_{D,\tilde{m}+k'} \\ & + \left(\varepsilon^{\bar{\mathcal{X}}}_{D,\tilde{m}} - \varepsilon^{\mathcal{X}}_{D,m} + (\delta_{\mathcal{X},S} - \delta_{\mathcal{X},C})\tilde{J}^{xy} - \frac{\tilde{t}}{2}\right)\hat{P}^{\mathcal{X}}_{u}, \end{aligned} \tag{3.13}$$

where the subscripts $m \pm x$ represent numbers $mod(D+1)$ and the following notations were used:

$$\bar{\mathcal{X}} = \begin{cases} S\,, & \text{if } \mathcal{X} = C\,, \\ C\,, & \text{if } \mathcal{X} = S\,, \end{cases} \qquad \beta_{D,m} = \begin{cases} \frac{4}{Z_2}\,, & \text{if } m = 0 \text{ or } D\,, \\ 1\,, & \text{otherwise}\,, \end{cases}$$

$$\alpha_l = \begin{cases} 1\,, & \text{if } J^{xy}_l \geq 0\,, \\ 3\,, & \text{if } J^{xy}_l < 0\,, \end{cases} \qquad sgn(J^{xy}_l) = \begin{cases} +\,, & \text{if } J^{xy}_l \geq 0\,, \\ -\,, & \text{if } J^{xy}_l < 0\,, \end{cases}$$

$$\tilde{J}^{xy} = \frac{1}{8}\sum_{l=1}^{2} \alpha_l |J^{xy}_l| Z_l\,, \qquad \tilde{t} = 4\sum_{l=1}^{2} -t_l Z_l\,.$$

Finally, in equation (3.13), $\tilde{m}$ represents the index which minimizes the energy $\varepsilon^{\bar{\mathcal{X}}}_{D,m}$ for given $\bar{\mathcal{X}}$ and D values respectively, that is $\tilde{m}$ satisfies the following equation:

$$\varepsilon^{\bar{\mathcal{X}}}_{D,\tilde{m}} = \min_{0 \leq m' \leq D} \{\varepsilon^{\bar{\mathcal{X}}}_{D,m'}\}. \tag{3.14}$$

We mention that $\varepsilon^{\bar{\mathcal{X}}}_{D,\tilde{m}}$ (for a given D and $\bar{\mathcal{X}}$) is uniquely determined by the coupling constant values. For further convenience we introduce the notation: $K = 2[\varepsilon^{S}_{D,\tilde{m}} -$

$(\varepsilon^C_{D,\tilde{m}'} - U/2)]$. The K quantity does not depend on U and t_l, but is uniquely determined by J^z_l, J^{xy}_l, V_l $(l = 1, 2)$ and the dimension D.

On the basis of equation (3.13) which has exactly the form of equation (3.3), one can deduce the stability domains for $\psi^{\mathcal{X}}_{D,m}$, i.e. we can delimit the phase diagram regions where the studied wave functions belong to the ground state.

3.5 Stability conditions for the considered phases

General conditions. The deduced equation (3.13) is valid only at $-t_l = X_l$ $(l = 1, 2)$ for arbitrary $D \geq 2$ dimensions on hypercubic lattices. Furthermore $\hat{P}^C_{D,D}$ is positive semidefinite only at $n = 1$ and every presented wave function $\psi^{\mathcal{X}}_{D,m}$ corresponds to half filling. Finally, the third term in equation (3.13) implies for every case that $t_l \leq 0$ $(l = 1, 2)$. The above mentioned conditions are general conditions valid for every case presented below. We remark that $\varepsilon^{\bar{\mathcal{X}}}_{D,\tilde{m}+1} \geq \varepsilon^{\bar{\mathcal{X}}}_{D,\tilde{m}}$ and $\varepsilon^{\bar{\mathcal{X}}}_{D,\tilde{m}-1} \geq \varepsilon^{\bar{\mathcal{X}}}_{D,\tilde{m}}$ inequalities which originate from the fifth term of equation (3.13) do not represent restrictions for the stability domain of the $\psi^{\mathcal{X}}_{D,m}$ functions. This is because these inequalities are satisfied automatically due to the definition of $\tilde{m}$ presented in equation (3.14).

Equation (3.13) gives several important results depending on the values of the indices and coupling constants. We discuss three different cases below.

(I) *Stability conditions for the $\psi^S_{D,m}$ phases in case of anisotropic Heisenberg interaction.* A $\psi^{\mathcal{X}}_{D,m}$ wave function with $0 \leq m \leq D$ is the exact ground state of the Hamiltonian defined in equation (3.1) with the $E^{\mathcal{X}}_{D,m}$ ground-state energy given in equations (3.6) under the following conditions:

(*A*) $J^{xy}_l = 0$, $(l = 1, 2)$. This implies that $\varepsilon^{\mathcal{X}}_{D,m} = \epsilon^{\mathcal{X}}_{D,m}$ and $\tilde{J}^{xy} = 0$.

(*B*) $\epsilon^S_{D,m} \leq \epsilon^S_{D,m+1}$ and $\epsilon^S_{D,m} \leq \epsilon^S_{D,m-1}$. This implies that $\epsilon^S_{D,m} \leq \epsilon^S_{D,m'}$ for arbitrary m'. These inequalities depend only on the value of J^z_1 and J^z_2, i.e. they describe the stability domain of $\psi^{\mathcal{X}}_{D,m}$ in the (J^z_1, J^z_2) parameter plane. Explicitly these conditions can be written as

$$\begin{aligned} J^z_1 \leq 0, \quad 2(D-1)J^z_2 \geq J^z_1, &\quad \text{if } m = 0, \\ J^z_1 \geq 0, \quad -2(D-1)J^z_2 \leq J^z_1, &\quad \text{if } m = D, \\ 2(D-2m+1)J^z_2 \leq J^z_1 \leq 2(D-2m-1)J^z_2, &\quad \text{otherwise.} \end{aligned}$$

(*C*) $\varepsilon^C_{D,\tilde{m}} - \varepsilon^S_{D,\tilde{m}} - \tilde{t}/2 \geq 0$. Here we used $\varepsilon^S_{D,m} = \varepsilon^S_{D,\tilde{m}}$. In this case the following condition is satisfied:

$$U \geq U^S_c \equiv K + \tilde{t}$$

(II) *Stability conditions for the ferromagnetic phase in case of isotropic Heisenberg interaction.* The fully saturated ferromagnetic state denoted by $\psi^S_{D,D}$ is the exact ground state of the Hamiltonian (3.1) with the ground-state energy $E^S_{D,D} = [(Z_1/2)V_1 + (Z_2/2)V_2 - (Z_1/8)J_1 - (Z_2/8)J_2]N_\Lambda$ if the following conditions are satisfied:

(*A*) $J^{xy}_l = J^z_l \equiv J_l \geq 0$, $(l = 1, 2)$. This implies that $\varepsilon^S_{D,m} = (Z_1/2)V_1 + (Z_2/2)V_2$ and $(Z_1/2)V_1 + (Z_2/2)V_2 - \tilde{J}^{xy} = \epsilon^S_{D,D}$.

(*B*) $U \geq U^S_c$

(III) *Stability conditions for $\psi^C_{D,m}$ phases.* A $\psi^C_{D,m}$ wave function is an exact ground states of the Hamiltonian (3.1) with energy $E^{\mathcal{X}}_{D,m}$ if the following conditions hold:

(*A*) $\epsilon^C_{D,m} \leq \epsilon^C_{D,m+1}$ and $\epsilon^C_{D,m} \leq \epsilon^C_{D,m-1}$ delimit the stability domains of $\psi^{\mathcal{X}}_{D,m}$ in (V_1, V_2) parameter plane. This condition is similar to (I.*B*), but here $-V_l$ plays the role of J^z_l taking into account the sign convention in the definition of Hamiltonian (3.1). Explicitly:

$$\begin{aligned} V_1 \geq 0, \quad 2(D-1)V_2 \leq J^z_1, &\quad \text{if } m = 0, \\ V_1 \leq 0, \quad -2(D-1)V_2 \geq V_1, &\quad \text{if } m = D, \\ 2(D-2m-1)V_2 \leq V_1 \leq 2(D-2m+1)V_2, &\quad \text{otherwise.} \end{aligned}$$

(*B*) The last term of equation (3.13) gives the following condition:

$$U \leq U^C_c \equiv K - \tilde{t}.$$

Examples of the obtained results for $D = 3$ dimensions are presented in Fig. 3.2 and Fig. 3.3. The previous one shows the (U, V_1) plane, and the later one the (U, J^z_1) plane of the parameter space.

In the following Section we present a study of the obtained results.

3.6 Study of the obtained results

We demonstrated the presence of

(*a*) a phase separation region

(*b*) different types of antiferromagnetic ordering

(*c*) fully saturated ferromagnetic phase and

(*d*) different types of charge-density waves

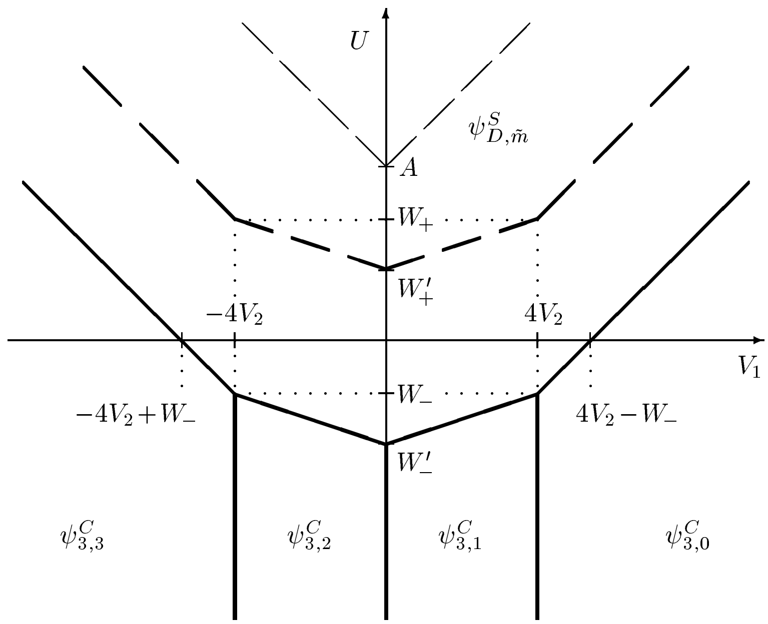

Figure 3.2: The (U, V_1) plane of the phase diagram for $V_2 \geq 0$ in $D = 3$ dimension. The bold solid and broken lines delimit the deduced stability domains of the ordered phases. The $\psi^S_{D,\tilde{m}}$ phase situated above the bold broken lines is present in the phase diagram only for $J^{xy}_l = 0$ or $J^{xy}_l = J^z_l \geq 0$. In the latter case, $\psi^S_{D,\tilde{m}} = \psi^S_{D,D}$ denotes the ferromagnetic phase. For comparison we present the thin broken line above which the ferromagnetic phase deduced in Ref. [84] for the isotropic Heisenberg coupling case emerges. The notations is as follows: $W_- = U^C_c|_{V_1=4V_2}$; $W'_- = U^C_c|_{V_1=0}$; $W_+ = W_- + 2\tilde{t}$; $W'_+ = W'_- + 2\tilde{t}$; $A = V_2 Z_2 + \tilde{t}$. For the definition of U^S_c and $\tilde{t}$ see the text.

in restricted domains of the phase diagram. Case (a) in our knowledge is for the first time signaled at the level of exact results in higher than one dimension in Ref.[1, 2, 3]; cases (b), (c) and (d) were found with enlarged stability domains in comparison with previous publications [84, 44, 43]. We obtained a complete phase diagram in all $D \geq 2$ dimensions in the localized limit, for special values of Heisenberg coupling constants. All obtained results emphasize the importance of the next to nearest-neighbour effects.

In the anisotropic case the x and y spin components are completely irrelevant because the Hamiltonian does not contain terms which depend on these spin projection. This means that the spins behave in this case as Ising spins. Therefore we refer to this anisotropic case also as Ising-type coupling.

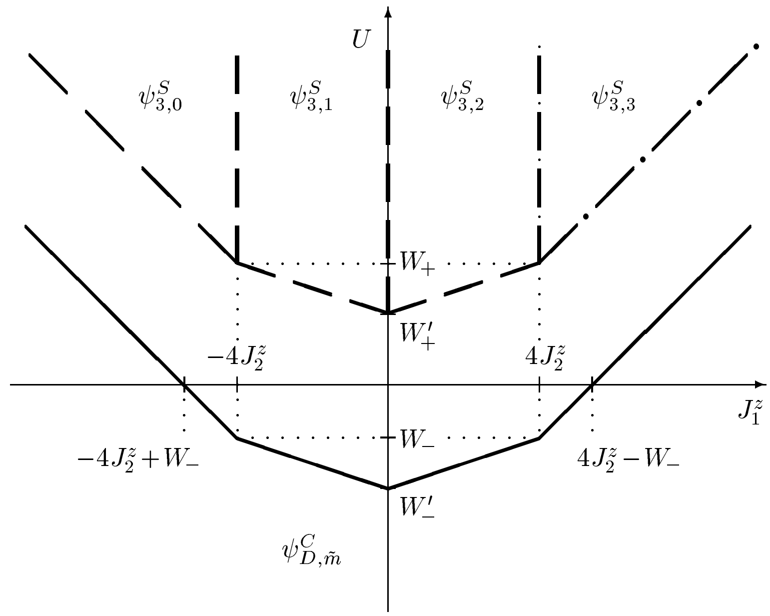

Figure 3.3: The (U, J^z_1) plane of the phase diagram for $J^z_2 \geq 0$ in $D = 3$ dimension. The bold solid and broken lines delimit the deduced stability domains of the ordered phases. The $\psi^S_{D,m}$ $(m = 0, 1, 2)$ states situated between the bold broken lines are present in the phase diagram only for $J^{xy}_l = 0$. The ferromagnetic phase $\psi^S_{3,3}$ situated in the right upper corner is present only for $J^{xy}_l = 0$ or $J^{xy}_l = J^z_l \geq 0$. The notation is as follows: $W_- = U^C_c|_{V_1=4V_2}$; $W'_- = U^C_c|_{V_1=0}$; $W_+ = W_- + 2\tilde{t}$; $W'_+ = W'_- + 2\tilde{t}$; For the definition of U^S_c and $\tilde{t}$ see the text.

We have written in Section 3.3. that the wave functions $\psi^S_{D,m}$ with $m < D$ describe commensurate spin density waves. As the spin polarization is considered to be along the z-axis, these are z-polarized antiferromagnetic phases. For Ising-type spin coupling the deduced results (case I.) state that if U is large enough, i.e. $U \geq U^S_c$, the ground state is either the fully saturated ferromagnetic state (if $J^z_1 \geq 0$ and $-2(D-1)J^z_2 \leq J^z_1$) or one of the possible spin-density wave states depending on the values of J^z_1 and J^z_2. The ferromagnetic phase can be stable for negative J^z_2, but J^z_1 has to be positive. Contrary to these results, for isotropic Heisenberg couplings we can state only that the fully saturated ferromagnetic phase is stable when $J^z_1, J^z_2 \geq 0$ and $U \geq U^S_c$, i.e. the stability domain is decreased, and the spin-density wave phases are completely missing from the phase diagram.

Our results in connection with the charge-density wave phases and the phase separation region are similar to the results obtained for the $\psi^S_{D,m}$ phases in the

Ising-type coupling case, but now $-V_l$ plays the role of J_l^z. The stability domains for the $\psi_{D,m}^C$ phases can be easily represented in this case in terms of V_2 and V_1. The phase delimitation lines are situated in the (V_2, V_1) plane in a similar manner to those present in the (J_2^z, J_1^z) plane (Ising case) for the $\psi_{D,m}^S$ phases. However, there are two important differences. The $\psi_{D,m}^S$ phases are stable for $U \geq U_c^S$ but the $\psi_{D,m}^C$ phases are stable for $U \leq U_c^C$. In other words the $\psi_{D,m}^S$ phases are situated at the top, and the $\psi_{D,m}^C$ phases at the bottom of the phase diagram with respect to the U axis. We mention that $U_c^S \geq U_c^C$, because $U_c^S - U_c^C = 2\tilde{t} \geq 0$. Emerging phases were not deduced in the region of the phase diagram between these delimitation bound U values. As a consequence, we cannot state anything about the stability of the $\psi_{D,m}^{\mathcal{X}}$ phases in this U domain, because our criteria for the emergence of a given phase are sufficient, but not necessary conditions. However, in the localized limit $\tilde{t} \to 0$ and Ising-type couplings, at $-t_l = X_l = J_l^{xy} = 0 (l = 1, 2)$, we have $U_c^C = U_c^S$. In this case, the deduced U_c^S value represents a first-order quantum phase transition point between a $\psi_{D,m}^S$ (spin-density wave or fully saturated ferromagnetic) and a $\psi_{D,m}^C$ (phase separation or charge-density wave) phases. We emphasize that in this case our calculations give the complete phase diagram of the system. For non-Ising-type couplings this statement remains valid only in case of isotropic ferromagnetic $J_l^{xy} = J_l^z \geq 0,\ (l = 1, 2)$ couplings. The condition $U_c^S = U_c^C$ remains valid only for this case, and in this situation, only the stability of the fully saturated ferromagnetic state can be stated ($\psi_{D,m}^S$ at $m = D$). For non-Ising couplings the spin-density wave phases are not stable therefore we do not know the phase diagram for large positive U if the couplings are not ferromagnetic.

Another important difference between the $\psi_{D,m}^S$ phases in Ising-type coupling case and the $\psi_{D,m}^C$ phases is that the former phases are stable only for $J_l^{xy} = 0$ ($l = 1, 2$), but every $\psi_{D,m}^C$ phase can be in principle stable for arbitrary Heisenberg coupling.

It is important to emphasize that, when two different deduced phases have common delimitation boundary, the stability conditions becomes necessary and sufficient conditions. For this reason for example, the surfaces separating the ferromagnetic phase from the antiferromagnetic phases $\psi_{D,0}^S$ and $\psi_{D,D-1}^S$, or the surfaces separating different spin-density wave phases each from other represent necessary and sufficient conditions for the emergence of the mentioned phases and indicate first-order quantum phase transitions. The same can be stated about the separation surfaces present between the $\psi_{D,m}^C$ phases.

Concerning the effect of the extended interaction range on the phase diagram, our results show that the longer-range terms increase the variety of ordered phases. In this case, the presence of several different charge and spin density waves is due to the non-zero next-nearest neighbour couplings. For example we mention that only the non-zero value of $\lambda_2^{\mathcal{X}}$ alone can stabilize all $\psi_{D,m}^{\mathcal{X}}$ phases for $1 \leq m \leq D - 1$. Furthermore, the stability domain of every phase strongly depends on the value of next-nearest couplings. Even more, the next-nearest neighbour couplings enhance the stability of those phases that are present in the phase diagram for vanishing next-nearest neighbour terms. This is the case for example for the phase separation region.

Concerning the effect of the increased interaction range, we mention that, for $\varepsilon^S_{D,m} - \tilde{J}^{xy} > 0$, the $V_2 \neq 0$ coupling increases the domain of the phase diagram in the region $U < 0$ from where the charge-density wave or phase separation is excluded, making room for other ordered phases (such as superconductivity), independently on the sign of V_1, if V_1 is small. However, if $\varepsilon^S_{D,m} - \tilde{J}^{xy}$ is comparable with V_2, based on V_2 it is possible to erase completely other domains than charge-density wave or phase separation in charge from the $U < 0$ region. In this balance, the effect of the hopping terms is also present given by $\tilde{t}$.

The presented criteria for the emergence of the spin-density wave $\psi^S_{D,0}$ and charge-density wave $\psi^C_{D,0}$ phases in the presence of next-nearest couplings are generalizations of the results obtained by other authors [83, 84, 44, 74, 43] taking into account only nearest-neighbour contributions.

Concerning the behaviour of the magnetic phases at $J_l = 0, (l = 1, 2)$, it can be shown that, in this case, the ferromagnetic and spin-density wave phases present in our phase diagram change into a highly degenerate solution of the form

$$\psi_P = \prod_{i \in \mathcal{B}} \hat{c}^\dagger_{i\uparrow} \prod_{i \notin \mathcal{B}} \hat{c}^\dagger_{i\downarrow} \mid 0\rangle, \tag{3.15}$$

with energy $\epsilon_P = (Z_1 V_1 + Z_2 V_2)/2$. This energy can be obtained from our $\epsilon^S_{D,m}$ in $J^z_l \to 0, (l = 1, 2)$ limit. In equation (3.15), $\mathcal{B}$ represents an arbitrary subdomain of the starting lattice. In this limit our results reproduce the results of Refs. [84, 44].

In connection with the D dependences one can see that, at $V_2 > 0$ and $|V_1| < 2(D-1)V_2$ case, increasing the dimensionality of the system, the $\psi^S_{D,m}$ phases penetrate more deeply in the phase diagram in the direction of the $U = 0$ point. At the same time, for $U < 0$, the region from where the phase separation and charge-density wave ordering are excluded becomes greater. These results emphasize that, in the presence of $V_2 > 0$, the U^S_c critical value above which the ferromagnetic domain is situated, decreases with increasing dimensions for $D \geq 2$, independently of the sign of V_1. Furthermore, at $U < 0$, the domain containing other orderings than phase separation or charge-density wave extends to higher $|U|$ values with increasing D, above $D = 2$, for $|V_1| \geq 2(D-1)V_2 > 0$. In this manner, concretely for the $X_l = -t_l$ restricted parameter region, we extended the stability domain of the ferromagnetic phase in comparison with the results deduced by Strack and Vollhardt [84].

Chapter 4

Periodic Anderson model in two dimensions

In this chapter we deal with a two-band Fermi system in two dimensions and look for exact solutions. It is some new interesting phases that we find, which show some characteristic features which differ from usual Fermi liquid behaviour.

We apply the method used in the previous Chapter, described in Section 3.2. We find that it can be done in this more complicated case, too. In fact we got two qualitatively different solutions: a completely localized and a non-localized one. The solutions are valid on two surfaces of the parameter space, i.e. on restricted, but continuous and infinite regions of the $T = 0$ phase diagram, extended from the low U to the high U regions up to $U = \infty$ at $U > 0$.

The derived non-Fermi liquid state is given by a flat band effect in multi-band systems with more than half filling. The obtained properties are extremely peculiar: the system in case of the described solution possesses a well defined Fermi energy e_F under the conditions in which the $\vec{k}_F$ Fermi momentum cannot be defined, and the $n_{\vec{k}}$ momentum distribution function is continuous together with its derivatives of any order.The state is paramagnetic and non-insulating. The state emerges in the proximity of a Mott insulating phase.

Concerning the flat-band features, we mention that such characteristics have been clearly observed in different systems where strong electron interactions and strong correlation effects play a main role. On numerical side, flat-band features are present for example in results connected to 2D Hubbard model [90, 91, 92], or 2D $t - J$ model [93]. Experimentally flat-band features are seen in angle-resolved photo-emission data of high T_c cuprates [94, 95]. For layered systems angle-resolved photo-emission often shows main bands without any sharp characteristics in $n_{\vec{k}}$ [96], or give results interpreted via flat-band features assumptions[97]. Band structure calculations for these systems often reflect a Fermi level positioned exactly at the bottom of a conduction band with large effective mass around its minimum, below which a gap is present [63]. We further wish to mention that connections between superconductivity and flat-band features were also clearly pointed out by Imada et al. [98], and flat-band features can be seen as well in experiments related to heavy-fermion materials[99]. On the technological side, for example Lammert et al. [100] have shown that squashing carbon nanotubes, flat-band features can be achieved around e_F, where a mismatch of nearly isoenergetic $\vec{k}$ states may have unexpected application possibilities.

4.1 Some basic notations and the Hamiltonian

In this Chapter we apply the notations for the lattice and sites introduced in Section 2.2 taking into account explicitly the two dimensional situation. We denote the two linearly independent unit length elements of $\Lambda := \mathbb{Z}^2/(L_x, L_y)$ by $\mathbf{x} = (1,0)$ and $\mathbf{y} = (0,1)$, the primitive lattice vectors by $\vec{d_x}$ and $\vec{d_y}$. We extend this kind of notation for the unit cells — in other words "plaquettes" — of the lattice. A plaquette will be labelled by boldface capitals, e.g. **I, J**, etc. We consider the center point of a plaquette as a coordinate of it, denoted by $\vec{R}_{\mathbf{I}}$. For the consistent uniform notation we consider $\mathbf{I}$ as an element of $\Lambda_{pl} := \left(\frac{1}{2}, \frac{1}{2}\right) + \Lambda$, [1] and similarly to the relation between $\mathbf{i}$ and $\vec{R}_{\mathbf{i}}$ we have $\vec{R}_{\mathbf{I}} = \mathbf{I}_x\vec{d_x} + \mathbf{I}_y\vec{d_y}$. The four corners of a plaquette $\mathbf{I}$ are $\{\mathbf{I} + \boldsymbol{\delta} \ : \ \boldsymbol{\delta} \in S_{\boldsymbol{\delta}}\}$ where $\boldsymbol{\delta} = (\boldsymbol{\delta}_x, \boldsymbol{\delta}_y)$ and $S_{\boldsymbol{\delta}} = \{\left(\frac{1}{2}, \frac{1}{2}\right), \left(-\frac{1}{2}, \frac{1}{2}\right), \left(\frac{1}{2}, -\frac{1}{2}\right), \left(-\frac{1}{2}, -\frac{1}{2}\right)\}$. On this line we denote $\vec{R}_{\boldsymbol{\delta}} = \boldsymbol{\delta}_x\vec{d_x} + \boldsymbol{\delta}_y\vec{d_y}$, and in the following $\sum_{\boldsymbol{\delta}}$ is a short notation instead of $\sum_{\delta \in S_{\boldsymbol{\delta}}}$.

Such as Λ, also Λ_{pl} is handled as ordered set, i.e., it is endowed with a greater than relation, which is coming down from the ordering of Λ by the following definition: $\mathbf{I} < \mathbf{J} \Leftrightarrow \mathbf{I} - \left(\frac{1}{2}, \frac{1}{2}\right) < \mathbf{J} - \left(\frac{1}{2}, \frac{1}{2}\right)$. If we do not say anything else, by definition, the multipliers of every non-commutative product over Λ_{pl} or some subsets of it stand in increasing order. The products of which multipliers stand in decreasing order is denoted by prime over the $\prod$, such as in equation (4.12).

We consider a 2D square lattice described by a two-band model. We denote these bands by c and f, and in expressions where we need a common notation by $b \in \{c, f\}$. The Hamiltonian is given in direct space as have been written in Section 2.5,

$$\hat{H} = \hat{H}_0 + \hat{U}, \qquad \hat{H}_0 = \hat{T}_c + \hat{T}_f + \hat{V}_0 + \hat{V} + \hat{E}_f, \tag{4.1}$$

[1] Here we consider Λ_{pl} as a subgroup of $\mathbb{R}^2/(L_x, L_y)$ and this defines the sum of its elements among themselves and with the elements of Λ.

where the non-interacting terms have been denoted together by $\hat{H}_0$, and the interaction term $\hat{U}$ is the usual Hubbard interaction at the f-electron level. The on-site energy E_f for the second band fixes the relative energy of the two bands. These terms together with the kinetic energy and hybridization terms can be written as in equations (2.32), but in this Chapter we take into account, beside the on-site hybridization $\hat{V}_0$, only nearest and next-nearest terms. Based on physical considerations detailed in Chapter 2 the long-range terms being considered negligible small. Therefore the set $\mathcal{N}$ — which determines the range of the interaction in equations (2.32) — in this chapter is $\mathcal{N} = \{\mathbf{x}, -\mathbf{x}, \mathbf{y}, -\mathbf{y}, \mathbf{x}+\mathbf{y}, -\mathbf{x}-\mathbf{y}, \mathbf{x}-\mathbf{y}, \mathbf{y}-\mathbf{x}\}$. We take into account different couplings along different lattice directions, which allow in fact the study of the system with distorted unit cell as well.

Our model is given by the following nineteen independent coupling constants. The hopping amplitudes in the c band are: $t^c_{\mathbf{x}}$, $t^c_{\mathbf{y}}$, $t^c_{\mathbf{x}+\mathbf{y}}$, $t^c_{\mathbf{x}-\mathbf{y}}$. The remaining four ones are determined by the Hermitian requirement of the Hamiltonian: $t^c_{-\mathbf{x}} = (t^c_{\mathbf{x}})^*$, $t^c_{-\mathbf{y}} = (t^c_{\mathbf{y}})^*$, $t^c_{-\mathbf{x}-\mathbf{y}} = (t^c_{\mathbf{x}+\mathbf{y}})^*$, $t^c_{\mathbf{y}-\mathbf{x}} = (t^c_{\mathbf{x}-\mathbf{y}})^*$. The hopping amplitudes in the f band are: $t^f_{\mathbf{x}}$, $t^f_{\mathbf{y}}$, $t^f_{\mathbf{x}+\mathbf{y}}$, $t^f_{\mathbf{x}-\mathbf{y}}$, and again $t^f_{-\mathbf{x}} = (t^f_{\mathbf{x}})^*$, etc. The eight plus one hybridization couplings are $V_{\mathbf{j}}$, $\mathbf{j} \in \mathcal{N}$ and V_0, furthermore E^f and U. The last two ones are clearly have to be real (again because of the Hermitian requirement), but for the generality we do not take any other assumptions for the above coupling constants.

Hereafter the operators of the total number of particles in a given band is denoted by $\hat{N}_b := \sum_{\mathbf{i},\sigma} \hat{b}^\dagger_{\mathbf{i},\sigma} \hat{b}_{\mathbf{i},\sigma}$, and $\hat{N} := \hat{N}_b + \hat{N}_f$.

4.2 Main idea of the method

Our starting $\hat{H}$ from equation (4.1) represents a prototype of an interacting two band system in 2D. To study this model we use the method described in Section 3.2. We express the Hamiltonian as can be seen in equation (3.3) and search for the ground state wave function as a vector in the kernel of positive semidefinite operators. For this purpose we write the interaction term as

$$\hat{U} = U\hat{P}' + U\hat{N}_f - UN_\Lambda, \tag{4.2}$$

where

$$\hat{P}' = \sum_{\mathbf{i}} \hat{P}'_{\mathbf{i}}, \qquad \hat{P}'_{\mathbf{i}} = (1 - \hat{n}^f_{\mathbf{i},\uparrow} - \hat{n}^f_{\mathbf{i},\downarrow} + \hat{n}^f_{\mathbf{i},\uparrow}\hat{n}^f_{\mathbf{i},\downarrow}). \tag{4.3}$$

In the decomposition presented in equation (4.2) the operator $\hat{P}'$ is a positive semidefinite operator, because it is a sum of positive semidefinite terms. The reason for this is simple. $\hat{P}'_{\mathbf{i}}$ applied to a wave function gives one if on the site $\mathbf{i}$ no f electrons are present, and gives zero, if on the site $\mathbf{i}$ at least one f electron is present. As a consequence, the spectrum of $\hat{P}'_{\mathbf{i}}$ is the set $\{0,1\}$, and $\hat{P}'$ measures the number of empty sites on the f-level, thus its kernel (null-space) consists of the wave functions which do not contain empty sites on the f-level.

An other positive semidefinite terms is expressed as $\sum_{\mathbf{I},\sigma} \hat{A}_{\mathbf{I},\sigma}\hat{A}^{\dagger}_{\mathbf{I},\sigma}$, — which is positive semidefinite by definition, — where the operator $\hat{A}^{\dagger}_{\mathbf{I},\sigma}$ is build up as a linear combination of the starting $\hat{b}^{\dagger}$ fermionic operators which create electrons on the corners of plaquette $\mathbf{I}$. The $\mathbf{I}$th plaquette operator for a fixed spin σ can be generally expressed as $\hat{A}_{\mathbf{I},\sigma} = \sum_{\boldsymbol{\delta},b} a_{\mathbf{I}+\boldsymbol{\delta},b}\hat{b}_{\mathbf{I}+\boldsymbol{\delta},\sigma}$. We will build up from these operators the Hamiltonian which is invariant under the lattice translations, therefore plaquette independence will be considered for the emerging eight complex coefficients present in $\hat{A}_{\mathbf{I},\sigma}$, i.e., $a_{\mathbf{I}+\boldsymbol{\delta},b} = a_{\boldsymbol{\delta},b}$. Thus the plaquette operators become

$$\hat{A}_{\mathbf{I},\sigma} = \sum_{\boldsymbol{\delta}} \sum_{b\in\{c,f\}} a_{\boldsymbol{\delta},b}\hat{b}_{\mathbf{I}+\boldsymbol{\delta},\sigma} \tag{4.4}$$

The $\hat{A}^{\dagger}_{\mathbf{I},\sigma}$ creates an electron into a one-particle state which is linear combination of the eight original electron state of a plaquette. These new one-particle states are not orthogonal, i.e., $g_{\mathbf{I},\mathbf{J}} := \langle 0|\hat{A}_{\mathbf{J},\sigma}\hat{A}^{\dagger}_{\mathbf{I},\sigma}|0\rangle \neq \delta_{\mathbf{I},\mathbf{J}}$. (As usual, the normal type letter δ denotes the Kronecker delta function of its discrete variables and has not any relation with the boldface letter $\boldsymbol{\delta}$, which is a discrete vector.) Therefore the operators $\hat{A}^{\dagger}_{\mathbf{I},\sigma}$ and $\hat{A}_{\mathbf{I},\sigma}$ do not satisfy the canonical fermionic anticommutation relations, instead

$$[\hat{A}^{\dagger}_{\mathbf{I},\sigma}, \hat{A}_{\mathbf{J},\sigma'}]_{+} = \delta_{\sigma,\sigma'} g_{\mathbf{I},\mathbf{J}}, \qquad [\hat{A}_{\mathbf{I},\sigma}, \hat{A}_{\mathbf{J},\sigma'}]_{+} = [\hat{A}^{\dagger}_{\mathbf{I},\sigma}, \hat{A}^{\dagger}_{\mathbf{J},\sigma'}]_{+} = 0, \tag{4.5}$$

where based on the definition (4.4) of the $\hat{A}$ operators the matrix g can be expressed with the parameters $a_{\boldsymbol{\delta},b}$

$$g_{\mathbf{I},\mathbf{J}} = \sum_{b\in\{c,f\}} \sum_{\substack{\boldsymbol{\delta},\boldsymbol{\delta}' \\ \boldsymbol{\delta}\text{-}\boldsymbol{\delta}'=\mathbf{J}\text{-}\mathbf{I}}} a^{*}_{\boldsymbol{\delta},b} a_{\boldsymbol{\delta}',b}. \tag{4.6}$$

Our strategy is the following. Beside the term $\hat{N}$ the operator $\sum_{\mathbf{I},\sigma} \hat{A}^{\dagger}_{\mathbf{I},\sigma}\hat{A}_{\mathbf{I},\sigma}$ contains the same terms than the noninteracting Hamiltonian $\hat{H}_0$, among them $\hat{E}_f$, which operator (with different coupling constant) also occurs in the (4.2) decomposition of the interaction. When the parameters $a_{\boldsymbol{\delta},b}$ can be chosen in such a way — because it is allowed by the starting parameters of the Hamiltonian — that the following equality holds,

$$-\sum_{\mathbf{I},\sigma} \hat{A}^{\dagger}_{\mathbf{I},\sigma}\hat{A}_{\mathbf{I},\sigma} + K\hat{N} = \hat{H}_0 + U\hat{N}_f, \tag{4.7}$$

where K is a parameter, then based on equations (4.2, 4.5, 4.6) we have

$$\hat{H} = \hat{P} + U\hat{P}' + K\hat{N} - 2N_\Lambda \sum_{\boldsymbol{\delta},b} |a_{\boldsymbol{\delta},b}|^2 - N_\Lambda U, \tag{4.8}$$

where

$$\hat{P} = \sum_{\mathbf{I},\sigma} \hat{A}_{\mathbf{I},\sigma} \hat{A}^\dagger_{\mathbf{I},\sigma} \tag{4.9}$$

is a positive semidefinite operator. We search for the ground state under the condition that the number of particles are fixed. The Hilbert space of the system of N particles is denoted by $\mathfrak{H}_N$. On this space $\hat{N}$ is a constant operator. When the following three conditions

- (a) there is a proper definition for $\hat{A}_{\mathbf{I},\sigma}$, i.e. for $a_{\boldsymbol{\delta},b}$, which make the equation (4.7) valid,
- (b) $U > 0$,
- (c) $\mathfrak{H}_{N,0} := \mathfrak{H}_N \cap \ker \hat{P} \cap \ker \hat{P}' \neq \{0\}$

are satisfied, then $\mathfrak{H}_{N,0}$ is the subspace of the ground states within $\mathfrak{H}_N$. There is some differences between the method sketched above and presented in Section 3.2. Now there has no coupling constant dependent multiplier of $\hat{P}$, but the expression (4.8), which gives the Hamiltonian in terms of positive semidefinite operators, is valid only in special values of the parameters, which allow the solution of equation (4.7) for the parameters $a_{\boldsymbol{\delta},b}$ and K. This gives the condition (a) which together with condition (b) gives a domain $\mathcal{D}_g$ in the parameter space where we can give lower bound for the ground state energy keeping only the constant and neglecting the positive semidefinite terms. The condition (c) assures the existence of a proper state which gives the same energy as an upper bound. This terminology would suggest that we follow the procedure written down in Section 3.2, namely that we find an upper bound for the ground state energy using the variational method. But the situation is not the same now. In the next Section we *deduce* the ground state subspace determining the kernel of $\hat{P}$ and $\hat{P}'$. We will see that the condition (c) is satisfied only in $N \geq 3N_\Lambda$ case, thus it leads to a condition for the band filling. Then in Section 4.4 we examine the conditions (a) and (b) which are conditions for the model parameters. We write down the system of equations comes from equation (4.7) and we discuss the physical properties of the model which allow the solution of it.

4.3 The ground state wave functions

Now we study the situation when $\{\hat{A}^\dagger_{\mathbf{I},\sigma}|0\rangle \, : \, \mathbf{I} \in \Lambda_{pl}\}$ is a linearly independent vector set. This is equivalent with $\det g \neq 0$. This is an additional condition which is needed for us to determine $\mathfrak{H}_{N,0}$. The above mentioned set can be linearly dependent, such a case will be discussed in Section 4.6. Now we can define a dual vector set which is created from the vacuum — by definition — with the operators $(\hat{A}^{\mathbf{I},\sigma})^\dagger$. The relation between the operators $\hat{A}$ with sub- and superscript is the following:

$$(\hat{A}^{\mathbf{I},\sigma})^\dagger|0\rangle = \sum_{\mathbf{J}} g^{\mathbf{J},\mathbf{I}} \hat{A}^\dagger_{\mathbf{J},\sigma}|0\rangle, \qquad \hat{A}^\dagger_{\mathbf{I},\sigma}|0\rangle = \sum_{\mathbf{J}} g_{\mathbf{J},\mathbf{I}}(\hat{A}^{\mathbf{J},\sigma})^\dagger|0\rangle, \tag{4.10}$$

where $g^{\mathbf{I},\mathbf{J}}$ is the inverse of $g_{\mathbf{I},\mathbf{J}}$, i.e., $\sum_{\mathbf{L}} g^{\mathbf{I},\mathbf{L}} g_{\mathbf{L},\mathbf{J}} = \delta_{\mathbf{I},\mathbf{J}}$. Due to the definition (4.10) the operators $\hat{A}$ with sub- and superscripts are anticommute,

$$[\hat{A}^\dagger_{\mathbf{I},\sigma}, \hat{A}^{\mathbf{J},\sigma'}]_+ = \delta_{\sigma,\sigma'}\delta_{\mathbf{I},\mathbf{J}}. \tag{4.11}$$

As a further consequence of the linear independence of the vector set $\{\hat{A}^\dagger_{\mathbf{I},\sigma}|0\rangle : \mathbf{I} \in \Lambda_{pl}\}$ we can realize that $\hat{G}^\dagger := \big(\prod_{\mathbf{I}} \hat{A}^\dagger_{\mathbf{I},\uparrow}\big)\big(\prod_{\mathbf{I}} \hat{A}^\dagger_{\mathbf{I},\downarrow}\big) \neq 0$. The operator $\hat{G}$, which is the adjoint of $\hat{G}^\dagger$ can be written as $\hat{G} = \big(\prod'_{\mathbf{I}} \hat{A}^\dagger_{\mathbf{I},\downarrow}\big)\big(\prod'_{\mathbf{I}} \hat{A}^\dagger_{\mathbf{I},\uparrow}\big)$, where the prime over the $\prod$ indicates that the multipliers of the product stand in reverse order.

A wave function $|\psi\rangle = \hat{G}^\dagger \hat{Z}^\dagger|0\rangle$ with arbitrary operator $\hat{Z}^\dagger$ is in the kernel of $\hat{P}$. It is simple consequence of the commutation relations (4.5), likewise the reverse statement, that every wave vector $|\psi\rangle = \hat{Z}^\dagger_1|0\rangle$ from the kernel of $\hat{P}$ can be written as $\hat{G}^\dagger \hat{Z}^\dagger|0\rangle$, where $Z^\dagger = \hat{G}\hat{Z}^\dagger_1/(\det g)^2$. For the proving of this latter statement take into account that from $\hat{P}\hat{Z}^\dagger_1|0\rangle = 0$ follows that $\hat{A}^\dagger_{\mathbf{I},\sigma}\hat{Z}^\dagger_1|0\rangle = 0$ for every $\mathbf{I}$ and σ, therefore

$$\begin{aligned}
\hat{G}^\dagger \hat{G} \hat{Z}^\dagger_1|0\rangle &= \prod_\sigma \Big(\Big(\prod_{\mathbf{I}} \hat{A}^\dagger_{\mathbf{I},\sigma}\Big)\Big(\prod_{\mathbf{J}}{}' \hat{A}_{\mathbf{J},\sigma}\Big)\Big)\hat{Z}^\dagger_1|0\rangle \\
&= \prod_\sigma \Big(\Big(\prod_{\mathbf{I}} \hat{A}^\dagger_{\mathbf{I},\sigma}\Big)\Big(\prod_{\mathbf{J}}{}' \Big(\sum_{\mathbf{L}} g^*_{\mathbf{L},\mathbf{J}} \hat{A}^{\mathbf{L},\sigma}\Big)\Big)\Big)\hat{Z}^\dagger_1|0\rangle \\
&= \prod_\sigma \Big(\Big(\prod_{\mathbf{I}} \hat{A}^\dagger_{\mathbf{I},\sigma}\Big)\Big(\sum_{\mathcal{P}\in S_{\Lambda_{pl}}} \prod_{\mathbf{J}}{}' g^*_{\mathcal{P}(\mathbf{J}),\mathbf{J}} \hat{A}^{\mathcal{P}(\mathbf{J}),\sigma}\Big)\Big)\hat{Z}^\dagger_1|0\rangle \\
&= \prod_\sigma \Big(\Big(\prod_{\mathbf{I}} \hat{A}^\dagger_{\mathbf{I},\sigma}\Big)\Big(\sum_{\mathcal{P}\in S_{\Lambda_{pl}}} (-1)^{|\mathcal{P}|} \prod_{\mathbf{J}}{}' g^*_{\mathcal{P}(\mathbf{J}),\mathbf{J}} \hat{A}^{\mathbf{J},\sigma}\Big)\Big)\hat{Z}^\dagger_1|0\rangle \\
&= \prod_\sigma \Big(\sum_{\mathcal{P}\in S_{\Lambda_{pl}}} (-1)^{|\mathcal{P}|} \prod_{\mathbf{J}} g_{\mathbf{J},\mathcal{P}(\mathbf{J})} \hat{A}^\dagger_{\mathbf{J},\sigma} \hat{A}^{\mathbf{J},\sigma}\Big)\hat{Z}^\dagger_1|0\rangle \\
&= (\det g)^2 \hat{Z}^\dagger_1|0\rangle,
\end{aligned} \tag{4.12}$$

where $\sum_{\mathcal{P}\in S_{\Lambda_{pl}}}$ means summation over all the permutations $\mathcal{P}$ of the the set Λ_{pl}, and $|\mathcal{P}|$ is the parity of a permutation. We used in equation (4.12) that $g_{\mathbf{I},\mathbf{J}} = g^*_{\mathbf{J},\mathbf{I}}$.

Thus we have determined the kernel of $\hat{P}$: every state vector from it has the form $\hat{G}^\dagger \hat{Z}^\dagger|0\rangle$, where $\hat{Z}^\dagger$ is an arbitrary operator. [2]

We have mentioned that a state vector $|\psi\rangle$ is in the kernel of $\hat{P}'$ if and only if there is no empty site in the f-level. More precisely it means that expressing $|\psi\rangle$ in terms of $\hat{b}_{\mathbf{i},\sigma}$ as a linear combination of operator products $\hat{b}^\dagger_{\mathbf{i}_1,\sigma_1}\hat{b}^\dagger_{\mathbf{i}_2,\sigma_2}\cdots$ every term of this linear combination have to contain the operators $\hat{f}^\dagger_{\mathbf{i},\sigma_\mathbf{i}}$ for all $\mathbf{i}$ with an arbitrary $\sigma_\mathbf{i}$. Taking into account that expressing $\hat{G}^\dagger$ in terms of $\hat{b}^\dagger_{\mathbf{i},\sigma}$ there is a term which does not contain $\hat{f}^\dagger$ operators at all, we conclude that a vector $|\psi\rangle = \hat{G}^\dagger\hat{Z}^\dagger|0\rangle \in \ker(\hat{P})$ is simultaneously in $\ker(\hat{P}')$ as well if and only if $\hat{Z}^\dagger$ is a linear combination of operators $\hat{F}^\dagger_{\boldsymbol{\sigma}}\hat{Z}^\dagger_{\boldsymbol{\sigma}}$, where we used the notation $\hat{F}^\dagger_{\boldsymbol{\sigma}} = \prod_\mathbf{i}\hat{f}^\dagger_{\mathbf{i},\sigma_\mathbf{i}}$ with $\boldsymbol{\sigma} = (\sigma_\mathbf{i})_{\mathbf{i=1}}^{\mathbf{N}_\Lambda}$, $\sigma_\mathbf{i} \in \{\uparrow,\downarrow\}$, and $\hat{Z}^\dagger_{\boldsymbol{\sigma}}$ are arbitrary operators. As a corollary, every ground state vector, which can be determined by our method corresponds to $N \geq 3N_\Lambda$, and the ground state vector at three-quarter filling can be written as a linear combination of the following ones

$$|\psi_{0,\boldsymbol{\sigma}}\rangle = \hat{G}^\dagger\hat{F}^\dagger_{\boldsymbol{\sigma}}|0\rangle \tag{4.13}$$

In the Appendix A we show that these vectors not only generate the ground state subspace but they are linearly independents, so these form a basis in $\mathfrak{H}_{3N_\Lambda,0}$.

With the condition that the particle number is N where $N \geq 3N_\Lambda$, a ground state can be written as

$$|\psi_0\rangle = \sum_{\boldsymbol{\sigma}}\hat{G}^\dagger\hat{F}^\dagger_{\boldsymbol{\sigma}}Z^\dagger_{\boldsymbol{\sigma}}|0\rangle, \tag{4.14}$$

where the operators $Z^\dagger_{\boldsymbol{\sigma}}$ create $N-3N_\Lambda$ particles from the vacuum, otherwise these are arbitrary operators, consist of not only a simple product of creation operators but its linear combination with complex numerical coefficients.

4.4 Conditions for the model parameters

In the previous Section we have seen that the condition (c) from Section 4.2 can be satisfied when $N \geq 3N_\Lambda$ assuming that $\det g \neq 0$. Now we examine the conditions (a) which is formulated in equation (4.7). Writing down explicitly the two sides of that equation we get the following system of nineteen equations for the parameters

[2] We need it later therefore we mention here that on the same manner like the computation (4.12) we can prove the equality $\hat{G}\hat{G}^\dagger|0\rangle = (\det g)^2|0\rangle$. For this purpose we neglect the operator $\hat{Z}^\dagger_1$ and interchange the $\hat{G}$ and $\hat{G}^\dagger$ operators, but the main concepts of the computation (4.12) remain unchanged. In the last step we use that $\hat{A}_{\mathbf{I},\sigma}|0\rangle = 0$ for arbitrary $\mathbf{I}$ and σ. As a consequence we have $||\hat{G}^\dagger|0\rangle|| = \det g$.

$a_{\boldsymbol{\delta},b}$ and K:

$$t_{\mathbf{j}}^b = -\sum_{\substack{\boldsymbol{\delta},\boldsymbol{\delta}' \\ \boldsymbol{\delta}\text{-}\boldsymbol{\delta}'=\mathbf{j}}} a^*_{\boldsymbol{\delta},b} a_{\boldsymbol{\delta}',b}, \quad b \in \{c, f\}, \;\; \mathbf{j} \in \{\mathbf{x}, \mathbf{y}, \mathbf{x}+\mathbf{y}, \mathbf{x}-\mathbf{y}\},$$

$$V_{\mathbf{j}} = -\sum_{\substack{\boldsymbol{\delta},\boldsymbol{\delta}' \\ \boldsymbol{\delta}\text{-}\boldsymbol{\delta}'=\mathbf{j}}} a^*_{\boldsymbol{\delta},c} a_{\boldsymbol{\delta}',f}, \quad \mathbf{j} \in \mathcal{N}, \qquad V_0 = -\sum_{\boldsymbol{\delta}} a^*_{\boldsymbol{\delta},c} a_{\boldsymbol{\delta},f},$$

$$E_f + U = \sum_{\boldsymbol{\delta}} (|a_{\boldsymbol{\delta},c}|^2 - |a_{\boldsymbol{\delta},f}|^2), \qquad K = \sum_{\boldsymbol{\delta}} |a_{\boldsymbol{\delta},c}|^2. \tag{4.15}$$

Before we analyze the physical meaning of the condition that these equations have to be solvable we make some remarks.

Choosing the parameters $a_{\boldsymbol{\delta},b}$ and U arbitrarily but satisfying the conditions $\det g \neq 0$ and $U > 0$ we can get proper model parameters from equations (4.15). From mathematical point of view equations (4.15) define a quadratic mapping from the space of eight complex variables $a_{\boldsymbol{\delta},b}$ and the real variable U into the original parameter space of the seventeen complex hybridization and hopping coupling constants and the real E_f and U. From the domain of this mapping we exclude the $U \leq 0$ half-space and the one dimensional complex submanifold in which $\det g = 0$. The image of this domain determines the values of the parameters in the original parameter space for which we can solve the model. This is clearly a submanifold which goes through the parameter space from small to large U.

Using the last two equations from (4.15) we can express the ground state energy from equation (4.8) in terms of the original model parameters and K.

$$E_0 = KN + (2E_f + U - 4K)N_\Lambda \tag{4.16}$$

This expression contains explicitly only two model parameters U and E_f, but they are implicitly influenced by the others via equations (4.15), and the other parameters influence the value of E_0 via K, too.

Summarizing, we can state the following: if (a) the system of equations (4.15) is solvable, (b) $U > 0$ and (c) from the solution of equations (4.15) we get $\det g \neq 0$, then fixing the particle number on a value $N \geq 3N_\Lambda$ the ground state of the Hamiltonian (4.1) is degenerated, the ground states can be written as in equation (4.14) and have energy (4.16).

To understand the physical background of condition (a) we Fourier transform the equation (4.7). From the right hand side we get the usual $\vec{k}$-space representation of the non-interacting Hamiltonian, but the energy level of the f-band is shifted by U due to the second term originated from the interaction. After Fourier transformation the non-interacting term is not diagonal either, unlike equation (2.9), because of the hybridization terms. As follows from the conventions of Section 2.2

the Fourier transform of the operator $\hat{b}_{\mathbf{i},\sigma}$ is (compare the equations (2.4, 2.5, 2.8) and (2.10))

$$\hat{b}_{\vec{k},\sigma} = \frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{i}} e^{i\vec{k}\vec{R}_\mathbf{i}} \hat{b}_{\mathbf{i},\sigma}, \tag{4.17}$$

and the inverse relation is

$$\hat{b}_{\mathbf{i},\sigma} = \frac{1}{\sqrt{N_\Lambda}} \sum_{\vec{k}} e^{-i\vec{k}\vec{R}_\mathbf{i}} \hat{b}_{\vec{k},\sigma}. \tag{4.18}$$

Thus the right hand side of the equation (4.7) takes on the form

$$\hat{H}_0 + U\hat{N}_f = \sum_{\vec{k},\sigma} \sum_{b,b'} h_{\vec{k};b,b'} \hat{b}^\dagger_{\vec{k},\sigma} \hat{b}'_{\vec{k},\sigma}, \tag{4.19}$$

where

$$h_{\vec{k};b,b'} := \begin{pmatrix} \epsilon_{\vec{k},c} & V_{\vec{k}} \\ V^*_{\vec{k}} & \epsilon_{\vec{k},f} + U \end{pmatrix} = \begin{pmatrix} \sum_{\mathbf{j}\in\mathcal{N}} t^c_\mathbf{j} e^{i\vec{k}\vec{R}_\mathbf{j}} & V_0 + \sum_{\mathbf{j}\in\mathcal{N}} V_\mathbf{j} e^{i\vec{k}\vec{R}_\mathbf{j}} \\ V^*_{\vec{k}} & U + E_f + \sum_{\mathbf{j}\in\mathcal{N}} t^f_\mathbf{j} e^{i\vec{k}\vec{R}_\mathbf{j}} \end{pmatrix} \tag{4.20}$$

To handle the left hand side of equation (4.7) we express $\hat{A}_{\mathbf{I},\sigma}$ with the Fourier transformed operators (4.17):

$$\hat{A}_{\mathbf{I},\sigma} = \sum_{\boldsymbol{\delta},b} a_{\boldsymbol{\delta},b} \frac{1}{\sqrt{N_\Lambda}} \sum_{\vec{k}} e^{-i\vec{k}\vec{R}_{\mathbf{I}+\boldsymbol{\delta}}} \hat{b}_{\vec{k},\sigma} = \frac{1}{\sqrt{N_\Lambda}} \sum_{\vec{k}} e^{-i\vec{k}\vec{R}_\mathbf{I}} \sum_b \alpha_{\vec{k},b} \hat{b}_{\vec{k},\sigma}, \tag{4.21}$$

where

$$\alpha_{\vec{k},b} := \sum_{\boldsymbol{\delta}} a_{\boldsymbol{\delta},b} e^{-i\vec{k}\vec{R}_{\boldsymbol{\delta}}}. \tag{4.22}$$

Based on equation (4.21) we have

$$-\sum_{\mathbf{I},\sigma} \hat{A}^\dagger_{\mathbf{I},\sigma} \hat{A}_{\mathbf{I},\sigma} + K\hat{N} = -\sum_{\vec{k},\sigma} \sum_{b,b'} \alpha^*_{\vec{k},b} \alpha_{\vec{k},b'} \hat{b}^\dagger_{\vec{k},\sigma} \hat{b}'_{\vec{k},\sigma} + K \sum_{\vec{k},\sigma} \sum_b \hat{b}^\dagger_{\vec{k},\sigma} \hat{b}_{\vec{k},\sigma}. \tag{4.23}$$

From the comparison of equations (4.19) and (4.23) we conclude that the equation (4.7), which is the formula of condition (a), in Fourier space can be written as

$$h_{\vec{k};b,b'} = -\alpha^*_{\vec{k},b} \alpha_{\vec{k},b'} + K\delta_{b,b'}. \tag{4.24}$$

From this expression of the matrix $h_{\vec{k}}$ one can immediately see that from the diagonalization of the Hamiltonian $\hat{H}_0 + U\hat{N}_f$ — which means the diagonalization of the matrix $h_{\vec{k}}$, as can be seen from equation (4.19) — two bands arise with dispersion relations

$$E_{\vec{k},1} = K - \Delta_{\vec{k}}, \qquad E_{\vec{k},2} = K, \tag{4.25}$$

where

$$\Delta_{\vec{k}} = \sum_b |\alpha_{\vec{k},b}|^2 = 2K - \epsilon_{\vec{k},c} - \epsilon_{\vec{k},f} - U \geq 0. \tag{4.26}$$

We mention here that in the ground state, because of $\hat{P}'|\psi_0\rangle = 0$, the effective Hamiltonian is $\hat{H}_{\mathit{eff}} = \hat{H}_0 + U\hat{N}_f$. With this notation we can write the Hamiltonian (4.1) as

$$\hat{H} = \hat{H}_{\mathit{eff}} + U\hat{P}' - UN_\Lambda. \tag{4.27}$$

Now we take into account the condition $\det g \neq 0$. As we have mentioned, in this case $\{\hat{A}^\dagger_{\mathbf{I},\sigma}|0\rangle \,:\, \mathbf{I} \in \Lambda_{pl}\}$ is a linearly independent vector set. The Fourier transformation is a regular linear transformation, i.e. preserves the linear independence. From equation (4.21) one can see that the Fourier transform of $\hat{A}_{\mathbf{I},\sigma}$ is $\sum_b \alpha_{\vec{k},b}\hat{b}_{\vec{k},\sigma}$, therefore $\{\sum_b \alpha^*_{\vec{k},b}\hat{b}^\dagger_{\vec{k},\sigma}|0\rangle \,:\, \vec{k} \in \Lambda\}$ is also a linearly independent set. As a simple consequence $\sum_b \alpha_{\vec{k},b}\hat{b}_{\vec{k},\sigma} \neq 0$ thus $\sum_b |\alpha_{\vec{k},b}|^2 \neq 0$ for all $\vec{k}$. It means that the diagonalized bands of $\hat{H}_{\mathit{eff}}$ with dispersions (4.25) are not degenerated, hence the operators given by this diagonalization, i.e., for which

$$\hat{H}_{\mathit{eff}} = \sum_{s=1}^{2} \sum_{\vec{k},\sigma} C^\dagger_{\vec{k},s,\sigma} C_{\vec{k},s,\sigma}, \tag{4.28}$$

are uniquely determined by the following expressions

$$\hat{C}_{\vec{k},1,\sigma} = \frac{\alpha_{\vec{k},c}\hat{c}_{\vec{k},\sigma} + \alpha_{\vec{k},f}\hat{f}_{\vec{k},\sigma}}{\sqrt{\Delta_{\vec{k}}}}, \qquad \hat{C}_{\vec{k},2,\sigma} = \frac{\alpha^*_{\vec{k},f}\hat{c}_{\vec{k},\sigma} - \alpha^*_{\vec{k},c}\hat{f}_{\vec{k},\sigma}}{\sqrt{\Delta_{\vec{k}}}}. \tag{4.29}$$

As we expect, but it can be checked by direct computation, the canonical anticommutation relations are hold for these operators and their adjoints, because $\hat{C}^\dagger_{\vec{k},s,\sigma}|0\rangle$ are eigenvectors with non-degenerated eigenvalues of the self-adjoint operator $\hat{H}_{\mathit{eff}}$ thus they are orthogonal each other, and they are also normalized due to the normalization constant $(\Delta_{\vec{k}})^{-1/2}$. Apart from this normalization the operators $\hat{C}_{\vec{k},1,\sigma}$ are the Fourier transforms of $\hat{A}_{\mathbf{I},\sigma}$. This is not surprising taking into account that $\hat{H}_{\mathit{eff}}$ can be written by $\hat{A}^\dagger_{\mathbf{I},\sigma}$ as the left hand side of equation (4.7).

In the light of the above we can consider the expression (4.19) of $\hat{H}_{\mathit{eff}}$ as a Hamiltonian of a non-interacting system which is similar to $\hat{H}_0$ but the value of E_f is substituted by $E_f + U$. As can be seen from the expression (4.28), this non-interacting Hamiltonian describes a two-band system with one completely flat band which energy is above the other, non flat band.

Finally we can restate our results in the following form: the ground states of the Hamiltonian (4.1) are the states from equation (4.14) with energy (4.16) when $N \geq 3N_\Lambda$, $U > 0$ and the Hamiltonian $\hat{H}_0 + U\hat{N}_f$ has two non-intersecting bands and the upper one is completely dispersionless.

In the following we discuss the physical properties of the deduced ground states.

4.5 Physical properties of the deduced ground state

4.5.1 Momentum distribution functions and ground state expectation values of the Hamiltonian terms

Now we compute the momentum distribution functions and ground state expectation values of the terms from Hamiltonian (4.1). For this purpose it is enough to compute the expectation value of $\sum_\sigma \hat{b}^\dagger_{\vec{k},\sigma} \hat{b}'_{\vec{k},\sigma}$ because the non-interacting terms can be easily expressed by them and based on the decomposition (4.2) of the interaction it can be seen that for the expectation value of $\hat{U}$ it is enough to compute the expectation value of $\hat{N}_f$, because $\hat{P}'$ — due to its definition — gives zero on the ground states. The operators $\hat{b}_{\vec{k},\sigma}$ can be expressed by $\hat{C}_{\vec{k},s,\sigma}$ via the inverse expressions of equations (4.29),

$$\hat{c}_{\vec{k},\sigma} = \frac{\alpha^*_{\vec{k},c}\hat{C}_{\vec{k},1,\sigma} + \alpha_{\vec{k},f}\hat{C}_{\vec{k},2,\sigma}}{\sqrt{\Delta_{\vec{k}}}}, \qquad \hat{f}_{\vec{k},\sigma} = \frac{\alpha^*_{\vec{k},f}\hat{C}_{\vec{k},1,\sigma} - \alpha_{\vec{k},c}\hat{C}_{\vec{k},2,\sigma}}{\sqrt{\Delta_{\vec{k}}}} \tag{4.30}$$

therefore we need the expectation values of $\hat{C}^\dagger_{\vec{k},s,\sigma}\hat{C}_{\vec{k},s',\sigma}$. To calculate them we express the ground state vectors with the operators $\hat{C}^\dagger_{\vec{k},s,\sigma}$.

For the operator $\hat{G}^\dagger$ it is easily can be done based on the observation that it contains product of $\hat{A}^\dagger_{\mathbf{I},\sigma}$ over all the plaquette indices, and the Fourier transform of $\hat{A}^\dagger_{\mathbf{I},\sigma}$ is $(\Delta_{\vec{k}})^{1/2}\hat{C}^\dagger_{\vec{k},1,\sigma}$, as we mentioned in the previous Section. Therefore

$$\hat{G}^\dagger = \Big(\prod_{\vec{k}} (\Delta_{\vec{k}})^{1/2}\hat{C}^\dagger_{\vec{k},1,\uparrow}\Big)\Big(\prod_{\vec{k}} (\Delta_{\vec{k}})^{1/2}\hat{C}^\dagger_{\vec{k},1,\downarrow}\Big) = \Big(\prod_{\vec{k}} \Delta_{\vec{k}}\Big)\Big(\prod_{\vec{k}} \hat{C}^\dagger_{\vec{k},1,\uparrow}\Big)\Big(\prod_{\vec{k}} \hat{C}^\dagger_{\vec{k},1,\downarrow}\Big). \tag{4.31}$$

The prefactor $\prod_{\vec{k}} \Delta_{\vec{k}}$ gives the norm of the state vector $\hat{G}^\dagger|0\rangle$ because the last two operatorial parts in equation (4.31) create a normalized state from the vacuum, since the operators $\hat{C}^\dagger_{\vec{k},1,\sigma}$ and their adjoints satisfy the canonical anticommutation relations. Comparing it with footnote 2 in page 43 we can realize that $\det g = \prod_{\vec{k}} \Delta_{\vec{k}}$. We derived this relation for $\det g \neq 0$ case but it remains valid in $\det g = 0$ case, too. It holds true because from the linear dependency of the vector set $\{\hat{A}_{\mathbf{I},\sigma} : \mathbf{I} \in \Lambda_{pl}\}$ follows the linear dependency of $\{(\Delta_{\vec{k}})^{1/2}\hat{C}^\dagger_{\vec{k},1,\sigma}|0\rangle : \vec{k} \in \hat{\Lambda}\}$, which involves $\Delta_{\vec{k}} = 0$ for at least one $\vec{k}$, since the non-zero vectors $\hat{C}^\dagger_{\vec{k},1,\sigma}|0\rangle$ are linearly independents. This again emphasizes that the condition $\det g \neq 0$ means that the gap between the bands of the Hamiltonian $\hat{H}_{\mathit{eff}}$ is non-vanishing. Therefore in case of $N > 2N_\Lambda$ every ground state of $\hat{H}_{\mathit{eff}}$ is simply built up from a completely filled lower band and a partially filled upper band in which the electrons can be situated arbitrarily because it is dispersionless. The particle distribution in this band is determined by the further condition that the interaction energy have to be minimal, i.e. the ground state has to be in $\ker \hat{P}'$. The state vectors (4.13-4.14) meet these two requirements simultaneously. The operator $\hat{G}^\dagger$ fills up the lower band of $\hat{H}_{\mathit{eff}}$ and $\hat{F}^\dagger_{\boldsymbol{\sigma}}$ assures that every site contains at least one electron.

Expressing $\hat{F}^\dagger_{\boldsymbol{\sigma}}$ in terms of $\hat{C}^\dagger_{\vec{k},s,\sigma}$ we get a linear combination of terms consisting of the products of these operators. In the building up of the ground states only those terms play role which consist of only $\hat{C}^\dagger_{\vec{k},2,\sigma}$, because $\hat{G}^\dagger$ contains $\hat{C}^\dagger_{\vec{k},1,\sigma}$ for every $\vec{k}$ and σ. The same is true for $\hat{Z}^\dagger_{\boldsymbol{\sigma}}$. The terms of its expression which contain $\hat{C}^\dagger_{\vec{k},1,\sigma}$ are cancel out. Based on the above we conclude that

$$\hat{C}^\dagger_{\vec{k},1,\sigma}\hat{C}_{\vec{k},1,\sigma}|\psi_0\rangle = |\psi_0\rangle, \qquad \hat{C}^\dagger_{\vec{k},1,\sigma}\hat{C}_{\vec{k},2,\sigma}|\psi_0\rangle = 0, \tag{4.32}$$

for arbitrary ground state vectors from equation (4.14).

If a physical quantity has the property that its quantum mechanical expectation value is uniform in the subspace of ground states then we denote it in this Chapter by $\langle . \rangle$. In other words $\langle \hat{X} \rangle := \frac{\langle\psi_0|\hat{X}|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}$, and the notation used on the left hand side includes that the right hand side does not depend on $\psi_0 \in \mathfrak{H}_{N,0}$.

From equations (4.32) we can see that $\langle \hat{C}^\dagger_{\vec{k},1,\sigma}\hat{C}_{\vec{k},1,\sigma}\rangle = 1$ and $\langle \hat{C}^\dagger_{\vec{k},1,\sigma}\hat{C}_{\vec{k},2,\sigma}\rangle = 0$. These results are valid for arbitrary $N \geq 3N_\Lambda$ cases. Furthermore, in case of 3/4 filling and with the additional condition that $\alpha_{\vec{k},c} \neq 0$ for all $\vec{k}$ in Appendix A based on the explicit expression of $\hat{F}^\dagger$ in terms of operators $\hat{C}^\dagger_{\vec{k},s,\sigma}$ we prove that

$$\langle \sum_\sigma \hat{C}^\dagger_{\vec{k},2,\sigma}\hat{C}_{\vec{k},2,\sigma}\rangle = 1. \tag{4.33}$$

When there exists $\vec{k}$ for which $\alpha_{\vec{k},c} = 0$ then the vectors (4.13) for all $\boldsymbol{\sigma}$ are not linearly independent, and the proof of equation (4.33) in Appendix A is not applicable. It seems to be not only a technical difficulty. It is a matter of fact that the result (4.33) with its all consequences equations (4.34) and (4.35) do not remain valid in this case. Therefore in the following part of this Section all discussion is related to the $\alpha_{\vec{k},c} \neq 0$ case, which involves $\Delta_{\vec{k}} \neq 0$, so hereafter this condition becomes more restrictive.

Now we can accomplish the program written down in the first paragraph of this Section. We use the equation (4.33) therefore the results below are related to the case of 3/4 filling and $\alpha_{\vec{k},c} \neq 0$. From the results of the previous paragraph and equations (4.30) we get

$$\begin{aligned} n_{\vec{k},c} &:= \Big\langle \sum_\sigma \hat{c}^\dagger_{\vec{k},\sigma}\hat{c}_{\vec{k},\sigma} \Big\rangle = 1 + \frac{|\alpha_{\vec{k},c}|^2}{\Delta_{\vec{k}}} = 1 + \frac{K - \epsilon_{\vec{k},c}}{2K - \epsilon_{\vec{k},c} - \epsilon_{\vec{k},f} - U} , \\ n_{\vec{k},f} &:= \Big\langle \sum_\sigma \hat{f}^\dagger_{\vec{k},\sigma}\hat{f}_{\vec{k},\sigma} \Big\rangle = 1 + \frac{|\alpha_{\vec{k},f}|^2}{\Delta_{\vec{k}}} = 1 + \frac{K - \epsilon_{\vec{k},f} - U}{2K - \epsilon_{\vec{k},c} - \epsilon_{\vec{k},f} - U} , \\ &\Big\langle \sum_\sigma \hat{f}^\dagger_{\vec{k},\sigma}\hat{c}_{\vec{k},\sigma} \Big\rangle = \frac{\alpha^*_{\vec{k},c}\alpha_{\vec{k},f}}{\Delta_{\vec{k}}} = -\frac{V_{\vec{k}}}{2K - \epsilon_{\vec{k},c} - \epsilon_{\vec{k},f} - U} , \end{aligned} \tag{4.34}$$

and the ground-state expectation values of different Hamiltonian terms become

$$\begin{aligned} \langle \hat{T}_c \rangle &= \sum_{\vec{k}} (K - |\alpha_{\vec{k},c}|^2)\Big(1 + \frac{|\alpha_{\vec{k},c}|^2}{\Delta_{\vec{k}}}\Big) = \sum_{\vec{k}} \epsilon_{\vec{k},c}\, \frac{K - \epsilon_{\vec{k},c}}{\Delta_{\vec{k}}}, \\ \langle \hat{T}_f \rangle &= \sum_{\vec{k}} (K - E_f - U - |\alpha_{\vec{k},f}|^2)\Big(1 + \frac{|\alpha_{\vec{k},f}|^2}{\Delta_{\vec{k}}}\Big) = \sum_{\vec{k}} (\epsilon_{\vec{k},f} - E_f)\frac{K - \epsilon_{\vec{k},f} - U}{\Delta_{\vec{k}}} , \\ \langle \hat{V} \rangle &= -\sum_{\vec{k}} \frac{(\alpha^*_{\vec{k},c}\alpha_{\vec{k},f} + V_0)\alpha^*_{\vec{k},f}\alpha_{\vec{k},c} + (\alpha^*_{\vec{k},f}\alpha_{\vec{k},c} + V_0^*)\alpha^*_{\vec{k},c}\alpha_{\vec{k},f}}{\Delta_{\vec{k}}} \\ &= -\sum_{\vec{k}} \frac{2|V_{\vec{k}}|^2 - (V^*_{\vec{k}}V_0 + V_0^* V_{\vec{k}})}{\Delta_{\vec{k}}} , \\ \langle \hat{V}_0 \rangle &= \sum_{\vec{k}} \frac{V_0\alpha^*_{\vec{k},f}\alpha_{\vec{k},c} + V_0^*\alpha^*_{\vec{k},c}\alpha_{\vec{k},f}}{\Delta_{\vec{k}}} = -\sum_{\vec{k}} \frac{V^*_{\vec{k}}V_0 + V_0^* V_{\vec{k}}}{\Delta_{\vec{k}}} , \\ \langle \hat{E}_f \rangle &= E_f \sum_{\vec{k}} \Big(1 + \frac{|\alpha_{\vec{k},f}|^2}{\Delta_{\vec{k}}}\Big) = E_f \sum_{\vec{k}} \Big(1 + \frac{K - \epsilon_{\vec{k},f} - U}{\Delta_{\vec{k}}}\Big) , \\ \langle \hat{U} \rangle &= U \sum_{\vec{k}} \frac{|\alpha_{\vec{k},f}|^2}{\Delta_{\vec{k}}} = U \sum_{\vec{k}} \frac{K - \epsilon_{\vec{k},f} - U}{\Delta_{\vec{k}}}, \end{aligned} \tag{4.35}$$

where we used that the dispersion relation $\epsilon_{\vec{k},b}$ summing over the whole Brillouin zone gives the meaning of the band, i.e. 0 for the c-band and E_f for the f-band.

The value of the constant K is given via the solution of equations (4.15) and $\Delta_{\vec{k}} > 0$ is also given in terms of the original coupling constants in equation (4.26) via equation (4.20).

First of all the most conspicuous feature of the above results that both bands are partially filled and the momentum distribution functions $n_{\vec{k},b}$ are continuous together with their derivatives of any order. Therefore Fermi momentum is not definable thus the system has not Fermi surface. These show that our system is not a usual Fermi liquid. To get more details about these properties we are motivated to examine the spin contributions to $n_{\vec{k},b}$. Investigating the ground state expectation value of $\hat{n}_{\vec{k},b,\sigma} = \hat{b}^{\dagger}_{\vec{k},\sigma}\hat{b}_{\vec{k},\sigma}$ we can realize that — due to the same feature of $\hat{C}^{\dagger}_{\vec{k},2,\sigma}\hat{C}_{\vec{k},2,\sigma}$ — it is not uniform in the subspace of the ground states either in $N = 3N_{\Lambda}$ case, but depends on the index $\boldsymbol{\sigma}$ of the basis vectors of $\mathfrak{H}_{N,0}$ from equation (4.13). Nevertheless, we can compute the limit $\langle\hat{n}_{\vec{k},b,\sigma}\rangle_0 := \lim_{T\to 0}\langle\hat{n}_{\vec{k},b,\sigma}\rangle_T$ which has a discontinuity at the Fermi surface for Fermi liquids. Here $\langle.\rangle_T$ denotes the finite temperature expectation value with the canonical density operator, i.e., for an observable $\hat{X}$ it is defined by

$$\langle\hat{X}\rangle_T := \frac{\mathrm{Tr}(\hat{X}\, e^{-\frac{\hat{H}}{k_B T}})}{\mathrm{Tr}(e^{-\frac{\hat{H}}{k_B T}})}, \tag{4.36}$$

therefore

$$\langle\hat{X}\rangle_0 := \lim_{T\to 0}\langle\hat{X}\rangle_T = \frac{\mathop{\mathrm{Tr}}_{\mathfrak{H}_{N,0}}\ \hat{X}}{\mathop{\mathrm{Tr}}_{\mathfrak{H}_{N,0}}\ \hat{1}}. \tag{4.37}$$

Here the subscript $\mathfrak{H}_{N,0}$ under the Tr means that the trace have to be taken over the ground state subspace, and not over the whole Hilbert space $\mathfrak{H}_N$. Based on the above one can see that from the existence of the expectation value $\langle\hat{X}\rangle$ follows that $\langle\hat{X}\rangle_0 = \langle\hat{X}\rangle$. That is why we immediately obtain from equations (4.32) that $\langle\hat{C}^{\dagger}_{\vec{k},1,\sigma}\hat{C}_{\vec{k},1,\sigma}\rangle_0 = 1$ and $\langle\hat{C}^{\dagger}_{\vec{k},1,\sigma}\hat{C}_{\vec{k},2,\sigma}\rangle_0 = 0$. Moreover, at the end of Appendix A we prove that $\langle\hat{C}^{\dagger}_{\vec{k},2,\sigma}\hat{C}_{\vec{k},2,\sigma}\rangle_0 = \frac{1}{2}$ independently on σ. All in all, we conclude that $n_{\vec{k},b,\sigma} = n_{\vec{k},b}/2$. Therefore neither $n_{\vec{k},b,\sigma}$ makes possible to define Fermi momentum.

In case of $N > 3N_{\Lambda}$ the quantum mechanical expectation value of $\sum_{\sigma}\hat{C}^{\dagger}_{\vec{k},2,\sigma}\hat{C}_{\vec{k},2,\sigma}$ is not uniform in $\mathfrak{H}_{N,0}$ any more, but the $T \to 0$ limit of its finite temperature expectation value is well defined and usable to study the momentum distribution functions in this case. By the same procedure than above we obtain continuous $n_{\vec{k},b}$ functions again. The reason is the same as in $3/4$ filling case. The electrons of a ground state wave function are created from the vacuum by three operators. As we have seen the electrons created by $\hat{F}^{\dagger}_{\boldsymbol{\sigma}}$ assure the minimalization of the interaction energy and do not cause any irregularity in k-space. Every other electron moves in the potential of these electrons driving by the effective Hamiltonian $\hat{H}_{eff}$. The lower band of this Hamiltonian is completely filled due to the electrons created by $\hat{G}^{\dagger}$, thus $\hat{Z}^{\dagger}_{\boldsymbol{\sigma}}$ can create electrons only in the upper band which is completely flat, so there is no reason to have Fermi momentum.

In the end we notice that the total momentum distribution function is completely uniform in $\vec{k}$-space: $n_{\vec{k}} := \langle \sum_b \hat{n}_{\vec{k},b} \rangle = 3$. As a check, from this result we get back $N = 3N_{\Lambda}$. Furthermore summing up all contributions from equations (4.35) we reobtain the ground state energy (4.16) with $N = 3N_{\Lambda}$. To prove it, based on equations (4.24,4.26) one can get for the sum of the terms from equations (4.35) — which is the ground state expectation value of the Hamiltonian (4.1) — that $E_0 = E_f N_{\Lambda} + \sum_{\vec{k}}(K - \Delta_{\vec{k}})$. The equivalence of this and equation (4.16) comes straightforward using the second expression of $\Delta_{\vec{k}}$ from (4.26) and $\sum_{\vec{k}} \epsilon_{\vec{k},c} = 0$ and $\sum_{\vec{k}} \epsilon_{\vec{k},f} = E_f N_{\Lambda}$.

4.5.2 Localized and non-localized solutions

Going on the discussion of the $N = 3N_{\Lambda}$ and $\alpha_{\vec{k},c} \neq 0$ case now we examine separately the on-site contribution to the ground state energy, and the contribution of the electron motion between the sites. For this purpose we decompose the Hamiltonian into sum of on-site — in other words localized — terms and non-localized terms which describe the moving of the electrons.

$$\hat{H} = \hat{H}_{loc} + \hat{H}_{mov}, \qquad \hat{H}_{loc} := \hat{V}_0 + \hat{E}_f + \hat{U}, \qquad \hat{H}_{mov} := \hat{T}_c + \hat{T}_f + \hat{V}. \tag{4.38}$$

Taking into account the equation (4.26) and that $\sum_{\vec{k}} \epsilon_{\vec{k},c} = \sum_{\vec{k}}(\epsilon_{\vec{k},f} - E_f) = 0$, from equations (4.35) we obtain the ground state expectation value of $\hat{H}_{mov}$:

$$\langle \hat{H}_{mov} \rangle = \sum_{\vec{k}} \frac{P_{\vec{k}}}{\Delta_{\vec{k}}} + 2\sum_{\vec{k}}(2K - E_f - U - \Delta_{\vec{k}}) = \sum_{\vec{k}} \frac{P_{\vec{k}}}{\Delta_{\vec{k}}} \tag{4.39}$$

where

$$P_{\vec{k}} = -[\,K|\alpha_{\vec{k},f}|^2 + (K - E_f - U)|\alpha_{\vec{k},c}|^2 + V_0 \alpha^*_{\vec{k},f}\alpha_{\vec{k},c} + V_0^* \alpha^*_{\vec{k},c}\alpha_{\vec{k},f}\,]. \tag{4.40}$$

Substituting into the above formula of $P_{\vec{k}}$ the last three equations from (4.15) which give the expressions of V_0, $E_f + U$ and K in terms of the parameters $a_{\boldsymbol{\delta},b}$, we obtain

$$P_{\vec{k}} = -\sum_{\boldsymbol{\delta}} |a_{\boldsymbol{\delta},c}\alpha_{\vec{k},f} - a_{\boldsymbol{\delta},f}\alpha_{\vec{k},c}|^2 \leq 0, \tag{4.41}$$

from which we get $\langle \hat{H}_{mov} \rangle \leq 0$ immediately.

We examine under which circumstances $\langle \hat{H}_{mov} \rangle$ can be zero. Clearly, it is zero if and only if $P_{\vec{k}} = 0$ for all $\vec{k}$, i.e., $a_{\boldsymbol{\delta},c}\alpha_{\vec{k},f} = a_{\boldsymbol{\delta},f}\alpha_{\vec{k},c}$ for all $\vec{k}$ and $\boldsymbol{\delta}$. In our case

($\alpha_{\vec{k},c} \neq 0$) it is equivalent with $a_{\boldsymbol{\delta},f} = p\, a_{\boldsymbol{\delta},c}$ where $p \in \mathbb{C}$ is a constant. Therefore in this case the definition (4.4) becomes

$$\hat{A}_{\mathbf{I},\sigma} = \sum_{\boldsymbol{\delta}} a_{\boldsymbol{\delta},c} \hat{d}_{\mathbf{I}+\boldsymbol{\delta},\sigma}, \quad \text{where} \quad \hat{d}_{\mathbf{i},\sigma} = \hat{c}_{\mathbf{i},\sigma} + p\hat{f}_{\mathbf{i},\sigma}. \tag{4.42}$$

The operators $\hat{d}^\dagger_{\mathbf{i},\sigma}$ anticommute with each other, therefore every non-vanishing term of the product $\prod_{\mathbf{I}} \hat{A}^\dagger_{\mathbf{I},\sigma}$ is proportional with the operator $\prod_{\mathbf{i}} \hat{d}^\dagger_{\mathbf{i},\sigma}$. Comparing the norm of the state vector created from the vacuum by $\hat{G}^\dagger$ and by $\prod_{\mathbf{i}} \hat{d}^\dagger_{\mathbf{i},\uparrow} \prod_{\mathbf{i}} \hat{d}^\dagger_{\mathbf{i},\downarrow}$ we conclude that contracting the numerical coefficients of these previously mentioned non-vanishing terms we have to get $\sqrt{\det g}$ apart from a factor coming from the normalization of the operators $\hat{d}^\dagger_{\mathbf{i},\sigma}$. All in all, we have

$$\hat{G}^\dagger = \frac{\det g}{(1+|p|^2)^{N_\Lambda}} \prod_{\mathbf{i}} \hat{d}^\dagger_{\mathbf{i},\uparrow} \prod_{\mathbf{i}} \hat{d}^\dagger_{\mathbf{i},\downarrow}. \tag{4.43}$$

We conclude that all ground state wave vectors from the equation (4.13) can be written as a product of one-site three particle states, so they describe a completely localized state. This means that from $\langle \hat{H}_{mov} \rangle = 0$ follows that $\hat{n}_{\mathbf{i}}|\psi_0\rangle = 3|\psi_0\rangle$, in other words, the ground-state vectors has no component in which the electron distribution is not uniform in the lattice.

The localization of the electrons implies under every circumstances that neither of any individual hopping term $\hat{T}^b_{\mathbf{j}}$ (its definition is a reasonable generalization of the definition (2.24) for c and f bands) or of any non-on-site hybridization term gives contribution to the ground state energy, therefore $\langle \hat{H}_{mov} \rangle = 0$. But in the studied case the reverse statement is also true, so we can say that $\langle \hat{H}_{mov} \rangle = 0$ holds if and only if every individual non-on-site term of the Hamiltonian has zero ground state expectation value, and it is equivalent to the fact that the ground state wave function is completely localized, i.e. it can be written as a product of on-site few-particle states, and finally the sufficient and necessary condition of it is that there exists a constant p which is independent of $\boldsymbol{\delta}$ for which

$$a_{\boldsymbol{\delta},f} = p\, a_{\boldsymbol{\delta},c}, \qquad p \in \mathbb{C}. \tag{4.44}$$

As a consequence, when (4.44) does not hold then the ground state wave function is not completely localized and the ground state expectation values of the moving terms give negative contribution to the ground state energy, since in this case the system preserves some movement of the electrons to decrease the ground state energy, while the momentum distribution function is continuous. Therefore the system is in a non-Fermi liquid normal state. (There is no any symmetry breaking to lead this situation.)

The localized case, in which the electrons are immovable, do not describe a liquid state of the electrons, instead it represents a Mott-insulator. The expectation values

(4.35,4.34) remain valid, but due to the validity of (4.44) which implies $\alpha_{\vec{k},f} = p\alpha_{\vec{k},c}$ these expectation values become simpler:

$$\begin{aligned} &n_{\vec{k},c} = \frac{2+|p|^2}{1+|p|^2}, && n_{\vec{k},f} = \frac{1+2|p|^2}{1+|p|^2}, && \Big\langle \sum_\sigma \hat{f}^\dagger_{\vec{k},\sigma}\hat{c}_{\vec{k},\sigma} \Big\rangle = \frac{p}{1+|p|^2}, \\ &\langle \hat{T}_c \rangle = 0, && \langle \hat{T}_f \rangle = 0, && \langle \hat{V} \rangle = 0, \\ &\langle \hat{V}_0 \rangle = \frac{(p^* V_0 + pV_0^*)N_\Lambda}{1+p^2}, && \langle \hat{E}_f \rangle = E_f N_\Lambda \frac{1+2|p|^2}{1+|p|^2}, && \langle \hat{U} \rangle = U N_\Lambda \frac{|p|^2}{1+|p|^2}. \end{aligned} \tag{4.45}$$

This is the situation in $N = 3N_\Lambda$ and $\alpha_{\vec{k},c} \neq 0$ case. However, the above distinction between the localized and non-localized situation is maintainable for arbitrary cases. The observation that the operator $\hat{G}^\dagger$ can be re-written in the form (4.43) makes us possible to generalize our localized solution to $\det g = 0$ case, when there exists $\vec{k}$ for which the gap $\Delta_{\vec{k}}$ between the flat and the other band of the effective Hamiltonian $\hat{H}_{eff}$ is zero. Further discussion of this gapless case is presented in Section 4.6.

4.5.3 Magnetic properties

As we have seen in Section 4.4 the effective Hamiltonian has a flat band. Flat band models are often used to explain ferromagnetism. [101] This fact, inter alia, motivate us to examine the magnetic properties of the ground states from equation (4.14). The important features of the above mentioned models, that the single electron ground state of the noninteracting Hamiltonian is very degenerated. The wave functions of these single electron ground states — however they have a small support, i.e, they vanish except on a small subset of the lattice containing few sites — overlap, therefore in general two electrons being in different single electron ground states can have interaction energy. The mechanism leading to ferromagnetic ground state is the following: switching on the repulsive on-site interaction the much degeneracy splits, and only those states remain ground states for which the interaction energy is minimal, in the most cases especially zero. Actually this is only the fully saturated ferromagnetic state in which the on-site interaction does not have effect on electrons because two electron can not be in the same site due to the Pauli principle.

The similarity between the above sketched situation and our case is that treating $\hat{H}_{eff}$ as the Hamiltonian of a non-interacting system we get a flat band. Though the lower band has normal dispersion, thus the single electron ground state is not very degenerated, putting more than $2N_\Lambda$ electrons into the system the lower band becomes fulfilled due to the first $2N_\Lambda$ electrons, and considering the remaining ones we can say that their single electron ground states are degenerated. Furthermore, the inverse Fourier transforms of the operators $\Delta_{\vec{k}}\hat{C}^{\dagger}_{\vec{k},2,\sigma}$ create from the vacuum such one particle eigenstates of $\hat{H}_{eff}$, of which wave functions are nonvanishing only in a small part of the lattice, namely on a plaquette.

However, the ground states from equation (4.14) show a typical paramagnetic behaviour, because our model essentially differs from the models of flat-band ferromagnetism. On the one hand, with the operator $\hat{H}_{eff}$ we have taken into account the interaction in some sort. The original non-interacting Hamiltonian $\hat{H}_0$ has no flat band, it describes a usual non-interacting Fermi system, which has a non-degenerated singlet ground state. Only the presence of the interaction leads to the degeneracy. Switching on U, when its value reaches the special value for which our solution is valid, i.e., for which the first equation of the last row of (4.15) becomes valid, then the one-particle eigenstates of $\hat{H}_{eff}$ become degenerated: every state in the upper band with arbitrary $\vec{k}$ and σ has the same energy. Nevertheless, it does not mean that in the ground states of the interacting system the electrons can be situated arbitrary in the upper band of $\hat{H}_{eff}$, because the ground states have to be in the kernel of $\hat{P}'$. The $U\hat{P}'$ term of the interacting Hamiltonian splits the very degenerated ground states of $\hat{H}_{eff}$. At first sight this is similar to the situation of the flat-band ferromagnetism, where $\hat{U}$ splits the large ground state degeneracy of the non-interacting Hamiltonian. But in our case the flat-band feature of $\hat{H}_{eff}$ and the switching on of $U\hat{P}'$ can not be distinguished; both are consequences of the interaction. On the other hand, the requirement that the ground state has to be in the kernel of $\hat{P}'$ leads to the presence of $\hat{F}^{\dagger}_{\boldsymbol{\sigma}}$ in the equation (4.14). This operator creates homogeneous particle distribution: one electron into every site, with arbitrary spin. In other words, this requirement determines the distribution of the particles, but not their spin states. In other point of view we can say that the lower band of $\hat{H}_{eff}$ is completely filled, therefore effectively the operator $\hat{F}^{\dagger}_{\boldsymbol{\sigma}}$ creates N_{Λ} electrons only in the upper band, and the distribution of these electrons in that flat band is uniquely determined by the fact that — taking into account also the $2N_{\Lambda}$ electrons in the lower band — there have not to be empty sites in the f-level. But the spin states each of these N_{Λ} electron in the flat band are completely arbitrary. It remains true for the other $N - 3N_{\Lambda}$ electrons created by $\hat{Z}^{\dagger}_{\boldsymbol{\sigma}}$, but their states are completely arbitrary, not only the spin state. They can occupy arbitrary state which the previous $3N_{\Lambda}$ electrons leaved empty. Clearly, such states there are only in the upper band.

So, while the electrons of the lower band are in singlet state, because this band is completely filled, the spin states of the electrons in the upper band are arbitrary. This is a typical paramagnetic behaviour, which usually occurs at high temperature. Every microscopic state has equal probability, the total spin is determined by the fact that which macroscopic spin state can be realized by most microscopic states, i.e., which has the greatest statistical weight. This is the state with minimal spin, which suppresses all the others in thermodynamic limit, and the expectation value of the total spin normalized with the number of particles (or with the number of sites) becomes zero. In other words the quantum mechanical expectation value of $\hat{S}^2$ is not uniform in the ground-state subspace $\mathfrak{H}_{N,0}$, but in thermodynamic limit we have $(1/N)\sqrt{\langle \hat{S}^2 \rangle_0} = 0$.

Now we show it explicitly in the $N = 3N_\Lambda$ and $\alpha_{\vec{k},c} \neq 0$ case. We can see that the state vectors from equation (4.13) are eigenvectors of $\hat{S}^z$, the eigenvalue is determined by $\boldsymbol{\sigma}$. It is due to the fact that $\hat{G}^\dagger$ creates singlet pairs in every plaquette, so it creates as many up electrons as down ones. Therefore supposing that the number of indices $\mathbf{i}$ for which $\sigma_\mathbf{i} =\uparrow$ is $N_\uparrow$, and the number of indices $\mathbf{i}$ for which $\sigma_\mathbf{i} =\downarrow$ is $N_\downarrow$, $(N_\uparrow + N_\downarrow = N_\Lambda,)$ then $\hat{S}^z|\psi_{0,\boldsymbol{\sigma}}\rangle = \frac{1}{2}(N_\uparrow - N_\downarrow)|\psi_{0,\boldsymbol{\sigma}}\rangle$. Therefore there are $N_\Lambda!/(N_\uparrow!N_\downarrow!)$ states among the states from equation (4.13) with a given S^z. These are linearly independent (see Appendix A), so they form a basis in $\mathfrak{H}_{3N_\Lambda,0}(S^z)$, of which dimension is therefore $N_\Lambda!/(N_\uparrow!N_\downarrow!)$. (Here $\mathfrak{H}_{N,0}(S^z)$ denotes the intersection of the ground sate subspace $\mathfrak{H}_{N,0}$ and the eigensubspace of the operator $\hat{S}^z$ described by the eigenvalue S^z.) Substituting the previous result into the formula

$$\langle \hat{S}^2 \rangle_0 = \frac{1}{\operatorname{Tr}_{\mathfrak{H}_{3N_\Lambda,0}} \hat{1}} \sum_S 6S^2 \operatorname{Tr}_{\mathfrak{H}_{3N_\Lambda,0}(S^z=S)} \hat{1} \tag{4.46}$$

which can be get by comparing equations (5.9, 5.10) from Chapter 5 and the formula (4.37) for the the zero temperature limit of the expectation value $\langle . \rangle_T$ we conclude that

$$\begin{aligned}\langle \hat{S}^2 \rangle_0 &= \frac{1}{\dim \mathfrak{H}_{3N_\Lambda,0}} \sum_S 6S^2 \dim \mathfrak{H}_{3N_\Lambda,0}(S^z\!=\!S) \\ &= \frac{1}{2^{N_\Lambda}} \sum_{N_\uparrow \geq \frac{N_\Lambda}{2}} 6\Big(N_\uparrow - \frac{N_\Lambda}{2}\Big)^2 \binom{N_\Lambda}{N_\uparrow} = \frac{1}{2^{N_\Lambda}} 6 \frac{N_\Lambda}{8} 2^{N_\Lambda} = \frac{3}{4} N_\Lambda. \end{aligned} \tag{4.47}$$

In the above formulas $\sum_S$ means summation over the all possible total spin values from $S_{min} = 0$ or $1/2$ to $S_{max} = N/2$.

In general case, when the ground state is not a single non-degenerated state, or $T \neq 0$, we define the expectation value of the total spin S by the implicit equation $\langle \hat{S}^2 \rangle = S(S+1)$. This is the natural generalization of the quantum mechanical definition for eigenvalues of $\hat{S}^2$. From the above result we can see that the expectation value of the total spin normalized with the number of particles is $S \sim 1/\sqrt{N_\Lambda}$, which goes to zero in thermodynamic limit.

In the above case the reason of the paramagnetic behaviour is that the spin states of every electron in the upper band of $\hat{H}_{eff}$ are arbitrary, thus the total spin of the system is also arbitrary between $S_{min} = 0$ or $1/2$ and $S_{max} = N_\Lambda/2$, moreover S_{min} has the greatest statistical weight. The situation becomes technically complicated when $N > 3N_\Lambda$ or $\exists\vec{k} : \alpha_{\vec{k},c} = 0$. In these cases some electrons of the upper band form singlet pairs, so S_{max} becomes less. But it remains true that below S_{max} all possible spin value occur among the ground states, and S_{min} has the greatest statistical weight. As a consequence, the system is paramagnetic.

4.6 The gapless case

As we proved in Section 4.3 the condition (c) formulated in Section 4.2 can be satisfied when $\det g \neq 0$. In this case the subspace of the ground states is generated by the vectors (4.14). The norm of these vectors are proportional with $\prod_{\vec{k}} \Delta_{\vec{k}}$ (see equation (4.31)) therefore when $\det g = \prod_{\vec{k}} \Delta_{\vec{k}} = 0$ then all these are the zero vector which does not describe physical state, and the satisfaction of condition (c) is not substantiated. Therefore up to this point only the $\det g \neq 0$ case was discussed, when the gap $\Delta_{\vec{k}}$ between the flat and the other band of $\hat{H}_{\mathit{eff}}$ is nonzero.

However, we can realize that under the circumstances when our solution describes localized state we can generalize the state vectors (4.13) for the gapless case. It is based on the the observation that in the mentioned case the formula (4.43) remains valid for $\hat{G}^\dagger$. Nevertheless the right hand side of that formula goes to zero as the gap goes to zero, but it is due to the scalar prefactor while the operator remains unchanged. Neglecting this prefactor and redefining $\hat{G}^\dagger$ as

$$\hat{G}^\dagger := \prod_{\mathbf{i}} \hat{d}^\dagger_{\mathbf{i},\uparrow} \prod_{\mathbf{i}} \hat{d}^\dagger_{\mathbf{i},\downarrow}, \qquad \text{when} \quad \det g = 0 \;\; \text{and} \;\; \exists p \in \mathbb{C} : a_{\boldsymbol{\delta},f} = p\, a_{\boldsymbol{\delta},c} \tag{4.48}$$

the definition (4.13) gives non-zero vectors which are in $\mathfrak{H}_{3N_\Lambda,0} = \ker \hat{P} \cap \ker \hat{P}'$. It can be easily seen rewriting the operator $\hat{P}$ in terms of $\hat{d}_{\mathbf{i},\sigma}$ based on the equation (4.42), and using that $\hat{d}^\dagger_{\mathbf{i},\sigma} d^\dagger_{\mathbf{i},\sigma} = 0$.

Actually the above means that in the localized case the ground state vectors valid in $\Delta \neq 0$ case survive the $\Delta \to 0$ limit, therefore every feature of these states remains valid, including the expectation values (4.45). The only difference is that the proof presented in Section 4.3 which prove that the states (4.13) generate the whole ground state subspace is does not survive.

4.7 Discussion

We have presented an exactly solvable case of a two band model of fermions in two dimensions. It is interesting in itself, regarding the absence of exact results even in one dimension, moreover our solution has some peculiar features. First of all, the momentum distribution functions $n_{\vec{k},b}$ are continuous together with their derivatives of any order. As a consequence, Fermi momentum — and so Fermi surface — can not be defined, nevertheless the Fermi energy is well defined. This is not valid for a usual Fermi liquid.

In case of $n = 3/4$ filling we found two kinds of solution. In the first case the electrons are immovable, each particle is localized to a site. The many-particle state vector is a product of uncorrelated localized three-particle states. The expectation values of every individual non-on-site term of the Hamiltonian are zero. Therefore this solution represents a Mott insulator phase. In spite of this, in the second case the many-particle state can not be built up from localized few-electron states; the Hamiltonian terms which are related to the moving of the electrons are strictly negative, i.e. the system preserves some electron motion to decrease the ground state energy. In this case the system is in a metal-like state. Take into account that the momentum distribution function is continuous, we can state that the system is in a non-Fermi liquid normal phase.

In our case the absence of the Fermi momentum is due to a flat-band feature in the following sense. Consider a model Hamiltonian $\hat{H}$ for which our solution is valid, i.e. $U > 0$ and the equations (4.15) have solution for $a_{\boldsymbol{\delta},b}$. The non-interacting Hamiltonian $\hat{H}_0$ defined by equation (4.1) describes a usual Fermi gas, but the formally non-interacting Hamiltonian $\hat{H}_{\mathit{eff}} = \hat{H}_0 + U\hat{N}_f$ describes a two band system of which upper band is completely flat. The Fig.(4.1) shows the relation of the Hamiltonians $\hat{H}$, $\hat{H}_0$ and $\hat{H}_{\mathit{eff}}$ in the (U, E_f) plane of the parameter space.

Starting from the parameter point of $\hat{H}_0$ and increasing the value of E_f through usual non-interacting Fermi systems we reach a special and somehow pathological parameter point of $\hat{H}_{\mathit{eff}}$. In spite of the usual non-interacting Fermi systems the ground state of $\hat{H}_{\mathit{eff}}$ is highly degenerated (when $n > 2$) due to the flat upper band. In ground states the lower band is completely filled, but the remaining $N - 2N_\Lambda$ electrons can be situated in $\binom{2N_\Lambda}{N-2N_\Lambda}$ different manner, because every momentum state with arbitrary spin has the same energy in the upper band. When the interaction is switching on and the model is modified along the solid line this degeneracy is splitting. The degeneracy becomes less, the ground states of the interacting system represent a negligible fraction of the ground state subspace of $\hat{H}_{\mathit{eff}}$, at least when $3 \lesssim n$. It is a qualitative changing. If we want to describe it by perturbation theory, we should use the technique valid in degenerated case. In our case it leads to a diagonalization of a matrix, which is as large as the degeneracy of the non-interacting ground state, and it is practically impossible. However, in the $n > 3$ case, — and this is the non-trivial feature of this model which makes possible the exact solution — there are $2^{4N_\Lambda - N}\binom{N_\Lambda}{N-3N_\Lambda}$ common ground state eigenvectors of $\hat{P}$ and $\hat{P}'$. These are the ground states of the interacting system. As we have written in Section 2.4 the non-interacting term of the Hamiltonian and the operator of the interaction do not commute with each other, therefore to find the spectrum and even the ground state of their sum is a highly nontrivial problem. In the

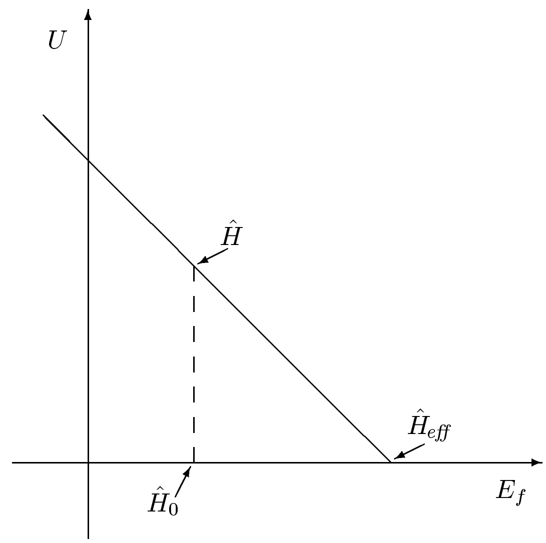

Figure 4.1: The (U, E_f) plane of the phase diagram. Our solution is valid on the half-line which starts from the $U = 0$, $E_f = \sum_{\boldsymbol{\delta}}(|a_{\boldsymbol{\delta},c}|^2 - |a_{\boldsymbol{\delta},f}|^2)$ point (this point is not contained by the half-line, yet) and crosses the U axis at the $U = \sum_{\boldsymbol{\delta}}(|a_{\boldsymbol{\delta},c}|^2 - |a_{\boldsymbol{\delta},f}|^2)$ point. The other parameters satisfy the requirement that the equations (4.15) have to be solvable.

special case presented in this Chapter, however, detaching a one-particle operator from the interaction and attaching it to the non-interacting term we get two terms of which have common ground states. Nevertheless the whole spectrum of the sum of these terms is complicated, the ground states can be given due to the flat band feature of the modified non-interacting term $\hat{H}_{\mathit{eff}}$.

The question may occur to somebody that what is the physical importance of a solution which is valid in a pathological point in the parameter space. Therefore important to emphasize the followings. First of all, this solution is valid in a wide range of the parameter space from small to large Hubbard U. Certainly there is a restriction among the parameters, but what remains is a hyper-surface in the parameter space, and not only a point at all. Furthermore, the non-Fermi liquid behaviour is always something special. The circumstances under which a system shows non-Fermi liquid features are well-determined. Changing the chemical compound or the pressure a little, the system returns to the normal Fermi liquid behaviour. As often said, the non-Fermi liquid behaviour is not "robust".

Chapter 5

Infinitely repulsive Hubbard model near half filling

The physics of holes moving in a background build up from a great number of electrons have received much attention in the last decade given by the connection of the problem with main questions arising from the study of strongly correlated systems [102]. Developments in several fields emphasize this aspect: the behaviour of holes in antiferromagnetic background [103], metal–insulator transition [104], doping effects [105], ferromagnetism [85], high-T_c superconductivity [106], colossal magnetoresistance [107], spiral states [108], generalized statistics [109, 110], pairing mechanism and bound states [38] and polaronic effects [111] are the main examples to be mentioned. From theoretical side the Hubbard-type models are especially involved in the theoretical description starting from the one-hole problem discussed by Nagaoka [32, 33], which has been continued with two-holes studies [30, 36, 37], and many-hole analysis in various configurations and circumstances [112, 31, 113, 39]. Despite the huge intellectual effort spent in the field, exact results related to the above mentioned problem are extremely rare [112] and concern mainly non-thermodynamic situations. However, in the above enumerated concrete applications mostly thermodynamic description is needed mainly in strong-coupling limit. These situations have been treated in the literature on the basis of various approximations (acceptable in restricted conditions) such as complete separation of charge and spin degrees of freedom [37], extended Gutzwiller wave functions [114], canonical transformations [115], generalization of one-dimensional results to higher dimensions [31], restriction related to the number of holes [113], unrestricted Hartree-Fock methods [105] or numerical procedures such as exact diagonalization of small clusters [116] and diagonalization within a retained portion of the Hilbert space [106]. There have also been studies on specific problems such as ferromagnetism [117].

Against the background of the above mentioned large spectrum of description attempts, we are presenting an interesting aspect of the hole-motion in the simple one-band Hubbard model in the limit of an infinitely large on-site repulsion U. For this reason first of all we have deduced and presented an exact and explicit Schrödinger equation for an arbitrary number of holes in the analyzed model. This equation clearly emphasizes the role played by the charge and spin degrees of freedom during the movement of the holes in the $U = \infty$ Hubbard model, being mathematically based on the representations of the symmetric group of degree N, where N represents the number of electrons within the system. The advantages of the description presented are emphasized by the observations that firstly, the emerging matrix elements can be found (or deduced in case of larger systems) from standard textbooks of the group theory and, secondly, the analysis reduced the concrete equation to be solved in subspaces fixed by a given but arbitrary total system spin S of the initial large Hilbert space, allowing comfortable numerical applications.

Our results clearly demonstrate that in the infinitely repulsive Hubbard model the movement of holes is intimately influenced by the spin-background of the electrons. As a consequence, in describing this process in the general case, the charge and spin degrees of freedom cannot be entirely separated. Within the frame of the presented formalism the Nagaoka mechanism of ferromagnetism becomes clear, and the reason why it cannot survive the generalization for more than one hole.

After this step we next study the $T \neq 0$ properties of the system by showing how the presented formalism helps us to deduce of the partition function Z and some physical quantities based on a loop summation (i.e. path integral on lattice) technique. Resembling technique was used in Refs. [118, 119]. The presented formulae have the advantage that the trace over the spin degrees of freedom has been taken exactly into account in terms of the characters of the representations of the symmetric group (again accessible from standard text-books on group theory). The emerging coefficients in our formulae can be reduced to coefficients obtainable from numerical methods. The procedure is described in detail which is able even to increase the efficiency of the usual Monte Carlo simulation methods.

In Ref. [119] the author have analyzed the magnetic behaviour of the system in thermodynamic limit. However, his result is valid in thermodynamic limit, only in the case $N_h/N_\Lambda \to 0$ where N_h denotes the number of holes, and not for finite hole concentration and $T \to 0$. With the purpose of enhancing the study of magnetic properties in the presence of a small hole concentration even at arbitrary finite temperatures, in this Chapter we investigate the behaviour of a small system with finite hole concentration, using Monte Carlo method at $T \neq 0$. The studied system is a 10×10 lattice with periodic boundary conditions containing two holes. The results show an increase of the magnetisation with the decrease of the temperature.

5.1 Representation of the Hilbert space and the Hamiltonian

Our Hamiltonian describes the one-band Hubbard model containing only nearest-neighbour hopping in $U = \infty$ limit:

$$\hat{H}_{\infty} = \sum_{\langle \mathbf{i},\mathbf{j} \rangle} t \hat{H}^{\mathbf{i},\mathbf{j}}_{\infty} = \sum_{\langle \mathbf{i},\mathbf{j} \rangle} t \hat{P} \sum_{\sigma} (\hat{c}^{\dagger}_{\mathbf{i},\sigma} \hat{c}_{\mathbf{j},\sigma} + \hat{c}^{\dagger}_{\mathbf{j},\sigma} \hat{c}_{\mathbf{i},\sigma}) \hat{P}, \tag{5.1}$$

where t is hopping matrix element for nearest neighbour sites. The double occupancy is projected out by $\hat{P} = \sum_{\mathbf{i}} (1 - \hat{n}_{\mathbf{i},\uparrow} \hat{n}_{\mathbf{i},\downarrow})$. We denote the number of electrons by N, so the number of holes becomes $N_h = N_{\Lambda} - N$. Furthermore, we need permutations, therefore we fix some notations about them in Appendix B. Here we notice only that the group of permutations of Λ is denoted by S_{Λ}, and the group of permutations of the set $\{\mathbf{1}, \ldots, \mathbf{N}\}$ is denoted shortly by $S_{\mathbf{N}}$ instead of $S_{\{\mathbf{1},\ldots,\mathbf{N}\}}$. In this Chapter $\mathfrak{H}_N$ denotes the subspace of the Hilbert space of N electrons with no doubly occupied site. The subspace of $\mathfrak{H}_N$ which is also eigensubspace of the operator $\hat{S}^z$ with eigenvalue S^z is denoted by $\mathfrak{H}_N(S^z)$, finally, when the total spin S is also a good quantum number, the subspace is denoted by $\mathfrak{H}_N(S^z, S)$.

5.1.1 The Hilbert space of the studied system

In our model the electrons can live only on lattice sites in two orthogonal states: spin up and down. Because of the kinetic energy term, an electron hops from one site to an other (while its spin state remains unchanged), changing, however, the locations of the empty and occupied sites. Hereafter, we call the fix positions of the occupied sites the charge configuration, which does not give an account the electronic spin states, only their places. We denote the set of occupied sites, which describes a particular charge configuration, by Λ_e, where $\Lambda_e \subset \Lambda$ and $|\Lambda_e| = N$. Iterating the action of the hopping term on a state several times, hopping around the lattice electrons produce different charge configurations; in particular they can produce the original configuration again. However, the spin up and spin down electrons are commingled; therefore the spin configuration can be different from that in the original state. We mean, that a spin configuration is described by the fact that which sites are occupied by spin up and which by spin down electrons. The spin configuration can be described by $\{\sigma_{\mathbf{i}}\}$. The state vectors

$$|\psi(\Lambda_e, \{\sigma_{\mathbf{i}}\})\rangle = \prod_{\mathbf{i} \in \Lambda_e} \hat{c}^{\dagger}_{\mathbf{i},\sigma_{\mathbf{i}}} \,|\, 0 \,\rangle \tag{5.2}$$

form a basis in $\mathfrak{H}_N$.

We would like to treat separately the spin and charge degrees of freedom, and to formulate it in our notations. However, above we denote the spin configuration by $\{\sigma_{\mathbf{i}}\}$, where the domain of the index $\mathbf{i}$ — which is Λ_e — depends on the charge configuration. To avoid this technical difficulty we introduce a bijective function $\mathcal{R} : \Lambda \to \Lambda$ which rearrange the label of sites in the following manner. By definition, the image of the set Λ_e by the map $\mathcal{R}$ is $\{\mathbf{1}, \ldots, \mathbf{N}\}$, and this map preserves the order.[1] The image of $\Lambda \backslash \Lambda_e$ (i.e. the indices of holes) is certainly $\{\mathbf{N}+\mathbf{1}, \ldots, \mathbf{N}_\Lambda\}$. Here the order is not important. Instead of Λ_e, hereafter we describe the charge configuration by $\tilde{\mathcal{R}}$ which is the collection (i.e. a set) of the possible functions $\mathcal{R}$ for a given Λ_e, differ from each other in the order of the indices of holes. The composition of $\tilde{\mathcal{R}}$ with a function $\mathcal{P}$ defined as $\mathcal{P}\tilde{\mathcal{R}} := \{\mathcal{P}\mathcal{R} : \mathcal{R} \in \tilde{\mathcal{R}}\}$ and similarly $\tilde{\mathcal{R}}^{-1} := \{\mathcal{R}^{-1} : \mathcal{R} \in \tilde{\mathcal{R}}\}$. In the followings when we refer to $\tilde{\mathcal{R}}(\mathbf{i})$ ($\mathbf{i} \in \Lambda_e$) we treat $\tilde{\mathcal{R}}$ through a representative $\mathcal{R}$, that is $\tilde{\mathcal{R}}(\mathbf{i}) := \mathcal{R}(\mathbf{i})$, $\mathcal{R} \in \tilde{\mathcal{R}}$. For $\mathbf{i} \in \Lambda_e$ it is well-defined, therefore none of our results depend on the choice of that representative.

Fixing a charge configuration, the spin configuration can be described by an ordered set of the up- and down-spin states: $(\sigma_{\mathbf{i}})_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}}$, where $\sigma_{\mathbf{i}} \in \{\uparrow, \downarrow\}$ indicates the spin state of the electron situated in the $\mathbf{i}$-*th occupied* lattice site, which was labelled by $\tilde{\mathcal{R}}^{-1}(\mathbf{i})$ originally. (Here we notice again, that $\tilde{\mathcal{R}}^{-1}(\mathbf{i})$ is well-defined for $\mathbf{i} \leq \mathbf{N}$). In this way, fixing the third component of the total spin S^z, every spin configuration can be obtained by a permutation from the following basic arrangement: $(\sigma^0(\mathbf{i}))_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}} = (\uparrow, \uparrow, \ldots, \uparrow, \downarrow, \downarrow, \ldots, \downarrow)$, where $\sigma^0(\mathbf{i}) = \uparrow$ if $\mathbf{i} = \mathbf{1}, \ldots, \mathbf{N}_\uparrow$ and $\sigma^0(\mathbf{i}) = \downarrow$ if $\mathbf{i} = \mathbf{N}_\uparrow + \mathbf{1}, \ldots, \mathbf{N}$. Here we use the notation $N_\uparrow = N/2 + S^z$. After it a spin configuration $(\sigma_{\mathbf{i}})_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}}$ can be described by a permutation $\mathcal{P} \in S_{\mathbf{N}}$ which rearranges the basic arrangement $(\sigma^0(\mathbf{i}))_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}}$ in such a way that $\sigma^0(\mathcal{P}(\mathbf{i})) = \sigma_{\mathbf{i}}$. We emphasize that here $\mathbf{i}$ denotes the $\mathbf{i}$-*th occupied site*. This means that, in a state described by a charge configuration $\tilde{\mathcal{R}}$ and a spin configuration $\mathcal{P}$, the electron situated in the site labelled *originally* by $\mathbf{i}$ is in the spin state $\sigma^0(\mathcal{P}\tilde{\mathcal{R}}(\mathbf{i}))$. More precisely, there is no one-to-one correspondence between the spin configurations and permutations, not even if we fix the value of S^z. A permutation uniquely determines a spin configuration, but the reverse is not true. Let $\mathcal{Q} \in S_{\mathbf{N}}$ be a permutation which rearranges the elements of the subset $(\sigma^0)^{-1}(\uparrow) = \{\mathbf{1}, \ldots, \mathbf{N}_\uparrow\}$, and rearranges the elements of $(\sigma^0)^{-1}(\downarrow) = \{\mathbf{N}_\uparrow + \mathbf{1}, \ldots, \mathbf{N}\}$ but does not interchange the elements of these two subsets. It is clear that for arbitrary permutation $\mathcal{P}$, $\mathcal{P}$ and $\mathcal{Q}\mathcal{P}$ describe the same spin configuration, because $\sigma^0(\mathcal{P}(\mathbf{i})) = \sigma^0(\mathcal{Q}\mathcal{P}(\mathbf{i}))$ for all $\mathbf{i} \leq \mathbf{N}$. Mathematically this means the following. The above defined permutations $\mathcal{Q}$ form a subgroup $K_{S^z} \subset S_{\mathbf{N}}$, and a right coset $\bar{\mathcal{P}}_{S^z} := \{\mathcal{Q}\mathcal{P} : \mathcal{Q} \in K_{S^z}\}$ is in one-to-one correspondence with a spin configuration. Furthermore, we have the possibility to define $\sigma^0(\bar{\mathcal{P}}_{S^z}(\mathbf{i})) := \sigma^0(\mathcal{P}(\mathbf{i}))$, where $\mathcal{P} \in \bar{\mathcal{P}}_{S^z}$ is arbitrary. Therefore we can label the basis vectors from equation (5.2) by $\tilde{\mathcal{R}}$ and $\bar{\mathcal{P}}_{S^z}$ as follows:

$$|\psi(\tilde{\mathcal{R}}, \bar{\mathcal{P}}_{S^z})\rangle = \prod_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}} \hat{c}^\dagger_{\tilde{\mathcal{R}}^{-1}(\mathbf{i}), \sigma^0(\bar{\mathcal{P}}_{S^z}(\mathbf{i}))} |0\rangle. \tag{5.3}$$

[1] Remember that Λ is an ordered set. (About this convention and the notations by boldface numbers see pg. 8.)

We mention that the sign of the right hand side is fixed by the order of the fermionic creation operators, which is determined by the fact that the map $\mathcal{R}$ restricted to Λ_e, which is a well-defined function, preserves the order of the ordered set Λ.

The above can be formulated in the following manner, too. The Hilbert space of the studied system is isomorphic with a product of two spaces: $\mathfrak{H}_N \cong \mathfrak{H}_c \otimes \mathfrak{H}_s$, where $\mathfrak{H}_c$ describes the charge degrees of freedom and $\mathfrak{H}_s$ describes the spin degrees of freedom. A basis of $\mathfrak{H}_c$ can be labelled by the different charge configurations which were denoted by $\tilde{\mathcal{R}}$, therefore we denote a basis vector of $\mathfrak{H}_c$ by $|\tilde{\mathcal{R}}\rangle$; thus $\mathfrak{H}_c$ is the complex Hilbert space generated by these elements as an orthonormal basis. We mention that $\mathfrak{H}_c$ represents in fact a Hilbert space of a system of hard-core spinless particles. We take into account the spin degrees of freedom by $\mathfrak{H}_s$. This space can be written as a direct sum of the spaces $\mathfrak{H}_s(S^z)$, that is, $\mathfrak{H}_s = \mathfrak{H}_s(-N/2) \oplus \ldots \oplus \mathfrak{H}_s(N/2)$; where $\mathfrak{H}_s(S^z)$ is generated by the vectors $|\bar{\mathcal{P}}_{S^z}\rangle$ as an orthonormal basis. Here $\bar{\mathcal{P}}_{S^z}$ is a right coset of $S_{\mathbf{N}}$ respect to the subgroup K_{S^z}. The spaces $\mathfrak{H}_s(S^z)$ are isomorphic with right ideals of the group algebra $\mathbb{C}[S_{\mathbf{N}}]$ (for more details see Appendix B). On this line the basis vectors defined by the usual creation operators in equation (5.3) can be written as

$$|\psi(\tilde{\mathcal{R}}, \bar{\mathcal{P}}_{S^z})\rangle = |\tilde{\mathcal{R}}\rangle \otimes |\bar{\mathcal{P}}_{S^z}\rangle. \tag{5.4}$$

Using this representation of the Hilbert space now we write down the Hamiltonian.

5.1.2 The Hamiltonian and Schrödinger equation

Now we study the change in a state vector from equation(5.3) during the motion of the particles. Let the starting state be $|\tilde{\mathcal{R}}\rangle \otimes |\bar{\mathcal{P}}_{S^z}\rangle$. When an electron hops from site $\mathbf{i}$ to $\mathbf{j}$, then the site $\mathbf{i}$ occupied earlier by an electron with spin $\sigma_{\mathbf{i}}$ becomes empty, and the site $\mathbf{j}$ which was empty earlier becomes occupied by an electron with spin $\sigma_{\mathbf{i}}$, because the spin of the electron remains unchanged during the hopping. The new charge configuration could be described by $\tilde{\mathcal{R}}\mathcal{P}^{\mathbf{i},\mathbf{j}}$ because the image of the set Λ_e' by $\tilde{\mathcal{R}}\mathcal{P}^{\mathbf{i},\mathbf{j}}$ is the set $\{\mathbf{1}, \ldots, \mathbf{N}\}$, and the image of $\Lambda \backslash \Lambda_e$ is $\{\mathbf{N}+\mathbf{1}, \ldots, \mathbf{N}_\Lambda\}$. Here we denoted by Λ_e' the set of the occupied sites after the hopping. But the map $\tilde{\mathcal{R}}\mathcal{P}^{\mathbf{i},\mathbf{j}}$ does not preserve the order of the labels of occupied sites sufficiently, therefore we need a permutation $\mathcal{C}(\tilde{\mathcal{R}}; \mathbf{i}, \mathbf{j})$ to write the new charge configuration as $\tilde{\mathcal{R}}' = \mathcal{C}(\tilde{\mathcal{R}}; \mathbf{i}, \mathbf{j})\tilde{\mathcal{R}}\mathcal{P}^{\mathbf{i},\mathbf{j}}$ which restricted to Λ_e' is already an order-preserving map. The permutation $\mathcal{C}(\tilde{\mathcal{R}}; \mathbf{i}, \mathbf{j})$ means in fact that in the expression (5.3) of the basis vectors we rearrange the creation operators which involves a sign $(-1)^{|\mathcal{C}(\tilde{\mathcal{R}}; \mathbf{i}, \mathbf{j})|}$. The permutation $\mathcal{C}(\tilde{\mathcal{R}}; \mathbf{i}, \mathbf{j})$ is an element of S_Λ but it rearranges only the first labels from $\mathbf{1}$ to $\mathbf{N}$, therefore it can be considered as an element of $S_{\mathbf{N}}$. In the notation I want to emphasize that this permutation depends on the starting configuration $\tilde{\mathcal{R}}$ too, not only on the bond $\langle \mathbf{i},\mathbf{j}\rangle$ along which the electron hops, and these two facts determine it uniquely.[2] Since the spin state of the electron remains unchanged during the hopping, the electron situated after the hopping in site $\mathbf{j} = \mathcal{P}^{\mathbf{i},\mathbf{j}}(\mathbf{i})$ is in the spin state $\sigma'_{\mathbf{j}} = \sigma_{\mathbf{i}} = \sigma^0(\bar{\mathcal{P}}_{S^z}\tilde{\mathcal{R}}(\mathbf{i})) = \sigma^0(\bar{\mathcal{P}}_{S^z}\tilde{\mathcal{R}}\mathcal{P}^{\mathbf{i},\mathbf{j}}(\mathbf{j}))$. The charge configuration after the hopping is $\tilde{\mathcal{R}}'$ as we have written above. To recognize the final spin state $\bar{\mathcal{P}}'_{S^z}$ we have to write the final spin state of the electron situated in site $\mathbf{j}$ as $\sigma'_{\mathbf{j}} = \sigma^0(\bar{\mathcal{P}}'_{S^z}\tilde{\mathcal{R}}'(\mathbf{j}))$, while the spin states of the electrons in the other sites $\mathbf{n}$, where $\mathbf{n} \in \Lambda_e \cup \Lambda'_e$, remains unchanged, i.e. $\sigma_{\mathbf{n}} = \sigma^0(\bar{\mathcal{P}}_{S^z}\tilde{\mathcal{R}}(\mathbf{n})) = \sigma^0(\bar{\mathcal{P}}'_{S^z}\tilde{\mathcal{R}}'(\mathbf{n})) = \sigma'_{\mathbf{n}}$. As a consequence, we have $\bar{\mathcal{P}}'_{S^z} = \bar{\mathcal{P}}_{S^z}[\mathcal{C}(\tilde{\mathcal{R}};\mathbf{i},\mathbf{j})]^{-1}$, and we find that while an electron hops from site $\mathbf{i}$ to $\mathbf{j}$ the initial state $|\tilde{\mathcal{R}}\rangle \otimes |\bar{\mathcal{P}}_{S^z}\rangle$ changing as follows:

$$\begin{aligned}\hat{H}^{\mathbf{i},\mathbf{j}}_{\infty}(|\tilde{\mathcal{R}}\rangle \otimes |\bar{\mathcal{P}}_{S^z}\rangle) &= |\tilde{\mathcal{R}}'\rangle \otimes |\bar{\mathcal{P}}'_{S^z}\rangle \\ &= |\,\mathcal{C}(\tilde{\mathcal{R}};\mathbf{i},\mathbf{j})\,\tilde{\mathcal{R}}\,\mathcal{P}^{\mathbf{i},\mathbf{j}}\,\rangle \otimes (-1)^{|\mathcal{C}(\tilde{\mathcal{R}};\mathbf{i},\mathbf{j})|}\,|\,\bar{\mathcal{P}}_{S^z}[\mathcal{C}(\tilde{\mathcal{R}};\mathbf{i},\mathbf{j})]^{-1}\rangle. \quad (5.5)\end{aligned}$$

The above expression holds only if the initial vector $|\tilde{\mathcal{R}}\rangle \otimes |\bar{\mathcal{P}}_{S^z}\rangle$ describes a state in which $\mathbf{i}$ is occupied and $\mathbf{j}$ is empty.[3]

The mapping $|\tilde{\mathcal{R}}\rangle \to |\tilde{\mathcal{R}}'\rangle$ is defined on the basis of $\mathfrak{H}_c$. Linearly extended it over the whole space we get a linear operator denoted by $\hat{H}^{\mathbf{i},\mathbf{j}}_{b,\infty}$. The index b refers to the word 'boson', because $\hat{H}_{b,\infty} = \sum_{\langle i,j\rangle} t\hat{H}^{\mathbf{i},\mathbf{j}}_{b,\infty}$ describes a hard-core spinless boson system of N particles (or equivalently N_h holes). In this context it can be said that the holes moving as hard-core bosons influence the spin background. The influence caused by a hopping of a hole along a bond $\langle \mathbf{i},\mathbf{j}\rangle$ is described by a linear operator which is the linear extension of the mapping $|\bar{\mathcal{P}}_{S^z}\rangle \to |\bar{\mathcal{P}}'_{S^z}\rangle$ to the whole $\mathfrak{H}_s(S^z)$. It is actually a linear representation of the symmetric group $S_{\mathbf{N}}$ on $\mathfrak{H}_s(S^z)$ (see Appendix B) hereafter is denoted by $\mathbb{T}^{S^z}$. Finally we write the action of the Hamiltonian (5.1) on the basis vector (5.4) as

$$\hat{H}_{\infty}(|\tilde{\mathcal{R}}\rangle \otimes |\bar{\mathcal{P}}_{S^z}\rangle) = \sum_{\langle \mathbf{i},\mathbf{j}\rangle} t\,\hat{H}^{\mathbf{i},\mathbf{j}}_{b,\infty}|\tilde{\mathcal{R}}\rangle \otimes \mathbb{T}^{S^z}[\mathcal{C}(\tilde{\mathcal{R}};\mathbf{i},\mathbf{j})]\bar{\mathcal{P}}_{S^z} \quad (5.6)$$

First of all we offer some remarks. We emphasize that the Hamiltonian presented in equation (5.1) cannot be written in the product form $\hat{H}_{\infty} \neq \hat{H}_c \otimes \hat{H}_s$ and the action of the Hamiltonian on $\mathfrak{H}_s(S^z)$ depends on the charge configuration $|\tilde{\mathcal{R}}\rangle$.

[2] Supposing that $\mathbf{i}$ is the site from where the electron hops to site $\mathbf{j}$, in fact $\mathcal{C}(\tilde{\mathcal{R}};\mathbf{i},\mathbf{j})$ is the cyclic permutation $\mathcal{C}^{\tilde{\mathcal{R}}(\mathbf{i})\to\tilde{\mathcal{R}}(\mathbf{j}')}$, where, in $\mathbf{j} > \mathbf{i}$ case $\mathbf{j}'$ is the least index among the indices greater than $\mathbf{j}$ for which $\tilde{\mathcal{R}}(\mathbf{j}') \le \mathbf{N}$ and, in $\mathbf{j} < \mathbf{i}$ case, $\mathbf{j}'$ is the greatest index among the indices smaller than $\mathbf{j}$ for which $\tilde{\mathcal{R}}(\mathbf{j}') \le \mathbf{N}$. In other words, $\mathbf{j}'$ labels the *occupied* lattice site whose index is closest to $\mathbf{j}$ among the indices situated between $\mathbf{i}$ and $\mathbf{j}$. By definition, the cyclic permutation $\mathcal{C}^{(\mathbf{k}\to\mathbf{l})}$ takes $\mathbf{m}$ to $\mathbf{m} + sgn(\mathbf{k} - \mathbf{l})$ if $\mathbf{m}$ is in the open interval $]\mathbf{k},\mathbf{l}[$, takes $\mathbf{k}$ to $\mathbf{l}$, and leaves $\mathbf{m}$ unchanged if $\mathbf{m}$ is out of the closed interval $[\mathbf{k},\mathbf{l}]$.

[3] When $\mathbf{j}$ is occupied and $\mathbf{i}$ is empty the equation (5.5) remains true with $\mathcal{C}(\tilde{\mathcal{R}};\mathbf{i},\mathbf{j}) = \mathcal{C}^{\tilde{\mathcal{R}}(\mathbf{j})\to\tilde{\mathcal{R}}(\mathbf{i}')}$. For the meaning of the notation $\mathbf{i}'$ see footnote 2.

In fact we have $\hat{H}^{\mathbf{i},\mathbf{j}}_{\infty} = \hat{H}^{\mathbf{i},\mathbf{j}}_{c} \otimes \hat{H}^{\mathbf{i},\mathbf{j}}_{s}(\tilde{\mathcal{R}})$, therefore the eigenstates of $\hat{H}$ in general case cannot be written in the form $|\varphi_c\rangle \otimes |\varphi_s\rangle$. As a consequence, there is no *a priori* charge spin separation taken into account at the level of the description. However, contrary to the Hamiltonian, the action of total spin operators does not depend on $|\mathcal{R}\rangle$, i.e. they act on $\mathfrak{H}_c$ as the identity operator. This is why the decomposition of the Hilbert space into sectors characterized by a fixed total spin S can be done within the space of the spin degrees of freedom: $\mathfrak{H}_s = \oplus_{S^z}(\oplus_{S=S^z}^{S_{max}} \mathfrak{H}_s(S^z, S))$. With this notation we have $\mathfrak{H}_N(S^z, S) = \mathfrak{H}_c \otimes \mathfrak{H}_s(S^z, S)$.

The subspaces $\mathfrak{H}_s(S^z, S)$ of the space $\mathfrak{H}_s(S^z)$ are invariant subspaces of the representation $\mathbb{T}^{S^z}$. The restriction of this representation to that subspaces is denoted by $\mathbb{T}_S$, which do not depend on S^z. Therefore the action of the Hamiltonian on $\mathfrak{H}_s(S^z, S)$ can be described by $\mathbb{T}_S$. It is the reflection of that simple fact that the Hamiltonian simultaneously commutes with the spin operators $\hat{S}^2$ and $\hat{S}^z$. Let us denote by $(\mathbb{T}_S[\mathcal{P}])_{nm}$ the matrix elements of the operator $\mathbb{T}_S[\mathcal{P}]$ in an orthogonal and normalized basis of $\mathfrak{H}_s(S^z, S)$ with arbitrary S^z, and by $(H^{\mathbf{i},\mathbf{j}}_{b,\infty})_{kl} = \langle \tilde{\mathcal{R}}_k | \hat{H}^{\mathbf{i},\mathbf{j}}_{b,\infty} | \tilde{\mathcal{R}}_l \rangle$ where $\tilde{\mathcal{R}}_k, \tilde{\mathcal{R}}_l \in \{| \tilde{\mathcal{R}}_i\rangle\}_{i=1}^{\binom{N_\Lambda}{N}}$ are the above defined basis vectors in $\mathfrak{H}_c$ indexed by integers. Now the Schrödinger equation becomes

$$\sum_{l,m} \alpha_{lm} \sum_{\langle \mathbf{i},\mathbf{j}\rangle} t(H^{\mathbf{i},\mathbf{j}}_{b,\infty})_{kl} (\mathbb{T}_S[\mathcal{C}(\tilde{\mathcal{R}}_l; \mathbf{i}, \mathbf{j})])_{nm} = E\alpha_{kn}. \tag{5.7}$$

Equation (5.7) gives the energy eigenvalues E connected to the eigenstates with given total spin S.

Equation (5.7) shows explicitly the role played by the total spin S in the Schrödinger equation. For example in the case when $S = S_{max}$, the representation $\mathbb{T}_{S_{max}}$ is the alternating representation. In this case the dimension of $\mathfrak{H}_s(S^z, S_{max})$ is 1, and the matrix representing every even permutation is 1 and every odd permutation is -1. For this reason, hard-core fermions with maximal spin do not differ from spinless fermions (see also Ref. [109, 110]). The on-site interaction has no effect on spinless fermions, therefore there is no difference between the behaviour of hard-core and free particles in this case.

Another simple example is the one-dimensional case with open boundary conditions. Numbering the sites of the chain in order one after another, the form of every nearest neighbour pair is simply $\langle \mathbf{i}, \mathbf{i}+\mathbf{1}\rangle$ in this case, and we have $\mathcal{C}(\tilde{\mathcal{R}}; \mathbf{i}, \mathbf{i}+\mathbf{1}) = 1 \in S_{\mathbf{N}}$ whose matrix is the unity matrix for arbitrary representation. Therefore there is no difference between the behaviour of hard-core bosons and fermions; so the energy spectrum is independent of the spin and the statistics of the particles, only every energy eigenvalue is $(2S+1)^N$-fold degenerate, S being the spin of the particles. We notice here also that in case of closed chain the occurring additional possibility that a particle can hop from site $\mathbf{1}$ to $\mathbf{N}$ (or vice versa) involves the permutation $\mathcal{C}(\tilde{\mathcal{R}}; \mathbf{1}, \mathbf{N}_\Lambda) = \mathcal{C}^{\mathbf{N}\to\mathbf{1}}$ (or $\mathcal{C}^{\mathbf{1}\to\mathbf{N}}$) which is odd when N is even and even when N is odd. Therefore using periodic boundary condition in the case when

N is odd, or antiperiodic boundary condition when N is even, the sign from the fermionic feature of the particles are compensated by the boundary condition, and thus the statistics does not play any role. The fermions behave as bosons in a ring (with periodic boundary condition).

If $D > 1$ and $S^z \neq S_{max}$, then the action of the Hamiltonian on the spin background is highly non-trivial and influences the mobility and interaction of holes. This type of situation was analyzed by a numerical technique by Trugman [106]. He showed that, on a Néel-type antiferromagnetic background, one hole is mobile but two holes are less mobile than was previously considered. In the language presented here this is due in fact to the permutation possibilities of spin positions with mobile hole positions. Trugman's results emphasized as well that the action of the Hamiltonian is clearly seen also on the spin background, which cannot be treated entirely separated from the movement of the holes within the system.

We note that the Schrödinger equation (5.7) essentially differs from Kuzmin's equation [37] for the purpose to solve the two-hole problem on singlet background. In the mentioned reference the Schrödinger equation has been solved supposing implicitly that the Hamiltonian has no action on the spin degrees of freedom, i.e. spin background. This explains why Kuzmin obtains the result that on bipartite lattices the Nagaoka state (the fully polarized ferromagnetic state) is degenerated with the singlet state even in the one-hole case, in contradiction to Nagaoka's original result [32]. In the one-hole case the spectrum given by Kuzmin is really related to a hard-core spinless boson system spectrum, instead of the singlet spectrum of an electron system as Kuzmin said. This spectrum is equivalent to the spectrum of a spinless fermion system. The latter is equivalent to the S_{max} spectrum of our original electron system as presented above. The first equivalence is due to the fact that — in case of bipartite lattice — for hard-core spinless particles (both bosons and fermions), the N-hole problem is equivalent to the N-particle problem, and in the one-particle case the statistics is unimportant. For more than one hole, it is not the same whether we deal with bosons or fermions even for the hard-core interaction. The ground-state energy of the bosons is always smaller [110]. In order to exemplify the above, we mention that the equality presented by Kuzmin, namely

$$0 = \sum_k \frac{1}{E - (\epsilon_k + \epsilon_{P-k})}, \tag{5.8}$$

gives the spectrum of a spinless hard-core boson system consisting of two particles (or equivalently two holes). Here ϵ_k is the one-particle dispersion relation and P is the total momentum of the system. For the ground-state energy of the simplest non-trivial two-dimensional case, the 2×3 lattice with periodic boundary conditions, for $t < 0$ equation (5.8) gives $E_0 = -6.6468|t|$ while from equation (5.7) one finds $E_0 = -6|t|$ which is connected to the $S = S_{max} = 2$ value of the total spin, and $E_{min}^{S=0} = -5.0212|t|$ is the lowest energy value on singlet background. Furthermore we note that in the two-particle case the spectrum of the hard-core spinless boson system is identical with the spin 1/2 fermion system's singlet spectrum, therefore it can be computed using equation (5.8). However, as presented here, in the $S \neq S_{max}$ case the behaviour of the system described by equation (5.1) cannot be described by hard-core particles and independent spin degrees of freedom. This is the reason why the N-particle and the N-hole problems are not generally equivalent, and the behaviour of a few holes is more complicated than the behaviour of a few particles.

5.2 Thermodynamic quantities

An asset of the representation presented in equation (5.6) is that the trace of $(\hat{H}_\infty)^l$ over the spin degrees of freedom can be computed with this relation exactly. This allows us to calculate the expectation values at $T \neq 0$ of different thermodynamic quantities. The procedure is presented as follows.

If we are interested in the magnetic properties of the model (5.1), we may express for example the expectation value of the square of the total spin. We have

$$\langle \hat{S}^2 \rangle = \frac{1}{Z} \operatorname{Tr} \left(\hat{S}^2 e^{-\frac{\hat{H}_\infty}{kT}} \right) = \frac{1}{Z} \sum_S S(S+1) \sum_{S^z=-S}^{S} \operatorname*{Tr}_{\mathfrak{H}_N(S^z,S)} e^{-\frac{\hat{H}_\infty}{kT}}$$
$$= \frac{1}{Z} \sum_{S^z=-\frac{N}{2}}^{\frac{N}{2}} 3(S^z)^2 \operatorname*{Tr}_{\mathfrak{H}_N(S^z)} e^{-\frac{\hat{H}_\infty}{kT}}, \tag{5.9}$$

where the partition function is given by

$$Z = \operatorname{Tr} e^{-\frac{\hat{H}_\infty}{kT}} = \sum_{S^z=-\frac{N}{2}}^{\frac{N}{2}} \operatorname*{Tr}_{\mathfrak{H}_N(S^z)} e^{-\frac{\hat{H}_\infty}{kT}}. \tag{5.10}$$

In equation (5.9) we used the fact that $\operatorname{Tr}_{\mathfrak{H}_N(S^z,S)} e^{-\frac{\hat{H}_\infty}{kT}}$ does not depend on S^z due to the SU(2) symmetry. The underscript of Tr means that the trace should be taken only over the indicated subspace.

For finite lattices the Tr operation means a finite sum which can be interchanged with the sum arising from the series expansion of the exponential function. This trace can be computed in the basis defined by equation (5.3) starting from equations (5.6). We have

$$\operatorname*{Tr}_{\mathfrak{H}_N(S^z)} e^{-\frac{\hat{H}_\infty}{kT}} = \sum_{l=0}^{\infty} \frac{1}{l!} \left(\frac{-t}{kT} \right)^l \times$$
$$\sum_{|\bar{\mathcal{P}}_{S^z}\rangle} \sum_{|\tilde{\mathcal{R}}\rangle} \sum_{|\tilde{\mathcal{R}}_1\rangle} \cdots \sum_{|\tilde{\mathcal{R}}_{l-1}\rangle} \sum_{\langle \mathbf{i}_1, \mathbf{j}_1 \rangle} \cdots \sum_{\langle \mathbf{i}_l, \mathbf{j}_l \rangle} \langle \tilde{\mathcal{R}} | \hat{H}_{b,\infty}^{\mathbf{i}_l,\mathbf{j}_l} | \tilde{\mathcal{R}}_{l-1} \rangle \ldots \langle \tilde{\mathcal{R}}_1 | \hat{H}_{b,\infty}^{\mathbf{i}_1,\mathbf{j}_1} | \tilde{\mathcal{R}} \rangle \times$$
$$\langle \bar{\mathcal{P}}_{S^z} | \mathbb{T}^{S^z} [\mathcal{C}(\tilde{\mathcal{R}}_{l-1}; \mathbf{i}_l, \mathbf{j}_l)] \ldots \mathbb{T}^{S^z} [\mathcal{C}(\tilde{\mathcal{R}}_1; \mathbf{i}_2, \mathbf{j}_2)] \mathbb{T}^{S^z} [\mathcal{C}(\tilde{\mathcal{R}}; \mathbf{i}_1, \mathbf{j}_1)] | \bar{\mathcal{P}}_{S^z} \rangle. \tag{5.11}$$

Hereafter let us denote by γ a sequence of charge configurations $\tilde{\mathcal{R}}$, i.e., $\gamma \equiv (\gamma(0), \gamma(1), \ldots, \gamma(l-1), \gamma(l)) = (\tilde{\mathcal{R}}, \tilde{\mathcal{R}}_1, \ldots, \tilde{\mathcal{R}}_{l-1}, \mathcal{R})$, for which $\gamma(l) = \gamma(0)$ and $\prod_{i=1}^{l} \langle \gamma(i) | \hat{H}_{b,\infty} | \gamma(i-1) \rangle \neq 0$. We call l the length of γ. The set of all the γ of length l of which starting (and so also the end) point is $\tilde{\mathcal{R}}$ will be denoted by $\Omega_{\tilde{\mathcal{R}}}(l)$.[4]

In the case when $\sum_{\langle \mathbf{i},\mathbf{j} \rangle} \langle \tilde{\mathcal{R}}' | \hat{H}^{\mathbf{i},\mathbf{j}}_{b,\infty} | \tilde{\mathcal{R}} \rangle \neq 0$ there is precisely one nearest-neighbour pair $\langle \mathbf{i}, \mathbf{j} \rangle$ for which $\langle \tilde{\mathcal{R}}' | \hat{H}^{\mathbf{i},\mathbf{j}}_{b,\infty} | \tilde{\mathcal{R}} \rangle \neq 0$. Therefore the loop γ uniquely determines a sequence of pairs of nearest-neighbour indices $\langle \mathbf{i}_1, \mathbf{j}_1 \rangle, \ldots, \langle \mathbf{i}_l, \mathbf{j}_l \rangle$ which gives the only one non-zero contribution of the sums $\sum_{\langle \mathbf{i}_1, \mathbf{j}_1 \rangle} \cdots \sum_{\langle \mathbf{i}_l, \mathbf{j}_l \rangle}$ in equation (5.11). Denoting the product of permutations $\mathcal{C}(\tilde{\mathcal{R}}; \mathbf{i}, \mathbf{j})$ obtained from this non-zero term by $\mathcal{P}_\gamma$, i.e. $\mathcal{P}_\gamma = \mathcal{C}(\tilde{\mathcal{R}}_{l-1}; \mathbf{i}_l, \mathbf{j}_l) \ldots \mathcal{C}(\tilde{\mathcal{R}}_1; \mathbf{i}_2, \mathbf{j}_2) \mathcal{C}(\tilde{\mathcal{R}}; \mathbf{i}_1, \mathbf{j}_1)$, we have

$$\begin{aligned} \operatorname*{Tr}_{\mathfrak{H}_N(S^z)} e^{-\frac{\hat{H}_\infty}{kT}} &= \sum_{l=0}^{\infty} \frac{1}{l!} \left(\frac{-t}{kT} \right)^l \sum_{\tilde{\mathcal{R}}} \sum_{\gamma \in \Omega_{\tilde{\mathcal{R}}}(l)} \sum_{|\bar{\mathcal{P}}_{S^z}\rangle} \langle \bar{\mathcal{P}}_{S^z} | \mathbb{T}^{S^z} [\mathcal{P}_\gamma] | \bar{\mathcal{P}}_{S^z} \rangle \\ &= \sum_{l=0}^{\infty} \frac{1}{l!} \left(\frac{-t}{kT} \right)^l \sum_{\tilde{\mathcal{R}}} \sum_{\gamma \in \Omega_{\tilde{\mathcal{R}}}(l)} \chi^{S^z}(\mathcal{P}_\gamma), \end{aligned} \tag{5.12}$$

where χ^{S^z} is the character of the representation $\mathbb{T}_{S^z}$.

By definition, $\mathcal{P}_\gamma$ is the permutation for which $\mathcal{P}_\gamma \tilde{\mathcal{R}} \mathcal{P}^{\mathbf{i}_1,\mathbf{j}_1} \ldots \mathcal{P}^{\mathbf{i}_l,\mathbf{j}_l} = \tilde{\mathcal{R}}$. This is due to the fact that the starting charge configuration, (i.e. the right hand side) and the final charge configuration (i.e. the left hand side) are the same, because the loop is closed. It implies that $\mathcal{P}_\gamma = \tilde{\mathcal{R}} \mathcal{P}^{\mathbf{i}_l,\mathbf{j}_l} \ldots \mathcal{P}^{\mathbf{i}_1,\mathbf{j}_1} \tilde{\mathcal{R}}^{-1}$, which means that $\mathcal{P}_\gamma$ and $\mathcal{P}^{\mathbf{i}_l,\mathbf{j}_l} \ldots \mathcal{P}^{\mathbf{i}_1,\mathbf{j}_1}$ are in the same conjugate class C. Every character is constant on an arbitrary conjugate class. Therefore the sum over $\Omega_{\tilde{\mathcal{R}}}(l)$ in equation (5.12) has $N^{(C)}_{\tilde{\mathcal{R}}}(l)$ identical members, where $N^{(C)}_{\tilde{\mathcal{R}}}(l)$ represents the number of the loops of length l and of starting point $\tilde{\mathcal{R}}$ for which $\mathcal{P}^{\mathbf{i}_l,\mathbf{j}_l} \ldots \mathcal{P}^{\mathbf{i}_1,\mathbf{j}_1} \in C$ or, which is the same, $\mathcal{P}_\gamma \in C$. Now we insert the results (B.7, B.8) related to the sum of the characters χ^{S^z} and the equation (5.12) into equations (5.9, 5.10) and we obtain the following expressions for the expectation value of the square of the total spin and the partition function:

$$\langle \hat{S}^2 \rangle = \frac{3}{4Z} \sum_{l=0}^{\infty} \frac{1}{l!} \left(\frac{-t}{kT} \right)^l \sum_{\tilde{\mathcal{R}}} \sum_{C \subset S_N} N^{(C)}_{\tilde{\mathcal{R}}}(l) \, (-1)^{|C|} \left(2^{\sum_{i=1}^{N} C_i} \right) \left(\sum_{i=1}^{N} i^2 C_i \right), \tag{5.13}$$

[4]Let consider now the lattice Λ_h consisting of every different hole configuration $\tilde{\mathcal{R}}$. We consider two lattice points $\tilde{\mathcal{R}}$ and $\tilde{\mathcal{R}}'$ nearest neighbours if they differ by only one hole position, and these different hole positions are nearest neighbours in the original lattice Λ. The lattice that we obtain in this way is a part of the DN_h-dimensional hypercubic lattice, and γ is a sequence of nearest-neighbour lattice points in Λ_h. For this reason, we call γ a 'loop'. In the $N_h = 1$ case γ is a loop in the original lattice Λ.

and

$$Z = \sum_{l=0}^{\infty} \frac{1}{l!} \left(\frac{-t}{kT} \right)^l \sum_{\tilde{\mathcal{R}}} \sum_{C \subset S_N} N_{\tilde{\mathcal{R}}}^{(C)}(l) \, (-1)^{|C|} \left(2^{\sum_{i=1}^{N} C_i} \right) . \tag{5.14}$$

In the above expressions $|C|$ is the parity of permutations from the conjugate class C and $(C_1, C_2, \ldots, C_N)$ describes their cycle structure, i.e. these permutations contain C_i cycles of length i.

From the partition function Z given in equation (5.14) we can compute the free energy $F = -T \ln Z$ and the specific heat $c = T \frac{\partial^2 (T \ln Z)}{\partial T^2}$.

From equation (5.13) we correctly obtain paramagnetic behaviour at high temperatures in thermodynamic limit. The first (i.e. $l = 0$) term of the l-sum becomes dominant if T increases; and $N_{\tilde{\mathcal{R}}}^{(C)}(0) = 1$ if $C = \{1\}$, otherwise $N_{\tilde{\mathcal{R}}}^{(C)}(0) = 0$. Therefore in high-temperature limit we have $\langle \hat{S}^2 \rangle = 3N/4$, so the value of the total spin per particle is proportional to $1/\sqrt{N}$.

Concerning the technical aspects in using equation (5.14) or equation (5.13) in concrete applications we mention that, in order to deduce the coefficients $N_{\tilde{\mathcal{R}}}^{(C)}(l)$, one should carry out the following procedure. We need to deduce a concrete $\sum_{C \subset S_{\mathbf{N}}}$ contribution at a fixed l value. For this:

1. Start from a fixed hole configuration $\tilde{\mathcal{R}}$, and denote with different numbers every site occupied by electrons.

2. A single step for a given hole means that we have to interchange the given hole with a nearest-neighbour number.

3. Take l steps with the holes in such a way, that finally get back the original hole configuration (this is a loop of length l). In this process an arbitrary hole can be moved in every step, the order of the steps being relevant. However, by interchanging holes between them, we do not obtain new loops.

4. Determine the cycle structure of the permutation of the numbers for the obtained loop (i.e. obtain the numbers C_i). As a result of this analysis, we have found one loop of length l and a given cycle structure $(C_1, C_2, \ldots, C_N)$.

5. Go back to step 3. and find a different loop of the same length l based on the same starting hole configuration $\tilde{\mathcal{R}}$. After this, we have another loop of length l, and another cycle structure.

6. If you have taken into account every possible different loop starting from the hole configuration $\tilde{\mathcal{R}}$, the quantity $N_{\tilde{\mathcal{R}}}^{(C)}(l)$ have the meaning of how many times this concrete C conjugate class (i.e. cycle structure) has been obtained in the procedure presented above. (A conjugate class C is uniquely determined by the common cycle structure of the permutations of that class.)

7. All this being done, the summation $\sum_{C\subset S_{\mathbf{N}}}$ at a fixed l and $\tilde{\mathcal{R}}$ means in fact a summation over all possible cycle structures. For a concrete cycle structure we may express $\sum_i C_i$ and $\sum_i i^2 C_i$. The number $|C|$ gives the parity of all permutations which give the same cycle structure C (as mentioned in Appendix B, all different permutations with the same cycle structure have the same parity).

Using this procedure up to a finite l, with a computer, a high temperature expansion can be obtained. A partition function, free energy, specific heat or a spin-square $T \neq 0$ expectation value can be deduced for a system with arbitrary number of holes. Evidently, the calculation time increases with the size of the system, with the number of holes and the order of the expansion.

5.3 The Nagaoka state

In order to analyze the temperature dependence of $\langle \hat{S}^2 \rangle$ we need the values of $N^{(C)}_{\tilde{\mathcal{R}}}(l)$ as functions of l. Comparing equation (5.14) with the formula for the partition function Z derived in first quantized formalism we obtain

$$\lim_{T\to 0} \frac{\sum_{l=0}^{\infty} \frac{1}{l!} \left(\frac{-t}{kT}\right)^l N^{(C)}_{\tilde{\mathcal{R}}}(l)}{e^{\frac{-E_0}{kT}}} = \frac{|C|}{N!} \tag{5.15}$$

for arbitrary conjugate class C which can occur in equations (5.13, 5.14), where E_0 is the ground-state energy of the N-particle hard-core boson system.

Knowledge of the asymptotic behaviour given by equation (5.15) is enough to analyze the T dependence of the Nagaoka ferromagnetism (i.e. $N_h = 1$ case). In this situation, $\Omega_{\tilde{\mathcal{R}}}(l)$ contains the loops of length l of the lattice Λ. For one hole, $\tilde{\mathcal{R}}$ is uniquely determined by the position of the hole. The positions of the hole described by $\gamma(0)$ at the starting point of the loop and $\gamma(l) = \mathcal{P}_\gamma \gamma(0) \mathcal{P}^{\mathbf{i}_1,\mathbf{j}_1} \dots \mathcal{P}^{\mathbf{i}_l,\mathbf{j}_l}$ at the end point of the loop are the same. In the cases when Nagaoka's theorem holds, namely for square, sc, bcc, fcc and hcp lattices, it can be seen that the parity $|\mathcal{P}_\gamma| = (-1)^l$ is always even when we use open boundary conditions, because there is no loop with odd length in these cases. This means that the dynamic evolution controlled by the Hamiltonian (5.1) is not able to permute the particles by odd permutations, given by the presence of the hard-core potential acting between them. As a consequence, the fermionic character of the particles has absolutely no effect in this case. This is fully consistent with our previous statement (presented before equation (5.8)) that the $S = S_{max}$ spectrum of our original fermion system is equivalent to the spectrum of a hard-core spinless boson system. Moreover, if bosons 'existed' with half spin, then there would be no differences between the system consisting of these particles with a hard-core potential on a square lattice and our original fermionic system in the one-hole case, because the permutations $\mathcal{C}(\mathcal{R}_l;\mathbf{i},\mathbf{j})$ occur in the Schrödinger equation (5.7) are always even, and in this case there is no difference between the Schrödinger equations connected to particles with bosonic and fermionic statistics if their spin is the same. As we mentioned above, the ground-state wave function of a boson system is always symmetric; therefore the spin wave function is also symmetric, i.e. the ground state is ferromagnetic. This is an interesting explanation of Nagaoka's theorem. Our formalism certainly gives back this result. It is obtained by taking the $T \to 0$ limit in equation (5.13), considering the asymptotic behaviour of the coefficients $N_{\tilde{\mathcal{R}}}^{(C)}(l)$ given by equation (5.15) for the conjugate classes with even parity and $N_{\tilde{\mathcal{R}}}^{(C)}(l) = 0$ for odd parity, furthermore using the result (B.6) from the Appendix B. When we use periodic boundary conditions, we still have $|\mathcal{P}_\gamma| = (-1)^l$ (l is the length of γ) which, however, can be odd, but only in the case when the linear length of the lattice is odd at least in one direction, and γ goes through the boundary in this direction. In $t > 0$ case, $(-t)^l(-1)^{|C|}$ is always positive; the sign coming from the odd parity of the permutation is compensated by the sign obtained during the movement around odd steps, and therefore the above arguments remains valid. The key feature now is the fact, that the parity of $\mathcal{P}_\gamma$ is in one-to-one correspondence with the parity of the length of γ.

5.4 Cases with more than one hole

The existence of more than one hole permits arbitrary (even and odd) permutations of the particles under dynamic evolution (independently of the length of the loop), therefore the fermionic feature of them plays an important role in building up the energy spectrum of the system. Using the asymptotic behaviour of $N_{\tilde{\mathcal{R}}}^{(C)}(l)$ from equation (5.15) and the results of the Appendix B presented after equation (B.6), the $\langle \hat{S}^2 \rangle$ value remains undetermined (i.e. 0/0), which in our interpretation is due to the fact that E_0 is not a possible energy for the fermionic system any longer. The special similarity of the behaviour of the particles with bosonic and fermionic statistics does not remain valid, therefore we can not draw conclusion about the magnetic property of the system based on Nagaoka's theorem. This is a qualitative difference between the one-hole and two-hole cases. It is similar to the case when the Hamiltonian has an extra symmetry at a special point, but the features of the model could be very different even close to this point owing to the symmetry breaking. If bosons had half spin, a system consisting of such hard-core bosons on a lattice would be ferromagnetic even for an arbitrary hole concentration. This statement remains valid for real bosons with integer (non-zero) spin as well and the expectation value of the total spin goes to a macroscopical (but not to the maximum) value when the temperature goes to zero, in this case.

In order to obtain information about the two-hole (or more-hole) case, a study of equation (5.13) is needed. The coefficients $N_{\tilde{\mathcal{R}}}^{(C)}(l)$ can be determined by the Monte Carlo method. By random sampling we can obtain the percentage of loops of a given length for which $\mathcal{P}_\gamma \in C$. Equations (5.14) and (5.13) have the advantage that the trace over the spin degrees of freedom has already been taken. Hence we need only to sample the loops, i.e. 'world lines' of holes, instead of the world lines of our original electron system. This is advantageous since, because of the presence of different possible electron spin configurations, the world lines of our original electron system have 2^N times more starting points than the hole loops.

We studied by this method a two-dimensional 10×10 lattice with periodic boundary conditions in the presence of two holes. We took into account every possible starting charge (hole) configuration. Because of the periodic boundary conditions and the translational, rotational and reflection symmetries of the lattice, there are 20 essentially different charge configurations instead of $\binom{100}{2}$. Because the contributions of the 2^{98} different spin configurations, corresponding to a fixed charge configuration, are taken into account analitycally by equations (5.14, 5.13), we have taken into account every possible starting point of world lines of our original electron system. Furthermore, starting from a charge configuration, we took into consideration every path up to the length $l = 14$. Thus, we counted exactly every loop up to $l \leq 14$; therefore the coefficients of our high-temperature expansion are exact up to 14th order in $|t|/kT$. Then, we continued every path with random directions up to $l = 100$.

The results can be seen in Fig. 5.1. The solid curves show the result of the high-temperature expansion with exact coefficients up to 14th order. Taking into account further coefficients determined by Monte Carlo method up to 50th order we obtain the broken (short-dash) curves, and up to 100th order we obtain the broken (long-dash) curves. The expectation value of the square of the total spin goes to $3N/4 = 73.5$ (and not to zero) as T goes to infinity. This is understandable, because at very high temperature the likelihood of all possible states becomes equal to $1/Z$. (The spectrum of the Hamiltonian is bounded.) Therefore, the expectation value of an arbitrary quantity goes to its simple algebraic average over all the states. This gives the result mentioned above for $\langle \hat{S}^2 \rangle$). This means in fact paramagnetic behaviour, because a smaller total spin value has greater thermodynamic weigh, i.e. the dimension of the eigensubspace of $\hat{S}^2$ is greater, therefore the $S = 0$ subspace is the greatest, and so this is the most probable value of the spin. For this reason, the total spin (but not $\langle \hat{S}^2 \rangle$) per particle is proportional to $1/\sqrt{N}$ which goes to zero in thermodynamic limit.

Because of the inaccuracy and the complete neglect of the higher-order coefficients in our expressions, the numerical error increases as the temperature decreases. Therefore we do not plot the $T \to 0$ temperature region in Fig. 5.1. Nevertheless, in the presented region the results are correct since the higher-order terms do not improve the lower-order contributions in this domain. At these temperatures, however, owing to the Monte Carlo method itself, small numerical errors

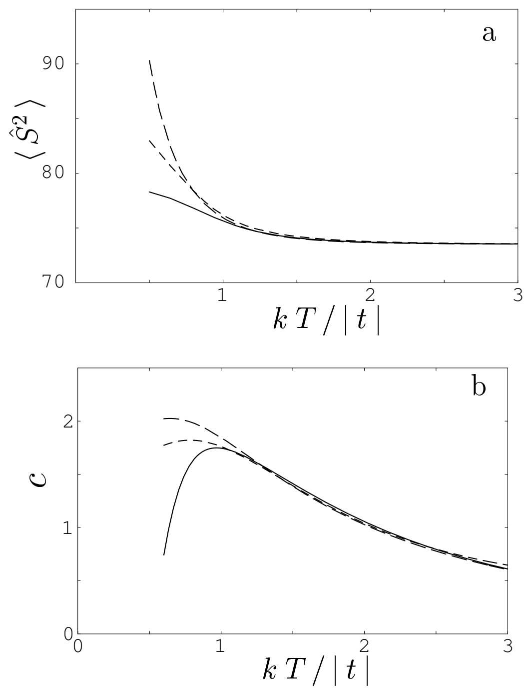

Figure 5.1: (a): Square of the total spin and (b): specific heat as functions of the temperature measured in $|t|$ units. The solid (lower) lines show the result of a 14th order high temperature expansion based on exact coefficients; the short-dash lines (in the middle) show the result of an 50-th order high temperature expansion, the long-dash (upper) lines of a 100-th order expansion based on coefficients determined by the described Monte Carlo method.

are present.

The obtained results show that the spontaneous magnetization increases as the temperature decreases. This tendency becomes stronger when we use more accurate approximation. In the same temperature range, when $\langle \hat{S}^2 \rangle$ starts to increase, the specific heat has a maximum. However this peak in the specific heat seems to be significant — also in higher-order approximations the curves break down since the specific heat has to go to zero in $T \to 0$ limit, — but the increase in $\langle \hat{S}^2 \rangle$ is small, nevertheless very fast.

Related to the-two and few-hole cases, in the literature it has been published that the ground state can not have maximal spin [30, 31, 36]. This statement is based on variational calculations. These calculations demonstrate that trial state exists with spin $S = S_{max} - 1$, which have a lower energy than the fully polarized state with spin S_{max}. However, until now it was not possible to construct variational state with spin $S \leq S_{max} - 2$, which would have a lower energy than the $S = S_{max} - 1$ state. Thus, the above mentioned results do not exclude ferromagnetic behaviour, only the highest spin value. None the less, our results suggest that the very low spin values can be excluded as well, and the ground state is not a singlet. As a conclusion, we may state that the system behaves at low temperature as a not fully saturated ferromagnet. This conclusion is consistent with exact diagonalization results for small clusters [120].

Summary

In this work I have presented exact results related to relevant and up-to-date problems of many-body physics. Important feature of these results are that they apply to higher than one dimensional systems. I emphasized the importance of the exact results, but I also underlined that in this field there are no standard well-tried methods.

My results can be summarized in the following points.

- I generalized Brandt and Giesekus's approach [77] to extended Hubbard model which contains next-nearest neighbour interaction terms and I deduced a ground state phase diagram of the system. My results are valid in all $D > 1$ spatial dimensions at half filling.
  - A completely saturated ferromagnetic phase, different types of commensurate spin density waves, commensurate charge-density waves and a region with phase separation were found, the last one being in our knowledge for the first time signaled at the level of approximation free results in $D > 1$ dimensions.
  - The stability domains of the fully saturated ferromagnetic phase, spin and charge density waves were extended in comparison with previous publications.
  - The presented phase diagram is complete in the localized limit $t_l = X_l \to 0$ in all dimensions $D > 1$ for arbitrary value of fully anisotropic or non-negative isotropic Heisenberg couplings.
  - The obtained results clearly emphasize that the next-nearest neighbour couplings have their role in building up the subtle balance between the stability domains of different ordered phases in the parameter space, introducing completely new phases or modifying considerably the emergence regions for other phases within the phase diagram.
- Under the conditions in which even the exact solution for the one dimensional periodic Anderson model is not known at finite U, I have presented exact

solutions for two dimensional periodic Anderson model in the interacting case. The described solutions are present on a surfaces of the $T = 0$ parameter space of the model. The physical properties of the solutions depend on the values of the coupling constants and the filling. Two types of solution emerge: a paramagnetic Mott insulator and a non-Fermi liquid type phase. Both solutions describe the interacting $U > 0$ model, and the deduced ground-state wave functions cannot be obtained perturbatively from the non-interacting case.

- The first solution emerges at 3/4 filling and represents a paramagnetic Mott insulator, the ground-state being completely localized.
- The second solution represents in two dimensions a new non-Fermi liquid normal (non-symmetry broken) phase and emerges at $N/N_\Lambda \geq 3/4$ filling. In this phase the $n_{\vec{k}}$ momentum distribution function is continuous together with its derivatives of any order; it is a well defined Fermi energy, but the Fermi momentum is not definable thus the system has no Fermi surface. In the parameter space this phase emerges in the vicinity of the above mentioned Mott insulating phase. The ground-state is paramagnetic with large spin degeneracy. The reason of this interesting behaviour is due to the fact, that the flat-band feature of the model — which is given by the diagonalization of the formally non-interacting Hamiltonian $\hat{H}_{eff} = \hat{H}_0 + U\hat{N}_f$ — remains valid also in the interacting case. This partially filled band is situated above a normal band with dispersion. Low lying excitations increases the number of particles at the Fermi energy. In this process particles are removed from the lower band and come up into the upper flat band.

• I presented a technique to deal with the simple Hubbar model in the case of infinitely repulsive interaction. The formalism treats separately the spin and charge degrees of freedom at the level of description, showing explicitly the effect of the spin background in the movement of the hole.

- The Hamiltonian can be reduced into invariant subspaces with given value of the total spin and its z-component. I explicitly showed that the matrix element of the Hamiltonian reduced into such a subspace can be given using matrix elements of an irreducible representation of the symmetric group of degree N. (N is the number of particles.) It can be useful for numerical diagonalization for small clusters.
- I developed a high-temperature expansion technique in which the sum over the spin degrees of freedom can be expressed exactly in terms of characters of the symmetric group. Based on this technique the efficiency of the world line Monte Carlo algorithm can be increased. By the limited

computer capacity available for me I attempted to study the magnetic properties of the model near half filling.

- Within the frame of the presented formalism the Nagaoka mechanism of ferromagnetism becomes clear, and also the reason why it cannot survive the generalization for more than one hole: the fermionic feature of particles does not play any role. The situation is similar for one dimensional system with open boundary condition (the number of particles is arbitrary), or in case of odd number of particles with periodic boundary conditions, or in case of even number of particles with anti-periodic boundary conditions.

Összefoglalás

(The Hungarian summary of the thesis.)

Napjaink szilárdtestfizikai és statisztikus fizikai kutatásainak sok központi kérdése az erősen kölcsönható, és ebből kifolyólag gyakran erősen korrelált állapotú elektronrendszer viselkedésének leírásához kapcsolódik. Prominens példák a magas hőmérsékletű szupravezetés, szuperfolyékonyság, kvantum Hall-effektus, nehéz-Fermion rendszerek, nem-Fermi-folyadék viselkedést mutató rendszerek, és a leghétköznapibb ide tartozó jelenség talán a ferromágnesség, amely ősidők óta ismert, de amelynek a teljes megértésétől még ma is messze vagyunk. Ennek a legfőbb oka abban rejlik, hogy a fent említett problémák sok erősen csatolt részecskét tartalmazó kvantummechanikai rendszerekhez kapcsolódnak, amelyekben a széles skálán változó és így nagy értéket is elérő csatolási állandók miatt a hagyományos közelítő eljárások (pl. perturbációszámítás) alkalmazása — ha egyáltalán lehetséges, — nehéz, az így adódó eredmények a paramétertérnek csak egy szűk tartományán érvényesek, és még ennek az érvényességi tartománynak a határai is sokszor nagyon bizonytalanok. Ezért ezen a területen különösen értékesek az egzakt megoldások, főleg akkor, ha ezek a paramétertér széles tartományán és nagy csatolási állandók esetén is érvényesek. Azonban az erősen korrelált rendszerek területén az ismert egzakt megoldási módszerek legnagyobb része csak egy dimenzióban alkalmazható (pl. Bethe Ansatz).

PhD munkám célja a fent leírt problematikus esetekben is alkalmazható új típusú egzakt módszerek kipróbálása erősen kölcsönható sokrészecskés rendszerek népszerű modelljein, illetve ha csak lehetséges, ilyen jellegű módszerek kifejlesztése vagy továbbfejlesztése. Az általam vizsgált modellek mindeddig a Hubbard-modell, illetve annak valamilyen kibővített változatai, valamint a periodikus Anderson-modell voltak.

Ennek keretében munkám első szakaszában egy szisztematikusan először Brandt és Giesekus által alkalmazott módszer [U. Brandt and A. Giesekus, Phys. Rev. Lett. **68**, 2648 (1992)] használhatóságát vizsgáltam. A módszer lényege, hogy a variációs elvet — melynek segítségével felső határ adható az alapállapoti energiára — kombinálva a Hamilton-operátor konstans ill. pozitív szemidefinit tagok összegére bontásával — amely a pozitív szemidefinit tagokat elhagyva alsó határt ad az alapállapoti energiára — meghatározható a paramétertér olyan tartománya, amelyben az alapállapoti energiára vonatkozó egzakt alsó ill. felső határok egybeesnek, így megadják annak pontos értékét. A hozzá tartozó hullámfüggvény — a variációs elv használatából adódóan — szintén ismert. Mivel korábban ezt a módszert csak első szomszéd kölcsönhatásokkal kibővített Hubbard-modell vizsgálatára használták, de bizonyos elméleti és kísérleti tények arra utaltak, hogy a második szomszéd kölcsönhatások fontossága ezzel összemérhető, ezért a cél ennek a kérdésnek a vizsgálata volt.

Később ennek a módszernek az alkalmazásával tanulmányoztam a periodikus Anderson-modellt két dimenzióban. Ennek a kérdésnek a nehézségét jól mutatja, hogy még az egydimenziós esetre vonatkozóan is nagyon kevés egzakt eredmény talalható az irodalomban. Az általam bemutatott megoldás kapcsolódik a nem-Fermi-folyadék jellegű viselkedést mutató rendszerek manapság hatalmas érdeklődést kiváltó kérdésköréhez.

Régóta nyitott kérdés az erősen korrelált rendszerek egyik legalapvetőbb modelljének tekinthető egyszerű Hubbard-modell ferromágneses tulajdonságainak kérdése. Habár mára bizonyossá vált, hogy nem ez a ferromágnesség általános modellje, de elméletileg továbbra is érdekes a ferromágnesességhez vezető mechanizmusok keresése. Továbbá a modell tulajdonságainak leírása az erősen kölcsönható határesetben félig töltött sáv közelében a magas hőmérsékletű szupravezetők megértése szempontjából is releváns lehet.

Eredmények

Tudományos eredményeimet az alábbi tézispontok tartalmazzák:

1. Általánosítottam Brandt és Giesekus módszerét második szomszéd kölcsönhatásokkal kibővített Hubbard-modellre, és ennek segítségével alapállapoti fázisdiagramot adtam a modellre. Eredményeim tetszőleges egynél nagyobb dimenzióban és félig töltött sáv esetén érvényesek.[1, 2, 3]

   (a) A fázisdiagramban teljesen telített ferromágneses fázis, különböző spin- és töltéssűrűség-hullámokat leíró fázisok stabilitási tartományait, valamint fázisszeparációt mutató tartományt sikerült körülhatárolnom. Ez utóbbira — közelítések használata nélkül — tudomásom szerint korábban nem volt példa az irodalomban $D > 1$ dimenziós rendszer esetén.

(b) A ferromágneses és a spin- illetve töltéssűrűség-hullám fázisok általam megadott stabilitási tartományai szélesebbek az irodalomban korábban megadottaknál, így azok javításának tekinthetők.

(c) Lokalizált határesetben — amikor a Hamilton-operátor semmilyen mozgást leíró tagot nem tartalmaz — a bemutatott fázisdiagram teljes, ha a Heisenberg-kölcsönhatás teljesen anizotróp, vagy izotróp és csatolási állandója nem negatív.

(d) Az eredmények alátámasztják, hogy a második szomszéd kölcsönhatásoknak jelentős szerepük van a rendezett fázisok stabilitási tartományainak kialakításában; erősen befolyásolják ezen tartományok határait, sőt olyan fázisok megjelenéséhez vezetnek, amelyek nélkülük nem lennének stabilak.

2. Mindeddig periodikus Anderson modellre egydimenziós egzakt megoldás sem volt ismert olyan esetben, amikor a kölcsönhatás erőssége véges. Ebben a dolgozatban én ismertettem egy két dimenzióra vonatkozó eredményt, amely az alapállapotot a paramétertér egy hiperfelületén adja meg, amelynek mentén a kölcsönhatás erőssége tetszőleges értékek között változhat. Az alapállapotot leíró hullámfüggvény perturbatív úton nem kapható meg. A megoldás fizikai tartalma a modellparaméterek értékétől függően kétféle lehet: paramágneses Mott-szigetelő, vagy nem-Fermi-folyadék típusú. [6]

   (a) Az egyik típusú megoldás háromnegyedig töltött sáv esetén jelenik meg, és paramágneses Mott szigetelőt ír le, lévén az alapállapoti hullámfüggvényben minden részecske teljesen lokalizált.

   (b) A másik megoldás egy új, nem-Fermi-folyadék jellegű normális (nem szimmetriasértő) fázist ír le háromnegyed vagy afeletti sávbetöltöttség esetén. Ebben a fázisban az elektronok impulzustérbeli eloszlásfüggvénye és az ő összes deriváltja folytonos, és emiatt — habár létezik Fermi-energia — Fermi-felület és hozzá tartozó Fermi-impulzus nem definiálható. Ez a fázis a paramétertérben a Mott szigetelőt leíró fázis közelében helyezkedik el, maga pedig erős spindegenerációval jellemezhető paramágnes. A fizikailag érdekes viselkedés bizonyos értelemben egy lapos sáv effektus eredménye. Ha a nemkölcsönható problémát úgy módosítjuk, hogy az f sáv magasságát U-val, a kölcsönhatás erősségével eltóljuk, az így adódó Hamilton-operátor diagonalizálásából egy teljesen lapos sáv adódik, amely a kölcsönhatás teljes figyelembevétele esetén is megmarad, és így divergenciát okoz az állapotsűrűségben a Fermi-energiánál. Ez a lapos sáv részlegesen betöltött, és egy másik sáv felett helyezkedik el, amely teljesen betöltött. Az alacsony energiájú gerjesztések a Fermi-energiájú részecskék számát növelik azáltal, hogy elektronok ugranak fel az alsó sávból a felső, lapos sávba.

3. Ismertettem egy olyan eljárást, amelynek a segítségével az egyszerű Hubbard-modell végtelen erős kölcsönhatás határesetében tanulmányozható. A formalizmus — a leírás szintjén — szeparáltan kezeli a spin és a töltés szabadsági fokokat, és explicit kifejezi a spinháttér hatását a mozgó lyukra.[4, 5]

   (a) Explicit megmutattam, hogyan fejezhetőek ki egy meghatározott spinnel és spin vetülettel jellemzett invariáns altérben adott bázisban a Hamilton-operátor mátrixelemei az N-ed fokú szimmetrikus csoport bizonyos irreducibilis ábrázolásainak mátrixelemeivel. (N a részecskék száma.) Ez hasznos lehet kis rendszerekre vonatkozó numerikusan egzakt diagonalizálási feladatok esetén.

   (b) Kidolgoztam egy magas hőmérsékletű sorfejtési eljárást, amelyben az állapotösszeg kiszámításához szükséges összegzésnek a spin szabadsági fokokra vonatkozó része analitikusan kifejezhető a szimmetrikus csoport karaktereinek segitségével. Erre alapozva növelhető a "world line" algoritmusú Monte Carlo szimuláció hatékonysága.

   (c) Az említett formalizmus keretében a ferromágnesesség Nagaoka-mechanizmusa könnyen interpretálható: a rendszert felépítő elektronok fermion jellege nem jut érvényre a végtelen erős kölcsönhatás miatt, ha csak egy lyuk van a rendszerben. A helyzet hasonló egy dimenzióban nyílt határfeltételek esetén (a részecskék száma tetszőleges), vagy páratlan számú részecske esetén periodikus határfeltételek mellett, és páros számú részecske esetén antiperiodikus határfeltételek mellett.

Appendix A

This Appendix contains some mathematical details related to the calculation of momentum distribution functions and of Hamiltonian terms when $N = 3N_\Lambda$ and $\alpha_{\vec{k},c} \neq 0$ for all $\vec{k} \in \hat{\Lambda}$. Firstly we prove that the state vectors defined in equation (4.13) form a basis in $\mathfrak{H}_{3N_\Lambda,0}$ in this case. For this purpose it is enough to show that the set $\{|\psi_{0,\boldsymbol{\sigma}}\rangle \,:\, \boldsymbol{\sigma} = (\sigma_{\mathbf{i}})_{\mathbf{i}=1}^{\mathbf{N}_\Lambda},\ \sigma_{\mathbf{i}} \in \{\uparrow,\downarrow\}\}$ consists of 2^{N_Λ} pieces of linearly independent vectors, since in Section 4.3 we have seen that every ground state can be written as a linear combination of $|\psi_{0,\boldsymbol{\sigma}}\rangle$. Secondly we prove that the quantum mechanical expectation value of the operator $\sum_\sigma \hat{C}^\dagger_{\vec{k},2,\sigma}\hat{C}_{\vec{k},2,\sigma}$ is uniform in $\mathfrak{H}_{3N_\Lambda,0}$ and equal with 1, independently from $\vec{k}$. Finally the equation $\langle \hat{C}^\dagger_{\vec{k},2,\sigma}\hat{C}_{\vec{k},2,\sigma}\rangle_0 = \frac{1}{2}$ will be verified, where the notation $\langle.\rangle_0$ means the $T \to 0$ limit of the finite temperature expectation value, according to the definition in Subsection 4.5.1.

The index $\boldsymbol{\sigma}$ can have 2^{N_Λ} different values, according to the 2^{N_Λ} different spin configurations of the N_Λ electrons situated in different sites. The operators $\hat{F}^\dagger_{\boldsymbol{\sigma}}$ creates orthogonal states from the vacuum: $\langle 0|\hat{F}_{\boldsymbol{\sigma}'}\hat{F}^\dagger_{\boldsymbol{\sigma}}|0\rangle = \delta_{\boldsymbol{\sigma}',\boldsymbol{\sigma}}$. The operators $\hat{F}^\dagger_{\boldsymbol{\sigma}}$ can be expressed in terms of operators $\hat{C}^\dagger_{\vec{k},s,\sigma_{\mathbf{i}}}$. Using equation (4.30) we obtain

$$\hat{F}^\dagger_{\boldsymbol{\sigma}} = \prod_{\mathbf{i}} \Big(\sum_{\vec{k}} e^{i\vec{k}\vec{R}_{\mathbf{i}}} \hat{f}^\dagger_{\vec{k},\sigma_{\mathbf{i}}} \Big) = \prod_{\mathbf{i}} \Bigg(\sum_{\vec{k}} e^{i\vec{k}\vec{R}_{\mathbf{i}}} (\Delta_{\vec{k}})^{-\frac{1}{2}} \big(\alpha_{\vec{k},f} \hat{C}^\dagger_{\vec{k},1,\sigma_{\mathbf{i}}} - \alpha^*_{\vec{k},c} \hat{C}^\dagger_{\vec{k},2,\sigma_{\mathbf{i}}} \big) \Bigg).$$

Substituting this result into the expression (4.13) of the ground state vectors the terms which contain operators $\hat{C}^\dagger_{\vec{k},1,\sigma}$ cancel out due to the fact that $\hat{G}$ contains these operators for all $\vec{k}$ and σ, as can be seen from equation (4.31). Therefore we obtain

$$|\psi_{0,\boldsymbol{\sigma}}\rangle = \hat{G}^\dagger \prod_{\mathbf{i}} \Bigg(\sum_{\vec{k}} e^{i\vec{k}\vec{R}_{\mathbf{i}}} (\Delta_{\vec{k}})^{-\frac{1}{2}} (-\alpha^*_{\vec{k},c}) \hat{C}^\dagger_{\vec{k},2,\sigma_{\mathbf{i}}} \Bigg) |0\rangle. \tag{A.1}$$

In equation (A.1) the ground state wave vectors are expressed by the operators $\hat{C}^\dagger_{\vec{k},s,\sigma_{\mathbf{i}}}$. (We get $\hat{G}^\dagger$ from equation (4.31).) This is an advantage when we compute the expectation values mentioned in the first paragraph of this Appendix. However, difficult to handle these state vectors because they are not orthonormal vectors. Further technical difficulty that in the formula (A.1) there is a sum under the product, therefore we are going to expand out the product. More convenient to handle separately the up and down spins. Therefore first of all we rearrange the order of the product. (As we mentioned on page 8 in Section 2.2 the notation $\prod_{\mathbf{i}}$ denotes an ordered product.) Considering an index $\boldsymbol{\sigma}$ we denote by $\mathcal{Q}$ a fix permutation[1] of Λ for which

$$(\sigma_{\mathcal{Q}(\mathbf{i})})_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}_\Lambda} \equiv (\sigma_{\mathcal{Q}(\mathbf{1})}, \sigma_{\mathcal{Q}(\mathbf{2})}, \ldots, \sigma_{\mathcal{Q}(\mathbf{N}_\Lambda)}) = (\overbrace{\uparrow, \uparrow, \ldots, \uparrow}^{N_\uparrow}, \overbrace{\downarrow, \downarrow, \ldots, \downarrow}^{N_\downarrow}).$$

As we indicated above, the number of up spins in $\boldsymbol{\sigma}$ is denoted by $N_\uparrow$ thus the number of down spins is $N_\downarrow = N_\Lambda - N_\uparrow$. Clearly $N_\uparrow$, $N_\downarrow$ and $\mathcal{Q}$ depend on $\boldsymbol{\sigma}$, but contrary to $N_\uparrow$ and $N_\downarrow$ the permutation $\mathcal{Q}$ is not uniquely determined by $\boldsymbol{\sigma}$. This ununiqueness does not influence our results. In the further formulas we regard $\mathcal{Q}$ as a fix permutation among which are allowed by $\boldsymbol{\sigma}$.

Using the above defined notations the rearranged product from equation (A.1) can be written as follows.

$$\hat{\mathcal{F}}_{\boldsymbol{\sigma}}^\dagger := \prod_{\mathbf{i}} \left(\sum_{\vec{k}} e^{i\vec{k}\vec{R}_{\mathbf{i}}} (\Delta_{\vec{k}})^{-\frac{1}{2}} (-\alpha^*_{\vec{k},c}) \hat{C}^\dagger_{\vec{k},2,\sigma_{\mathbf{i}}} \right) =$$

$$= (-1)^{|\mathcal{Q}|} \prod_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}_\uparrow} \left(\sum_{\vec{k}_{\mathbf{i}}} e^{i\vec{k}_{\mathbf{i}}\vec{R}_{\mathcal{Q}(\mathbf{i})}} \frac{-\alpha^*_{\vec{k}_{\mathbf{i}},c}}{(\Delta_{\vec{k}_{\mathbf{i}}})^{\frac{1}{2}}} \hat{C}^\dagger_{\vec{k}_{\mathbf{i}},2,\uparrow} \right) \prod_{\mathbf{i}=\mathbf{N}_\uparrow+\mathbf{1}}^{\mathbf{N}_\Lambda} \left(\sum_{\vec{k}_{\mathbf{i}}} e^{i\vec{k}_{\mathbf{i}}\vec{R}_{\mathcal{Q}(\mathbf{i})}} \frac{-\alpha^*_{\vec{k}_{\mathbf{i}},c}}{(\Delta_{\vec{k}_{\mathbf{i}}})^{\frac{1}{2}}} \hat{C}^\dagger_{\vec{k}_{\mathbf{i}},2,\downarrow} \right)$$

Here $|\mathcal{Q}|$ denotes the parity of the permutation $\mathcal{Q}$. To avoid the confusion when expanding out the products, we label the momentum summation indices by $\mathbf{i}$ for the purpose to distinct the different summation indices occur in different multipliers of the product $\prod_{\mathbf{i}}$. For a fix value of $\mathbf{i}$, $\vec{R}_{\mathbf{i}}$ denotes a fix vector as defined in Section 2.2, contrary to $\vec{k}_{\mathbf{i}}$ of which value is not determined by $\mathbf{i}$; $\vec{k}_{\mathbf{1}}, \ldots, \vec{k}_{\mathbf{N}_\Lambda}$ run over the whole $\hat{\Lambda}$.

Now we expand out the products in the previous expression of $\hat{\mathcal{F}}_{\boldsymbol{\sigma}}^\dagger$.

$$\hat{\mathcal{F}}_{\boldsymbol{\sigma}}^\dagger = (-1)^{|\mathcal{Q}|} \sum_{\vec{k}_{\mathbf{1}},\ldots,\vec{k}_{\mathbf{N}_\uparrow}} \prod_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}_\uparrow} \left(e^{i\vec{k}_{\mathbf{i}}\vec{R}_{\mathcal{Q}(\mathbf{i})}} \frac{-\alpha^*_{\vec{k}_{\mathbf{i}},c}}{(\Delta_{\vec{k}_{\mathbf{i}}})^{\frac{1}{2}}} \hat{C}^\dagger_{\vec{k}_{\mathbf{i}},2,\uparrow} \right) \times$$

$$\sum_{\vec{k}_{\mathbf{N}_\uparrow+\mathbf{1}},\ldots,\vec{k}_{\mathbf{N}_\Lambda}} \prod_{\mathbf{i}=\mathbf{N}_\uparrow+\mathbf{1}}^{\mathbf{N}_\Lambda} \left(\sum_{\vec{k}_{\mathbf{i}}} e^{i\vec{k}_{\mathbf{i}}\vec{R}_{\mathcal{Q}(\mathbf{i})}} \frac{-\alpha^*_{\vec{k}_{\mathbf{i}},c}}{(\Delta_{\vec{k}_{\mathbf{i}}})^{\frac{1}{2}}} \hat{C}^\dagger_{\vec{k}_{\mathbf{i}},2,\downarrow} \right)$$

[1] We treat a permutation as a bijective map from Λ onto itself.

Because of the anticommutation relation of the operators $\hat{C}^\dagger_{\vec{k},2,\sigma}$ every non-zero term of the above sums fulfills that $\vec{k}_{\mathbf{1}} \neq \vec{k}_{\mathbf{2}} \neq \cdots \neq \vec{k}_{\mathbf{N}_\uparrow}$ and $\vec{k}_{\mathbf{N}_\uparrow+\mathbf{1}} \neq \vec{k}_{\mathbf{N}_\uparrow+\mathbf{2}} \neq \cdots \neq \vec{k}_{\mathbf{N}_\Lambda}$. Furthermore every term of the first sum for which the set $\{\vec{k}_{\mathbf{1}}, \ldots, \vec{k}_{\mathbf{N}_\uparrow}\}$ is the same consists of the same operator multiplied by different scalar coefficients which we contract. Doing the similar procedure also in the second sum we get

$$\begin{aligned}
\mathcal{F}^\dagger_{\boldsymbol{\sigma}} = (-1)^{|\mathcal{Q}|} & \sum_{\vec{k}_{\mathbf{1}}<\cdots<\vec{k}_{\mathbf{N}_\uparrow}} \left[\prod_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}_\uparrow} \left(\sum_{\mathcal{P}\in S_1} (-1)^{|\mathcal{P}|} e^{i\vec{k}_{\mathcal{P}(\mathbf{i})}\vec{R}_{\mathcal{Q}(\mathbf{i})}} \frac{-\alpha_{\vec{k}^*_{\mathcal{P}(\mathbf{i}),c}}}{(\Delta_{\vec{k}_{\mathcal{P}(\mathbf{i})}})^{\frac{1}{2}}} \right) \hat{C}^\dagger_{\vec{k}_{\mathbf{i}},2,\uparrow} \right] \times \\
& \sum_{\vec{k}_{\mathbf{N}_\uparrow+\mathbf{1}}<\cdots<\vec{k}_{\mathbf{N}_\Lambda}} \left[\prod_{\mathbf{i}=\mathbf{N}_\uparrow+\mathbf{1}}^{\mathbf{N}_\Lambda} \left(\sum_{\mathcal{P}\in S_2} (-1)^{|\mathcal{P}|} e^{i\vec{k}_{\mathcal{P}(\mathbf{i})}\vec{R}_{\mathcal{Q}(\mathbf{i})}} \frac{-\alpha_{\vec{k}^*_{\mathcal{P}(\mathbf{i}),c}}}{(\Delta_{\vec{k}_{\mathcal{P}(\mathbf{i})}})^{\frac{1}{2}}} \right) \hat{C}^\dagger_{\vec{k}_{\mathbf{i}},2,\downarrow} \right] \\
= & \sum_{\substack{\vec{k}_{\mathbf{1}} < \cdots < \vec{k}_{\mathbf{N}_\uparrow} \\ \vec{k}_{\mathbf{N}_\uparrow+\mathbf{1}} < \ldots < \vec{k}_{\mathbf{N}_\Lambda}}} \left(\sum_{\mathcal{P}\in S_1\otimes S_2} (-1)^{|\mathcal{Q}\mathcal{P}|} e^{i\sum_{\mathbf{i}}\vec{k}_{\mathcal{P}(\mathbf{i})}\vec{R}_{\mathcal{Q}(\mathbf{i})}} \right) \left(\prod_{\mathbf{i}} \frac{-\alpha^*_{\vec{k}_{\mathbf{i}},c}}{(\Delta_{\vec{k}_{\mathbf{i}}})^{\frac{1}{2}}} \right) \times \\
& \left(\prod_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}_\uparrow} \hat{C}^\dagger_{\vec{k}_{\mathbf{i}},2,\uparrow} \right) \left(\prod_{\mathbf{i}=\mathbf{N}_\uparrow+\mathbf{1}}^{\mathbf{N}_\Lambda} \hat{C}^\dagger_{\vec{k}_{\mathbf{i}},2,\downarrow} \right),
\end{aligned} \tag{A.2}$$

where S_1 denotes the group of permutations of the set $\{\mathbf{1}, \ldots, \mathbf{N}_\uparrow\}$, S_2 denotes the group of permutations of the set $\{\mathbf{N}_\uparrow + \mathbf{1}, \ldots, \mathbf{N}_\Lambda\}$, and $S_1 \otimes S_2$ denotes the product of these groups. The $<$ relation among the momentum summation indices is defined by an arbitrary but fix order of $\hat{\Lambda}$ (see pg. 8).

In a very similar way as equation (A.2) was deduced one can get analogous formula for $\hat{F}^\dagger_{\boldsymbol{\sigma}}$:

$$\hat{F}^\dagger_{\boldsymbol{\sigma}} = \sum_{\substack{\vec{k}_{\mathbf{1}} < \cdots < \vec{k}_{\mathbf{N}_\uparrow} \\ \vec{k}_{\mathbf{N}_\uparrow+\mathbf{1}} < \ldots < \vec{k}_{\mathbf{N}_\Lambda}}} \left(\sum_{\mathcal{P}\in S_1\otimes S_2} (-1)^{|\mathcal{Q}\mathcal{P}|} e^{i\sum_{\mathbf{i}}\vec{k}_{\mathcal{P}(\mathbf{i})}\vec{R}_{\mathcal{Q}(\mathbf{i})}} \right) \left(\prod_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}_\uparrow} \hat{f}^\dagger_{\vec{k}_{\mathbf{i}},\uparrow} \right) \left(\prod_{\mathbf{i}=\mathbf{N}_\uparrow+\mathbf{1}}^{\mathbf{N}_\Lambda} \hat{f}^\dagger_{\vec{k}_{\mathbf{i}},\downarrow} \right). \tag{A.3}$$

Now we prove the following statement which will serve as a lemma in the followings.

Lemma: Assuming that we have two operators $\hat{X}_2$ and $\hat{X}_f$ of which the state vectors $\prod_{\mathbf{i}} \hat{C}^\dagger_{\vec{k}_{\mathbf{i}},2,\sigma_{\mathbf{i}}}|0\rangle$ and $\prod_{\mathbf{i}} \hat{f}^\dagger_{\vec{k}_{\mathbf{i}},\sigma_{\mathbf{i}}}|0\rangle$ are eigenvectors with the same eigenvalue for all possible values of $\vec{k}_{\mathbf{i}} \in \hat{\Lambda}$ and $\sigma_{\mathbf{i}} \in \{\uparrow,\downarrow\}$ ($\mathbf{i} \in \Lambda$), i.e.,

$$\begin{aligned}
\hat{X}_2 \prod_{\mathbf{i}} \hat{C}^\dagger_{\vec{k}_{\mathbf{i}},2,\sigma_{\mathbf{i}}}|0\rangle &= x(\vec{k}_{\mathbf{1}}, \sigma_{\mathbf{1}}, \ldots, \vec{k}_{\mathbf{N}_\Lambda}, \sigma_{\mathbf{N}_\Lambda}) \prod_{\mathbf{i}} \hat{C}^\dagger_{\vec{k}_{\mathbf{i}},2,\sigma_{\mathbf{i}}}|0\rangle, \\
\hat{X}_f \prod_{\mathbf{i}} \hat{f}^\dagger_{\vec{k}_{\mathbf{i}},\sigma_{\mathbf{i}}}|0\rangle &= x(\vec{k}_{\mathbf{1}}, \sigma_{\mathbf{1}}, \ldots, \vec{k}_{\mathbf{N}_\Lambda}, \sigma_{\mathbf{N}_\Lambda}) \prod_{\mathbf{i}} \hat{f}^\dagger_{\vec{k}_{\mathbf{i}},\sigma_{\mathbf{i}}}|0\rangle,
\end{aligned} \tag{A.4}$$

then

$$\langle 0|\hat{\mathcal{F}}^{\boldsymbol{\sigma}'}\hat{X}_2\hat{\mathcal{F}}^{\dagger}_{\boldsymbol{\sigma}}|0\rangle = \langle 0|\hat{F}_{\boldsymbol{\sigma}'}\hat{X}_f\hat{F}^{\dagger}_{\boldsymbol{\sigma}}|0\rangle, \tag{A.5}$$

where the $\hat{\mathcal{F}}$ operators labelled by superscript $\boldsymbol{\sigma}$ are defined as

$$(\hat{\mathcal{F}}^{\boldsymbol{\sigma}})^{\dagger} := \prod_{\mathbf{i}}\left(\sum_{\vec{k}} e^{i\vec{k}\vec{R}_{\mathbf{i}}}\frac{(\Delta_{\vec{k}})^{\frac{1}{2}}}{-\alpha_{\vec{k},c}}\hat{C}^{\dagger}_{\vec{k},2,\sigma_{\mathbf{i}}}\right). \tag{A.6}$$

For the proof of the above lemma first of all one can see that expanding equation (A.6) we get a similar formula than equation (A.2):

$$(\hat{\mathcal{F}}^{\boldsymbol{\sigma}})^{\dagger} = \sum_{\substack{\vec{k}_{\mathbf{1}} < \cdots < \vec{k}_{\mathbf{N}_\uparrow} \\ \vec{k}_{\mathbf{N}_\uparrow+\mathbf{1}} < \ldots < \vec{k}_{\mathbf{N}_\Lambda}}} \left(\sum_{\mathcal{P}\in S_1\otimes S_2}(-1)^{|\mathcal{QP}|}e^{i\sum_{\mathbf{i}}\vec{k}_{\mathcal{P}(\mathbf{i})}\vec{R}_{\mathcal{Q}(\mathbf{i})}}\right)\left(\prod_{\mathbf{i}}\frac{(\Delta_{\vec{k}_{\mathbf{i}}})^{\frac{1}{2}}}{-\alpha^{*}_{\vec{k}_{\mathbf{i}},c}}\right)\times$$
$$\left(\prod_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}_\uparrow}\hat{C}^{\dagger}_{\vec{k}_{\mathbf{i}},2,\uparrow}\right)\left(\prod_{\mathbf{i}=\mathbf{N}_\uparrow+\mathbf{1}}^{\mathbf{N}_\Lambda}\hat{C}^{\dagger}_{\vec{k}_{\mathbf{i}},2,\downarrow}\right). \tag{A.7}$$

The remaining part of the proof is a straightforward calculation based on the observation that from $\vec{k}_{\mathbf{1}} < \cdots < \vec{k}_{\mathbf{N}_\uparrow}$ and $\vec{k}_{\mathbf{N}_\uparrow+\mathbf{1}} < \cdots < \vec{k}_{\mathbf{N}_\Lambda}$, furthermore $\vec{k}'_{\mathbf{1}} < \cdots < \vec{k}'_{\mathbf{N}'_\uparrow}$ and $\vec{k}'_{\mathbf{N}'_\uparrow+\mathbf{1}} < \cdots < \vec{k}'_{\mathbf{N}_\Lambda}$ follows that

$$\langle 0|\prod_{\mathbf{i}=\mathbf{N}_\Lambda}^{\mathbf{N}_\uparrow+\mathbf{1}}{}' \hat{C}_{\vec{k}_{\mathbf{i}},2,\downarrow}\prod_{\mathbf{i}=\mathbf{N}_\uparrow}^{\mathbf{1}}{}' \hat{C}_{\vec{k}_{\mathbf{i}},2,\uparrow}\prod_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}_\uparrow}\hat{C}^{\dagger}_{\vec{k}_{\mathbf{i}},2,\uparrow}\prod_{\mathbf{i}=\mathbf{N}_\uparrow+\mathbf{1}}^{\mathbf{N}_\Lambda}\hat{C}^{\dagger}_{\vec{k}_{\mathbf{i}},2,\downarrow}|0\rangle =$$
$$= \langle 0|\prod_{\mathbf{i}=\mathbf{N}_\Lambda}^{\mathbf{N}_\uparrow+\mathbf{1}}{}' \hat{f}_{\vec{k}_{\mathbf{i}},\downarrow}\prod_{\mathbf{i}=\mathbf{N}_\uparrow}^{\mathbf{1}}{}' \hat{f}_{\vec{k}_{\mathbf{i}},\uparrow}\prod_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}_\uparrow}\hat{f}^{\dagger}_{\vec{k}_{\mathbf{i}},\uparrow}\prod_{\mathbf{i}=\mathbf{N}_\uparrow+\mathbf{1}}^{\mathbf{N}_\Lambda}\hat{f}^{\dagger}_{\vec{k}_{\mathbf{i}},\downarrow}|0\rangle = \delta_{N_\uparrow,N'_\uparrow}\prod_{\mathbf{i}=\mathbf{1}}^{\mathbf{N}_\Lambda}\delta_{\vec{k}_{\mathbf{i}},\vec{k}'_{\mathbf{i}}}\ , \tag{A.8}$$

where the prime over $\prod$ indicates that the product is in reverse order (see the convention described in page 8 in Section 2.2). Therefore expanding both sides of equation (A.5) using the expressions (A.2, A.7, A.3) the sums over the momentum indices $\vec{k}_{\mathbf{1}}, \ldots, \vec{k}_{\mathbf{N}_\Lambda}$ which occur twice on both sides of equation (A.5) are reduced to only one sum, and the second multipliers from equations (A.2) and (A.7) are reduced to 1, hence the differences between the right and left hand side of equation (A.5) vanish.

Herewith we directly certify the statements of the first paragraph of this Appendix. The state vectors from equation (A.1) are not orthonormal vectors. However the above results give us the possibility to define a set of vectors denoted by superscript $\boldsymbol{\sigma}$ for which $\langle\psi_0^{\boldsymbol{\sigma}}|\psi_{0,\boldsymbol{\sigma}'}\rangle = \delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}'}$. It follows that the vectors from

(A.1) are linearly independent and so form a basis in $\mathfrak{H}_{3N_\Lambda,0}$ of which dual basis is $\{|\psi_0^{\boldsymbol{\sigma}}\rangle \, : \, \boldsymbol{\sigma} = (\sigma_{\mathbf{i}})_{\mathbf{i}=1}^{\mathbf{N}_\Lambda}, \, \sigma_{\mathbf{i}} \in \{\uparrow, \downarrow\}\}$, where

$$|\psi_0^{\boldsymbol{\sigma}}\rangle = \frac{\hat{G}^\dagger}{\det g} (\hat{\mathcal{F}}^{\boldsymbol{\sigma}})^\dagger |0\rangle. \tag{A.9}$$

To compute the inner product of the ground state vectors with sub- and superscript $\boldsymbol{\sigma}$ we take into account that the operator $\hat{G}$ consists of only operators $\hat{C}_{\vec{k},1,\sigma}$ which anticommute all $\hat{C}_{\vec{k},2,\sigma}$ consisted by $\hat{\mathcal{F}}_{\boldsymbol{\sigma}}$ and $\hat{\mathcal{F}}^{\boldsymbol{\sigma}}$, therefore we can use the result (4.12). Then we use the Lemma with $\hat{X}_2 = \hat{X}_f = \hat{1}$, where $\hat{1}$ denotes the identity operator therefore the conditions (A.4) are trivially satisfied.

$$\langle \psi_0^{\boldsymbol{\sigma}'} | \psi_{0,\boldsymbol{\sigma}} \rangle = \langle 0 | \hat{\mathcal{F}}^{\boldsymbol{\sigma}'} \frac{\hat{G}\hat{G}^\dagger}{(\det g)^2} \hat{\mathcal{F}}_{\boldsymbol{\sigma}}^\dagger |0\rangle = \langle 0 | \hat{\mathcal{F}}^{\boldsymbol{\sigma}'} \hat{\mathcal{F}}_{\boldsymbol{\sigma}}^\dagger |0\rangle = \langle 0 | \hat{F}_{\boldsymbol{\sigma}'} \hat{F}_{\boldsymbol{\sigma}}^\dagger |0\rangle = \delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} \tag{A.10}$$

A very similar computation based on the Lemma with $\hat{X}_2 = \hat{C}^\dagger_{\vec{k},2,\sigma} \hat{C}_{\vec{k},2,\sigma}$ and $\hat{X}_f = \hat{f}^\dagger_{\vec{k},\sigma} \hat{f}_{\vec{k},\sigma}$ gives that

$$\langle \psi_0^{\boldsymbol{\sigma}'} | \hat{C}^\dagger_{\vec{k},2,\sigma} \hat{C}_{\vec{k},2,\sigma} | \psi_{0,\boldsymbol{\sigma}} \rangle = \langle 0 | \hat{F}_{\boldsymbol{\sigma}'} \hat{f}^\dagger_{\vec{k},\sigma} \hat{f}_{\vec{k},\sigma} \hat{F}^\dagger_{\boldsymbol{\sigma}} |0\rangle. \tag{A.11}$$

Based on this result we obtain that

$$\begin{aligned}
\langle \psi_0^{\boldsymbol{\sigma}'} | \sum_\sigma \hat{C}^\dagger_{\vec{k},2,\sigma} \hat{C}_{\vec{k},2,\sigma} | \psi_{0,\boldsymbol{\sigma}} \rangle &= \langle 0 | \hat{F}_{\boldsymbol{\sigma}'} \sum_\sigma \hat{f}^\dagger_{\vec{k},\sigma} \hat{f}_{\vec{k},\sigma} \hat{F}^\dagger_{\boldsymbol{\sigma}} |0\rangle \\
&= \frac{1}{N_\Lambda} \sum_{\mathbf{j},\mathbf{j}'} e^{-i\vec{k}(\vec{R}_{\mathbf{j}} - \vec{R}_{\mathbf{j}'})} \sum_\sigma \langle 0 | \hat{F}_{\boldsymbol{\sigma}'} \hat{f}^\dagger_{\mathbf{j},\sigma} \hat{f}_{\mathbf{j}',\sigma} \hat{F}^\dagger_{\boldsymbol{\sigma}} |0\rangle \\
&= \frac{1}{N_\Lambda} \sum_{\mathbf{j},\mathbf{j}'} e^{-i\vec{k}(\vec{R}_{\mathbf{j}} - \vec{R}_{\mathbf{j}'})} \sum_\sigma \delta_{\sigma,\sigma_{\mathbf{j}}} \delta_{\mathbf{j},\mathbf{j}'} \delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} \\
&= \delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}'}.
\end{aligned}$$

From this result immediately follows that the quantum mechanical expectation value of the operator $\sum_\sigma \hat{C}^\dagger_{\vec{k},2,\sigma} \hat{C}_{\vec{k},2,\sigma}$ is uniform in $\mathfrak{H}_{3N_\Lambda,0}$ and equal with 1, independently from $\vec{k}$. An arbitrary element of $\mathfrak{H}_{3N_\Lambda,0}$ can be written as $|\psi_0\rangle =$

$\sum_{\boldsymbol{\sigma}} c_{\boldsymbol{\sigma}} |\psi_{0,\boldsymbol{\sigma}}\rangle$ ($c_{\boldsymbol{\sigma}} \in \mathbb{C}$), thus

$$\begin{aligned}
\frac{\langle\psi_0| \sum_\sigma \hat{C}^\dagger_{\vec{k},2,\sigma} \hat{C}_{\vec{k},2,\sigma} |\psi_0\rangle}{\langle\psi_0|\psi_0\rangle} &= \frac{\sum_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} c^*_{\boldsymbol{\sigma}'} c_{\boldsymbol{\sigma}} \langle\psi_{0,\boldsymbol{\sigma}'}| \sum_\sigma \hat{C}^\dagger_{\vec{k},2,\sigma} \hat{C}_{\vec{k},2,\sigma} |\psi_{0,\boldsymbol{\sigma}}\rangle}{\sum_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} c^*_{\boldsymbol{\sigma}'} c_{\boldsymbol{\sigma}} \langle\psi_{0,\boldsymbol{\sigma}'}|\psi_{0,\boldsymbol{\sigma}}\rangle} \\
&= \frac{\sum_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} c^*_{\boldsymbol{\sigma}'} c_{\boldsymbol{\sigma}} \sum_{\boldsymbol{\sigma}''} \langle\psi_{0,\boldsymbol{\sigma}'}|\psi_{0,\boldsymbol{\sigma}''}\rangle\langle\psi_0^{\boldsymbol{\sigma}''}| \sum_\sigma \hat{C}^\dagger_{\vec{k},2,\sigma} \hat{C}_{\vec{k},2,\sigma} |\psi_{0,\boldsymbol{\sigma}}\rangle}{\sum_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} c^*_{\boldsymbol{\sigma}'} c_{\boldsymbol{\sigma}} \langle\psi_{0,\boldsymbol{\sigma}'}|\psi_{0,\boldsymbol{\sigma}}\rangle} \\
&= 1. \qquad\qquad (A.12)
\end{aligned}$$

Finally we compute the zero temperature limit of the finite temperature expectation value of $\hat{C}^\dagger_{\vec{k},2,\sigma} \hat{C}_{\vec{k},2,\sigma}$. As we have written in Subsection 4.5.1 this can be expressed with trace over the subspace of the ground states.

$$\begin{aligned}
\lim_{T\to 0} \frac{\mathrm{Tr}\, e^{-\beta\hat{H}} \hat{C}^\dagger_{\vec{k},2,\sigma} \hat{C}_{\vec{k},2,\sigma}}{\mathrm{Tr}\, e^{-\beta\hat{H}}} &= \frac{\mathrm{Tr}_{\mathfrak{H}_{3N_\Lambda,0}} \hat{C}^\dagger_{\vec{k},2,\sigma} \hat{C}_{\vec{k},2,\sigma}}{\mathrm{Tr}_{\mathfrak{H}_{3N_\Lambda,0}} \hat{1}} \\
&= \frac{\sum_{\boldsymbol{\sigma}} \langle\psi_0^{\boldsymbol{\sigma}}| \hat{C}^\dagger_{\vec{k},2,\sigma} \hat{C}_{\vec{k},2,\sigma} |\psi_{0,\boldsymbol{\sigma}}\rangle}{\sum_{\boldsymbol{\sigma}} \langle\psi_0^{\boldsymbol{\sigma}}|\psi_{0,\boldsymbol{\sigma}}\rangle} \\
&= \frac{1}{2^{N_\Lambda}} \sum_{\boldsymbol{\sigma}} \langle 0| \hat{F}_{\boldsymbol{\sigma}} \hat{f}^\dagger_{\vec{k},\sigma} \hat{f}_{\vec{k},\sigma} \hat{F}^\dagger_{\boldsymbol{\sigma}} |0\rangle \\
&= \frac{1}{2^{N_\Lambda}} \sum_{\boldsymbol{\sigma}} \frac{1}{N_\Lambda} \sum_{\mathbf{j},\mathbf{j}'} e^{-i\vec{k}(\vec{R}_{\mathbf{j}}-\vec{R}_{\mathbf{j}'})} \langle 0| \hat{F}_{\boldsymbol{\sigma}} \hat{f}^\dagger_{\mathbf{j},\sigma} \hat{f}_{\mathbf{j}',\sigma} \hat{F}^\dagger_{\boldsymbol{\sigma}} |0\rangle \\
&= \frac{1}{2^{N_\Lambda}} \frac{1}{N_\Lambda} \sum_{\mathbf{j},\mathbf{j}'} e^{-i\vec{k}(\vec{R}_{\mathbf{j}}-\vec{R}_{\mathbf{j}'})} \delta_{\mathbf{j},\mathbf{j}'} \sum_{\boldsymbol{\sigma}} \delta_{\sigma,\sigma_{\mathbf{j}}} \\
&= \frac{1}{2}, \qquad\qquad (A.13)
\end{aligned}$$

where we used the results (A.10) and (A.11).

Appendix B

In this Appendix we present mathematical details related to the formulae deduced and presented in Chapter 5. To begin we present an overview of the notations and definitions used; then rather technical proofs follow. For more mathematical details connected to the deduction procedure we refer the reader to the book by Hamermesh [121].

A permutation of a set Λ is a bijective function $\mathcal{P} : \Lambda \to \Lambda$. We said that $\mathcal{P}$ is a permutation of degree N_Λ where N_Λ is the cardinality of Λ. The product of two permutations is defined by the standard composition of them as functions (from right to left): $(\mathcal{P}\mathcal{Q})(i) := \mathcal{P}(\mathcal{Q}(i))$. The set of all the permutations of Λ endowed by this product form a group which is the symmetric group of degree N_Λ. It is denoted by S_Λ. We denote the transposition by $\mathcal{P}^{\mathbf{i},\mathbf{j}}$ which interchanges two elements $\mathbf{i}, \mathbf{j} \in \Lambda$. When Λ is an ordered set, and this is our case, we can use the notation $\mathcal{C}^{\mathbf{i}\to\mathbf{j}}$ for the cyclic permutation (shortly cycle) which takes $\mathbf{m}$ to $\mathbf{m} + sgn(\mathbf{i} - \mathbf{j})$ if $\mathbf{m}$ is in the open interval $]\mathbf{i}, \mathbf{j}[$, takes $\mathbf{i}$ to $\mathbf{j}$, and leaves $\mathbf{m}$ unchanged if $\mathbf{m}$ is out of the closed interval $[\mathbf{i}, \mathbf{j}]$. When $\mathcal{C}^{\mathbf{i}\to\mathbf{j}}$ moves n symbols, i.e. $\mathbf{i} - \mathbf{j} + \mathbf{1} = \mathbf{n}$, then we call $\mathcal{C}^{\mathbf{i}\to\mathbf{j}}$ an n-cycle.

Any permutation can be resolved into a product of transpositions. If this resolution have an even (odd) number of factors, then the permutation is said to be even (odd). The parity of a permutation $\mathcal{P}$ is denoted by $|\mathcal{P}|$ which is 1 if $\mathcal{P}$ is even and -1 if $\mathcal{P}$ is odd. However, the resolution of a permutation is not unique, its parity is well defined. Moreover, any permutation can be resolved uniquely into *independent* cycles. The cycle structure of a permutation $\mathcal{P}$ is a sequence $(C_1, C_2, \dots)$ which means that $\mathcal{P}$ can be resolved into C_1 1-cycle, C_2 2-cycle, etc. Certainly there is no cycle of length l which is greater than the degree of the permutation.

For $\Lambda_e \subset \Lambda$ we treat the group S_{Λ_e} as a natural subgroup of S_Λ, that is the restriction of a permutation $\mathcal{P} \in S_{\Lambda_e} \subset S_\Lambda$ to Λ_e is a bijection onto Λ_e and the restriction of $\mathcal{P}$ to $\Lambda \setminus \Lambda_e$ is the identity function. As a short notation we use $S_{\mathbf{N}} := S_{\{\mathbf{1},\dots,\mathbf{N}\}} \subset S_\Lambda$.

An element $\mathcal{P}$ of the group $S_{\mathbf{N}}$ is said to be conjugate to the element $\mathcal{P}'$ if we can find an element $\mathcal{Q} \in S_{\mathbf{N}}$ such that $\mathcal{Q}^{-1}\mathcal{P}'\mathcal{Q} = \mathcal{P}$. This is an equivalence relation between the elements of $S_{\mathbf{N}}$. This can be used to separate $S_{\mathbf{N}}$ into classes of elements which are conjugate to one another. These are the conjugate classes. A conjugate class can be described by the cycle structure of the permutations contained by it because two permutations have the same cycle structure if and only if they are in the same conjugate class. Therefore we denote a conjugate class of $S_{\mathbf{N}}$ by $C = (C_1, \dots C_N)$. Here the cycle structure of a permutation $\mathcal{P} \in S_{\mathbf{N}}$ is defined as the cycle structure of the function $\mathcal{P}$ restricted to the set $\{\mathbf{1}, \dots, \mathbf{N}\}$, i.e. the $N_\Lambda - N$ pieces of the 1-cycles are neglected. Thus we have $\sum_{i=1}^{N} i\, C_i = N$. From the above also follows that all permutations in the same conjugate class have the same parity.

The group algebra $\mathbb{C}[S_{\mathbf{N}}]$ is a complex Hilbert space generated by the elements of $S_{\mathbf{N}}$ as an orthonormal basis. The associative but noncommutative product of two elements of the group algebra defined by the convolution:

$$\begin{aligned} a\, b &\equiv \Big(\sum_{\mathcal{P}\in S_{\mathbf{N}}} \alpha_{\mathcal{P}}\mathcal{P}\Big)\Big(\sum_{\mathcal{Q}\in S_{\mathbf{N}}} \beta_{\mathcal{Q}}\mathcal{Q}\Big) \\ &= \sum_{\mathcal{P}\in S_{\mathbf{N}}}\sum_{\mathcal{Q}\in S_{\mathbf{N}}} \alpha_{\mathcal{P}}\beta_{\mathcal{Q}}\mathcal{P}\mathcal{Q} = \sum_{\mathcal{P}\in S_{\mathbf{N}}}\Big(\sum_{\mathcal{Q}\in S_{\mathbf{N}}} \alpha_{\mathcal{Q}}\beta_{\mathcal{Q}^{-1}\mathcal{P}}\Big)\mathcal{P}. \end{aligned}$$

If a subalgebra $\Im$ has the property that, for a in $\Im$, ab is also in $\Im$ for any elements b of the whole algebra, then $\Im$ is called a right ideal. If e is an idempotent element of the algebra ($ee = e$), then $e\mathbb{C}[S_{\mathbf{N}}] = \{e\ a\ :\ a \in \mathbb{C}[S_{\mathbf{N}}]\}$ is a right ideal, because of the associativity of the group algebra. It remains true if e is only essentially idempotent ($e\ e = ce, c \in \mathbb{C}$) because $e' = e/c$ is idempotent.

Now we verify that the Hilbert space generated by all the vectors $|\bar{\mathcal{P}}_{S^z}\rangle$ is isomorphic with a proper right ideal of the group algebra $\mathbb{C}[S_{\mathbf{N}}]$. (In the following N and S^z are fixed.) We recall that for fixed S^z we denote by σ^0 the following function: $\sigma^0(\mathbf{i}) :=\uparrow$ if $\mathbf{i} \in \{\mathbf{1}, \dots, \mathbf{N}_\uparrow\}$ (here $N_\uparrow = N/2 + S^z$) and $\sigma^0(\mathbf{i}) :=\downarrow$ if $\mathbf{i} \in \{\mathbf{N}_\uparrow\mathbf{+1}, \dots, \mathbf{N}\}$. Let us denote the subgroup of $S_{\mathbf{N}}$ the elements of which permute the labels of the set $(\sigma^0)^{-1}(\uparrow)$ by $K_\uparrow = S_{(\sigma^0)^{-1}(\uparrow)}$. Similarly, the permutations of $K_\downarrow = S_{(\sigma^0)^{-1}(\downarrow)}$ permute only the $(\sigma^0)^{-1}(\downarrow)$ labels. The direct product of $K_\uparrow$ and $K_\downarrow$ was denoted in Subsection 5.1.1 by K_{S^z}, that is $K_{S^z} = K_\uparrow \times K_\downarrow$. Now one can see that

$$e_{S^z} := \frac{1}{\sqrt{|K_{S^z}|}} \sum_{\mathcal{P}\in K_{S^z}} \mathcal{P} \tag{B.1}$$

is essentially idempotent, ($|K_{S^z}| = N_\uparrow! N_\downarrow!$ is the order of the subgroup K_{S^z}); therefore $\Im(S^z) := e_{S^z}\mathbb{C}[S_{\mathbf{N}}]$ is a right ideal. For different permutations $\mathcal{P}$ and $\mathcal{Q}$ the elements $e_{S^z}\mathcal{P}$ and $e_{S^z}\mathcal{Q}$ of the ideal $\Im(S^z)$ are the same if and only if the permutations are in the same right coset with respect to the subgroup K_{S^z} (i.e. we can find an element $\mathcal{P}' \in K_{S^z}$ such that $\mathcal{P} = \mathcal{P}'\mathcal{Q}$), because in the expression $\sum_{\mathcal{P}\in K_{S^z}} \mathcal{P}\mathcal{P}'\mathcal{Q} = \sum_{\mathcal{P}''\in K_{S^z}} \mathcal{P}''\mathcal{Q} = \sum_{\mathcal{Q}'\in\bar{\mathcal{Q}}} \mathcal{Q}'$ the sum is taken over the right coset $\bar{\mathcal{Q}} = K_{S^z}\mathcal{Q}$, and they form a disjoint cover of the group.

The previous paragraph prove that the map $|\bar{\mathcal{P}}_{S^z}\rangle \to e_{S^z}\mathcal{P}$ is well-defined and injective. Let us extend this map linearly over the whole $\mathfrak{H}_s(S^z)$, which is the space generated by the vectors $|\bar{\mathcal{P}}_{S^z}\rangle$ as an orthonormal basis. Certainly we get a surjective map onto $\Im(S^z)$, since the elements $e_{S^z}\mathcal{P}$ generate this ideal. Now we show that this linear isomorphism also preserves the inner product. In the proof we denote the inner product in the group algebra by $(.,.)$.

$$\begin{aligned}(e_{S^z}\mathcal{P}, e_{S^z}\mathcal{Q}) &= \left(\frac{1}{\sqrt{|K_{S^z}|}}\sum_{\mathcal{S}_1\in K_{S^z}} \mathcal{S}_1\mathcal{P}, \frac{1}{\sqrt{|K_{S^z}|}}\sum_{\mathcal{S}_2\in K_{S^z}} \mathcal{S}_2\mathcal{Q}\right) \\ &= \frac{1}{|K_{S^z}|}\sum_{\mathcal{P}'\in\bar{\mathcal{P}}}\sum_{\mathcal{Q}'\in\bar{\mathcal{Q}}} (\mathcal{P}', \mathcal{Q}'). \end{aligned} \tag{B.2}$$

If the right cosets $\bar{\mathcal{P}}_{S^z} = K_{S^z}\mathcal{P}$ and $\bar{\mathcal{Q}}_{S^z} = K_{S^z}\mathcal{Q}$ are different, then they have no common elements; therefore $(\mathcal{P}', \mathcal{Q}') = 0$. (The elements $\mathcal{P} \in S_{\mathbf{N}}$ are orthonormals by definition.) If the right cosets $\bar{\mathcal{P}}_{S^z}$ and $\bar{\mathcal{Q}}_{S^z}$ are the same then the sums have $|K_{S^z}|$ different members which give 1 (in the case $\mathcal{P}' = \mathcal{Q}'$), and the rest are zero; so the final result is 1.

We showed that the Hilbert space $\mathfrak{H}_s(S^z)$ generated by the vectors $|\bar{\mathcal{P}}_{S^z}\rangle$ as an orthonormal basis is isomorphic with $\Im(S^z)$. Based on the above defined Hilbert space isomorphism we identify $\mathfrak{H}_s(S^z)$ with $\Im(S^z)$ and we no longer distinguish between the notations for the inner product and the operators that act on them. We can regard a linear operator defined on $\Im(S^z)$ as an operator on $\mathfrak{H}(S^z)$ and vice versa.

A homomorphism $\mathbb{T}$ from a group G into the group of the regular linear transformations of a linear space is called a (linear) representation of the group. The trace of the linear operator $\mathbb{T}[g]$ is called the character of the group element $g \in G$ in the representation $\mathbb{T}$ and is denoted by $\chi(g)$. Every character is constant on an arbitrary conjugate class therefore we can define $\chi(C) := \chi(g)$ where $g \in C$ is arbitrary. The formula

$$\mathbb{T}[\mathcal{Q}]\mathcal{P} := (-1)^{|\mathcal{Q}|}\mathcal{P}\mathcal{Q}^{-1} \tag{B.3}$$

defines a representation of the symmetric group in the group algebra. Here $\mathbb{T}[\mathcal{Q}]$ is a linear operator associated the $\mathcal{Q} \in S_{\mathbf{N}}$ by the representation $\mathbb{T}$, and $\mathcal{P}$ is a vector as an element of $\mathbb{C}[S_{\mathbf{N}}]$. This representation is fully reducible. It is clear from the definition that every right ideal is an invariant subspace of this representation; thus restricted the above defined linear operators $\mathbb{T}[\mathcal{Q}]$ to the subspace $\Im(S^z)$ we obtain also a representation (with lower dimension) of the symmetric group in $\Im(S^z)$.

Taking into account the above defined identification of $\Im(S^z)$ and $\mathfrak{H}(S^z)$ we have found a linear representation of $S_{\mathbf{N}}$ in $\mathfrak{H}(S^z)$; we denote this reduced representation by $\mathbb{T}^{S^z}$. Comparing this representation and the effect of the Hamiltonian on a basis vector $|\tilde{\mathcal{R}}\rangle \otimes |\bar{\mathcal{P}}_{S^z}\rangle$ as can be seen from equation (5.5), it is clear that the effect on the spin configuration can be described by the operator $\mathbb{T}^{S^z}[\mathcal{C}(\mathcal{R};\mathbf{i},\mathbf{j})]$, and we obtain equation (5.6).

Now we compute the character of the representation $\mathbb{T}^{S^z}$.

$$\begin{aligned}\chi^{S^z}(\mathcal{P}) &= \sum_{\bar{\mathcal{Q}}_{S^z}} \langle \bar{\mathcal{Q}}_{S^z} | \mathbb{T}^{S^z}[\mathcal{P}] | \bar{\mathcal{Q}}_{S^z}\rangle = \frac{1}{|K_{S^z}|} \sum_{\mathcal{Q}\in S_{\mathbf{N}}} \langle e_{S^z}\mathcal{Q}|\mathbb{T}^{S^z}[\mathcal{P}]|e_{S^z}\mathcal{Q}\rangle \\ &= \frac{1}{|K_{S^z}|}\sum_{\mathcal{Q}\in S_{\mathbf{N}}} \langle e_{S^z}\mathcal{Q}|(-1)^{|\mathcal{P}|} e_{S^z}\mathcal{Q}\mathcal{P}^{-1}\rangle = \frac{(-1)^{|\mathcal{P}|}}{|K_{S^z}|^2}\sum_{\mathcal{Q}\in S_{\mathbf{N}}}\sum_{\mathcal{S}_1,\mathcal{S}_2\in K_{S^z}} \langle \mathcal{S}_1\mathcal{Q}|\mathcal{S}_2\mathcal{Q}\mathcal{P}^{-1}\rangle \\ &= \frac{(-1)^{|\mathcal{P}|}}{|K_{S^z}|^2}\sum_{\mathcal{Q}\in S_{\mathbf{N}}}\sum_{\mathcal{S}_1,\mathcal{S}_2\in K_{S^z}} \delta_{\mathcal{S}_1\mathcal{Q},\mathcal{S}_2\mathcal{Q}\mathcal{P}^{-1}} = \frac{(-1)^{|\mathcal{P}|}}{|K_{S^z}|}\sum_{\mathcal{Q}\in S_{\mathbf{N}}}\sum_{\mathcal{S}\in K_{S^z}} \delta_{\mathcal{Q}\mathcal{P}\mathcal{Q}^{-1},\mathcal{S}}. \end{aligned} \tag{B.4}$$

Let us denote by $C^{\mathcal{P}}$ the conjugate class which contains $\mathcal{P}$. Every element $\mathcal{P}'$ of the conjugate class $C^{\mathcal{P}}$ appears as $\mathcal{Q}\mathcal{P}\mathcal{Q}^{-1}$ the same number of times. That is why there are $|S_{\mathbf{N}}| \,/\, |C^{\mathcal{P}}|$ permutations $\mathcal{Q}$ for which $\mathcal{Q}\mathcal{P}\mathcal{Q}^{-1} = \mathcal{P}'$. ($|X|$ means the number of the elements of the set X.) If $\mathcal{P}'$ is in K_{S^z}, then the second sum in the last row of equation (B.4) has one non-zero element; otherwise it does not. Therefore the character

$$\begin{aligned}\chi^{S^z}(\mathcal{P}) &= (-1)^{|\mathcal{P}|}\frac{|S_{\mathbf{N}}||C^{\mathcal{P}}\cap K_{S^z}|}{|K_{S^z}||C^{\mathcal{P}}|} \\ &= (-1)^{|\mathcal{P}|} \sum_{\substack{c'_1,\,c''_1,\,\ldots,\,c'_N,\,c''_N \\ c'_1+c''_1 = C^{\mathcal{P}}_1,\,\ldots,\,c'_N+c''_N = C^{\mathcal{P}}_N \\ c'_1+2c'_2+\cdots+Nc'_N = N/2+S^z \\ c''_1+2c''_2+\cdots+Nc''_N = N/2-S^z}} \frac{C^{\mathcal{P}}_1!}{c'_1!c''_1!}\cdots\frac{C^{\mathcal{P}}_N!}{c'_N!c''_N!} \\ &= (-1)^{|\mathcal{P}|}\sum_{\substack{c_1,\,\ldots,\,c_N \\ \sum_{i=1}^N ic_i = N/2+S^z}} \prod_{i=1}^{N}\binom{C^{\mathcal{P}}_i}{c_i}, \end{aligned} \tag{B.5}$$

where the cycle structure of the permutations of the conjugate class $C^{\mathcal{P}}$ is described by $(C^{\mathcal{P}}_1, C^{\mathcal{P}}_2, \ldots, C^{\mathcal{P}}_N)$. For the second equality see the equation (7-16) in Section 7-2 of Ref.[121]; the third can be obtained with simple computation.

We need the sum of these characters on an arbitrary conjugate class $C \subset A_N$ where A_N is the alternating group formed by all the even permutations of $S_{\mathbf{N}}$. Based on the first line of equation (B.5) we can see that

$$\sum_{C\subset A_N} |C|\chi^{S^z}(C) = \frac{N!}{|K_{S^z}|}|A_N\cap K_{S^z}| = \frac{N!}{2}. \tag{B.6}$$

A similar sum over the conjugate class which has no common element with A_N gives the result $-N!/2$. The even permutations form an invariant subgroup in $S_{\mathbf{N}}$; therefore every conjugate class is in A_N or disjoint from it. Hence $\sum_{C\subset S_{\mathbf{N}}} |C|\chi^{S^z}(C) = 0$.

Based on the last line of equation (B.5) we can obtain:

$$\sum_{S^z=-N/2}^{N/2} \chi^{S^z}(C) = (-1)^{|C|} 2^{\sum_{i=1}^{N} C_i}. \tag{B.7}$$

Furthermore

$$\sum_{S^z=-N/2}^{N/2} (S^z)^2 \chi^{S^z}(C) = (-1)^{|C|} 2^{\sum_{i=1}^{N} C_i} \left(\frac{1}{4} \sum_{i=1}^{N} i^2 C_i \right). \tag{B.8}$$

The representation $\mathbb{T}^{S^z}$ is not irreducible if $S^z \neq \pm S^z_{max}$ (hereafter we use the notations $S^z_{max} = S_{max} = N/2$). Certainly it can be verified in pure mathematical way, but physically it is due to the SU(2) rotational symmetry in the spin space. The operator $\hat{S}^-$ realizes a linear bijection between the spaces $\mathfrak{H}_s(S^z, S)$ and $\mathfrak{H}_s(S^z - 1, S)$ if $-S + 1 \leq S^z \leq S$. Moreover $[\hat{H}_\infty, \hat{S}^-] = 0$, therefore the effect of the Hamiltonian is equivalent on the space $\mathfrak{H}_s(S^z, S)$ and $\mathfrak{H}_s(S^z - 1, S)$. The effect of the Hamiltonian on the space $\mathfrak{H}_s(S^z_{max}) = \mathfrak{H}_s(S^z_{max}, S_{max})$ can be described by the representation $\mathbb{T}^{S^z_{max}} =: \mathbb{T}_{S_{max}}$; hence it is true for the space $\mathfrak{H}_s(S^z_{max} - 1, S_{max})$. However, the effect of the Hamiltonian on $\mathfrak{H}_s(S^z_{max} - 1)$ is described by the representation $\mathbb{T}^{S^z_{max}-1}$. According to the above, the operators $\mathbb{T}^{S^z_{max}-1}[\mathcal{P}]$ restricted to $\mathfrak{H}_s(S^z_{max} - 1, S_{max})$ forms the representation $\mathbb{T}_{S_{max}}$, thus $\mathfrak{H}_s(S^z_{max} - 1, S_{max})$ is an invariant subspace of the representation $\mathbb{T}^{S^z_{max}-1}$. Therefore $\mathbb{T}^{S^z_{max}-1}$ is not irreducible and thus it is fully reducible (because it is a finite dimensional representation of a finite group). Therefore the orthogonal complement of $\mathfrak{H}_s(S^z_{max} - 1, S_{max})$ which is $\mathfrak{H}_s(S^z_{max} - 1, S_{max} - 1)$ is also an invariant subspace. The restriction of $\mathbb{T}^{S^z_{max}-1}$ to this subspace we denote by $\mathbb{T}_{S_{max}-1}$. Continuing this process along this line, acting by $\hat{S}^-$ again and again, we obtain: $\mathbb{T}^{S^z} \cong \oplus_{S=|S^z|}^{N/2} \mathbb{T}_S$.

In other words this means that the restriction of the linear operators $\mathbb{T}^{S^z}[\mathcal{P}]$ to $\mathfrak{H}_s(S^z, S)$ form a representation of the symmetric group. This above defined representation depending only on the value of S is denoted by $\mathbb{T}_S$, and the effect of the Hamiltonian on the spin configuration can be described by this representation. The matrices of the representations $\mathbb{T}_S$ can be given by algebraic methods, see e.g. [121]. These methods are usable only in case of few particles. In this case we can use the Schrödinger equation (5.7) to obtain numerically exact energy eigenvalues.

Bibliography

[1] P. Gurin and Zs. Gulácsi, Low Temp. Phys. 21 Conference, Prague, published in: Czech. J. Phys. **46 S5**, 2643 (1996).

[2] P. Gurin and Zs. Gulácsi, Phil. Mag. B **76**, 827 (1997).

[3] P. Gurin and Zs. Gulácsi, Phil. Mag. B **78**, 315 (1998).

[4] P. Gurin and Zs. Gulácsi, Phil. Mag. B **81**, 321 (2001).

[5] P. Gurin and Zs. Gulácsi, Phil. Mag. B, in press

[6] P. Gurin and Zs. Gulácsi, Phys. Rev. B, in press

[7] J. Hubbard, Proc. Roy. Soc. A **276**, 238 (1963).

[8] M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963).

[9] J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963).

[10] P. W. Anderson, Science **235**, 1196 (1987).

[11] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).

[12] H. Frahm and V. E. Korepin, Phys. Rev. B **42**, 10553 (1990).

[13] J. Sólyom, Adv. Phys. **28**, 201 (1979).

[14] S. R. Julian, P. A. A. Teunissen and S. A. J. Wiegers, Phys. Rev. B **46**, 9821 (1992).

[15] S. Doniach, Physica B **91**, 231 (1977).

[16] H. von Löhneysen, A. Shröder, M. Sieck and T. Trappmann, Phys. Rev. Lett. **72**, 3262 (1994).

[17] D. L. Cox, Phys. Rev. Lett. **59**, 1240 (1987); J. Phys. Cond. Mat. **8**, 9825 (1996).

[18] A. Rosch, A. Schröder, O. Stockert and H. von Löhneysen, Phys. Rev. Lett. **79**, 159 (1997).

[19] V. Dobrosavljevic, T. R. Kirkpatrick and G. Kotliar, Phys. Rev. Lett. **69**, 1113 (1992).

[20] A. J. Millis, Phys. Rev. B **48**, 7183 (1993).

[21] C. M. Varma, Phys. Rev. Lett. **83**, 3538 (1999).

[22] E. H. Lieb and D. C. Mattis, Phys. Rev. **125**, 164 (1962).

[23] E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).

[24] R. Shankar, Rev. Mod. Phys. **66**, 129 (1994).

[25] R. Strack and D. Vollhardt, J. of Low Temp. Phys. **99**, 385 (1995).

[26] A. Mielke and H. Tasaki, Commun. Math. Phys. **158**, 341 (1993).

[27] D. K. Campbell, J. T. Gammel and E. Y. Loh, Jr., Phys. Rev. B **38**, 12043 (1988); *ibid.* **42**, 475 (1990).

[28] P. Fazekas, B. Menge and E. Müller-Hartmann, Z. Phys. **78**, 69 (1990).

[29] B. S. Shastry, H. R. Krishnamurthy and P. W. Anderson, Phys. Rev. B **41**, 2375 (1990).

[30] A. Sütő, Commun. Math. Phys. **140**, 43 (1991).

[31] B. Doucot and X. G. Wen, Phys. Rev. B **40**, 2719 (1989).

[32] Y. Nagaoka, Phys. Rev. **147**, 392 (1966).

[33] Y. Nagaoka, Solid State Commun. **3**, 409 (1965).

[34] D. J. Thouless, Proc. Phys. Soc. **86**, 893 (1965).

[35] H. Tasaki, Phys. Rev. B **40**, 9192 (1989).

[36] B. Tóth, Lett. in Math. Phys. **22**, 321 (1991).

[37] E. V. Kuzmin, Pis'ma Zh. Eksp. Teor. Fiz. **57**, 575 (1993).

[38] S. A. Trugman, Phys. Rev. B **42**, 6612 (1990).

[39] G. S. Tian, Phys. Rev. B **44**, 4444 (1991).

[40] S. Q. Shen, Z. M. Qiu and G. S. Tian, Phys. Lett. A **178**, 426 (1993).

[41] E. H. Lieb, Advances in Dynamical Systems and Quantum Physics, World Scientific, (1995), cond-mat/9311033.

[42] R. Strack and D. Vollhardt, Phys. Rev. Lett. **72**, 3425 (1994).

[43] A. Montorsi and D. K. Campbell, Phys. Rev. B **53**, 5153 (1996).

[44] J. de Boer and A. Schadschneider, Phys. Rev. Lett. **75**, 4298 (1995).

[45] C. Verdozzi and M. Cini, Phys. Rev. B **51**, 7412 (1995).

[46] C. Verdozzi, NATO Advanced Study Institute Series B, Physics, Kluwer and Dordrecht, pg. 237 (1993).

[47] D. M. King, Z.-X. Shen, D. S. Dessau, B. O. Wells, W. E. Spicer, A. J. Arko, D. S. Marshall, J. DiCarlo, A. G. Loeser, C. H. Park, E. R. Ratner, J. L. Peng, Z. Y. Li and R. L. Greene, Phys. Rev. Lett. **70**, 3159 (1993).

[48] W. Bering, Phys. Rep. **251**, 155 (1995).

[49] R. R. P. Singh, P. A. Fleury, K. B. Lyons and P. E. Sulewski, Phys. Rev. Lett. **62**, 2736 (1989).

[50] A. P. Kampf, Phys. Rep. **249**, 222 (1994).

[51] D. J. Scalapino, Phys. Rep. **250**, 331 (1995).

[52] T. Koma and H. Tasaki, Phys. Rev. Lett. **68**, 3248 (1992).

[53] A. F. Veilleux, A. M. Daré, L. Chen, Y. M. Vilk and A. M. S. Tremblay, Phys. Rev. B **52**, 16255 (1995).

[54] R. Strack, Phys. Rev. Lett. **70**, 833 (1993).

[55] J. Kondo, Prog. Theor. Phys. Jap. **32**, 37 (1964).

[56] J. R. Schrieffer and P. A. Wolf, Phys. Rev. **149**, 491 (1966).

[57] N. Read and D. m. Newns, Adv. Phys. **36**, 799 (1987).

[58] T. M. Rice and K. Ueda, Phys Rev. Lett. **55**, 995 (1985); **55**, 2093(E) (1985); Phys. Rev. B **34**, 6420 (1986).

[59] H. J. Leder and B. Mühlschlegel, Z. Phys. B **29**, 341 (1978).

[60] W. Metzner, Advances in Phys. **47**, 317 (1998).

[61] P. W. Anderson, Phys. Rev. Lett. **64**, 1839 (1990); *ibid.* **65**, 2306 (1991).

[62] N. D. Mathur, F. M. Grosche, S. R. Julian, I. R. Walker, D. M. Freye, R. K. W. Haselwimmer and G. G. Lonzarich, Nature **394**, 39 (1998).

[63] P. K. de Boer and R. A. de Groot, Phys. Rev. B **60**, 10758 (1999).

[64] M. Gulácsi, Phil. Mag. B **76**, 731 (1996).

[65] D. Vollhardt and P. Wolfle, The superfluid phases of Helium 3, Taylor and Francis, (1990).

[66] L. D. Landau, Sov. Phys. JETP. **8**, 70 (1959).

[67] P. Nozieres, Theory of Interacting Fermi Systems, New York, Benjamin, (1964).

[68] G. D. Mahan, Many Body Physics, Plenum, (1990).

[69] J. M. Luttinger, Phys. Rev. **119**, 1153 (1960).

[70] D.Koelle, R. Kleiner, F. Ludwig, E. Dantsker and J. Clarke, Rev. Mod. Phys. **71**, 631 (1999); L. Degiorgi *ibid.* **71**, 687 (1999).

[71] D. R. Temprano, J. Mesot, S. Janssen, K. Conder, A. Furrer, H. Mutka and K. A. Müller, Phys. Rev. Lett. **84**, 1990 (2000).

[72] P. Nozieres and F. Pistolesi, Eur. Phys. Jour. B **10**, 649 (1999).

[73] F. D. M. Haldane, Jour. Phys. C **14**, 2585 (1994).

[74] A. A. Aligia, L. Arrachea and E. R. Gagliano, Phys. Rev. B **51**, 13774 (1995).

[75] J. Appel, M. Grodzicky and F. Paulsen, Phys. Rev. B **47**, 2812 (1993).

[76] J. de Boer, V. Korepin and A. Schadschneider, Phys. Rev. Lett. **74**, 789 (1995).

[77] U. Brandt and A. Giesekus, Phys. Rev. Lett. **68**, 2648 (1992).

[78] W. Brenig, Physics Reports **251**, 155 (1995).

[79] R. Fehrenbacher and M. R. Norman, Phys. Rev. Lett. **74**, 3884 (1995).

[80] F. D. M. Haldane, Phys. Rev. Lett. **60**, 635 (1988).

[81] F. D. M. Haldane and B. S. Shastry, Phys. Rev. Lett. **60**, 639 (1988).

[82] U. Löw, V. J. Emery, K. Fabritius and S. A. Kivelson, Phys. Rev. Lett. **72**, 1918 (1994).

[83] A. A. Ovchinikov, Mod. Phys. Lett. B **7**, 1397 (1993).

[84] R. Strack and D. Vollhardt, Phys. Rev. Lett. **70**, 2637 (1993).

[85] M. Kollar, R. Strack and D. Vollhardt, Phys. Rev. B **53**, 9225 (1996).

[86] Zs. Szabo and Zs. Gulácsi, Phil. Mag. B **76**, 911 (1997).

[87] M. Troyer, H. Tsunetsugu and T. M. Rice, Phys. Rev. B **53**, 251 (1996).

[88] F. Wenger and S. Östlund, Phys. Rev. B **47**, 5977 (1993).

[89] I. Orlik and Zs. Gulácsi, Phil. Mag. Lett. **78**, 177 (1998).

[90] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994); A. Nazarenko, K. J. E. Vos, S. Haas, E Dagotto and R. J. Gooding, Phys. Rev. B. **51**, 8676 (1995).

[91] N. Bulut, D. J. Scalapino and S. R. White, Phys. Rev. B. **50**, 7215 (1994).

[92] R. Preuss, W. Hanke, C. Grober and H. G. Evertz, Phys. Rev. Lett. **79**, 1122 (1997).

[93] F. F. Assaad and M. Imada, Eur. Phys. Jour. B. **10**, 595 (1999).

[94] K. Gofron, J. C. Campuzano, A. A. Abrikosov, M. Lindroos, A. Bansil, H. Ding, D. Koelling and B. Dabrowski, Phys. Rev. Lett. **73**, 3302 (1994).

[95] Z.-X. Shen and D. S. Dessau, Phys. Rep. **253**, 1 (1995).

[96] H. Ding, A. F. Bellman, J. C. Campuzano, M. Randeria, M. R. Norman, T. Yokoya, T. Takahashi, H. Katayama-Yoshida, T. Mochiku, K. Kadowaki, G. Jennings and G. P. Brivio, Phys. Rev. Lett. **76**, 1533 (1996).

[97] Y.-D. Chuang, A. D. Gromko, D. S. Dessau, Y. Aiura, Y. Yamaguchi, K. Oka, A. J. Arko, J. Joyce, H. Eisaki, S. I. Uchida, K. Nakamura and Yoichi Ando, Phys. Rev. Lett. **83**, 3717 (1999).

[98] M. Imada and M. Kohno, Phys. Rev. Lett. **84**, 143 (2000).

[99] T. Ito, H. Kumigashira, Hyeong-Do Kim, T. Takahashi, N. Kimura, Y. Haga, E. Yamamoto, Y. Onuki and H. Harima, Phys. Rev. B **59**, 8923 (1999).

[100] P. E. Lammert, P. Zhang and V. H. Crespi, Phys. Rev. Lett. **84**, 2453 (2000).

[101] A. Mielke, Phys. Lett. A **174**, 443 (1993); H. Tasaki, Phys. Rev. Lett. **69**, 1608 (1992).

[102] A. L. Chernyshev and P. W. Leung, Phys. Rev. B **60**, 1592 (1999).

[103] P. W. Anderson, Adv. in Phys. **46**, 3 (1997).

[104] S. A. Trugman, Phys. Rev. B **41**, 892 (1990).

[105] E. Louis, F. Guinea, S. M. P. López and J. A. Vergés, Phys. Rev. B **59**, 14005 (1999).

[106] S. A. Trugman, Phys. Rev. B **37**, 1597 (1988).

[107] S. Ishihara, M. Yamanaka and N. Nagaosa, Phys. Rev. B **56**, 686 (1997).

[108] Y. Watanabe and S. Miyashita, Jour. Phys. Soc. Jpn. **68**, 3086 (1999).

[109] M. W. Long and X. Zotos, Phys. Rev. B **45**, 9932 (1992).

[110] M. W. Long and X. Zotos, Phys. Rev. B **48**, 317 (1993).

[111] E. Louis, G. Chiappe, F. Guinea, J. A. Vergés and E. V. Anda, Phys. Rev. B **48**, 9581 (1993).

[112] D. C. Mattis, Rev. Mod. Phys. **58**, 361 (1986).

[113] A. Barbieri, J. A. Riera and A. P. Young, Phys. Rev. B **41**, 11697 (1990).

[114] F. Gebhard and X. Zotos, Phys. Rev. B **43**, 1176 (1991).

[115] A. L. Chernyshev, P. W. Leung and R. J. Gooding, cond-mat 9806018.

[116] M. Takahashi, Jour. Phys. Soc. Jpn. **51**, 8475 (1982).

[117] D. Vollhardt, N. Blümer, K. Held, M. Kollar, J. Schlipf, M. Ulmke and J. Wahle, Advances in Solid State Physics, Vol. 38. (1998).

[118] E. H. Lieb and M. Aizenman, Phys. Rev. Lett. **65**, 1470 (1990).

[119] A. Sütő, Phys. Rev. B **43**, 8779 (1991).

[120] L. Arrachea, Phys. Rev. B **62**, 10033 (2000).

[121] M. Hamermesh, Group theory and its application to physical problems, Addison-Wesley Publishing Company, Inc. (1962).