Many-Body Effects in the Persistent-Current Problem

by

Tilmann Hickel

A Master's Thesis

Submitted in partial fulfilment of the requirements for the award of Master of Philosophy of Loughborough University

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Abstract

In this work some many-body properties of isolated mesoscopic rings are investigated. Second quantization and tight-binding models for systems of spinless fermions and fermions with spin are used to derive an expression for the persistent current. The results obtained for non-interacting systems are in satisfactory agreement with both experimental measurements and other theoretical results. Then a Coulomb repulsion is considered for a system of interacting fermions and a variational approach is adopted. We attempt to improve the description of the system by introducing rotations of the spin-quantization axis on each site. Then we go on to show how the emergent Hartree-Fock equations may be treated, what kind of effects have to be considered and how the trial wave functions can be chosen accordingly.

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Introduction

Within the last few years a rapid development of technology has stimulated many interesting investigations in condensed matter physics. The ability to manage temperatures well below 1 Kelvin and to create systems of dimensionality of a few micrometers allows the observation of quantum effects which were hidden before. Even in normal conducting metals it is now possible to obtain situations where the coherence length of the electron wave function becomes comparable to the system size; this is called **mesoscopics**.

In this field the **persistent-current problem** has aroused particular interest. It provides an excellent possibility to compare the results of complicated theoretical many-body descriptions of these materials with real experimental measurements. A persistent current appears when single, isolated normal-metal rings are threaded by a magnetic flux. The basic observation is that this current depends on the flux in a characteristic way: a linearly increased magnetic field leads to an oscillation in the current. The period of this oscillation is the elementary flux quantum $\Phi_0 = \frac{hc}{e}$. Here h is the Planck constant, c is the speed of light and e is the charge of an electron.

The History of the Persistent Current

Observation

It is interesting that the history of the persistent current had already started a long time before the experimental evidence was found. For instance, a work by **Aharonov** and **Bohm** from 1959 [1] is mentioned very often when flux-dependent fluctuations of currents are investigated. These authors actually tried to prove

the physical existence of the vector potential **A** by suggesting an experiment in which an electron beam is split in two separate beams that enclose a solenoid and is recombined afterwards. Although the electrons only move in field-free space they still experience the vector potential connected to the flux Φ through the solenoid. Simple considerations as well as exact solutions of the scattering problem led to the result that the current of the recombined beam depends on the phase difference $\Delta S/\hbar = \frac{e}{\hbar c}\Phi$. Thus, the current is periodic with respect to the flux in the middle of the two beams.

The work of **Büttiker, Imry** and **Landauer** [2] in 1983 is usually quoted to be the first paper that predicted the existence of a persistent current in small one-dimensional rings. They pointed out that closing a random potential to a ring results in a periodic potential with the typical Bloch-like band structure in reciprocal space. An accelerating electrical field E forces the charged particles to move within the first Brillouin zone. As soon as the field is switched off the movement stops, and the current remains with a fixed momentum, which does not necessarily have to be zero. According to Büttiker, Imry and Landauer this effect leads to a persistent current within the ring. It is also mentioned in the paper that the existence of an accelerating field is equivalent to the appearance of an external flux through the ring which increases linearly in time. Furthermore, the frequency of the movement through the band is the same as for superconducting rings with a Josephson junction, except that $2e$ is replaced by e.

In 1990 **Lévy** *et al* [3] were the first to provide clear evidence for the existence of persistent currents with their results of measurements on mesoscopic copper rings. They used 10^7 "rings" of copper, which actually had a square shape and were located within an area of 7mm^2. The circumference of each of the rings was $L \approx 2.2\mu\text{m}$. The measured quantity was the magnetisation within a SQUID magnetometer. Lévy *et al* considered not only the value of the second and third harmonics of the momentum, $\mu_{2,3}$, for $T = 0$, but also their temperature dependence over an interval of 7 to 400 mK. Theoretical assumptions predict an exponential decrease according to the law $\mu_{2,3}(T) = \mu_{2,3}(0)\exp\left[-\frac{k_B T}{L_c}\right]$ leaving only $\mu_{2,3}(0)$ as a free parameter for fits. (E_c is the correlation energy and can be estimated.) The results in general confirm the theory used. Especially, an

oscillatory behaviour in the flux dependence of the magnetic moment was clearly observed, which indicates the existence of a persistent current. The magnitude of the moment is estimated to be $1.2 \cdot 10^{-15}\mathrm{Am}^2$, corresponding to an ensemble-averaged current of $0.4\mathrm{nA} \approx 3 \cdot 10^{-3}\frac{ev_F}{L}$ per ring. However, probably because of the necessary averaging over a whole system of rings the period of oscillation was found to be $\Phi_0/2$ (not Φ_0).

Only one year later **Chandrasekhar** *et al.* [4] published the results of their experiments on the magnetic response of a single, isolated gold loop. Because of the absence of an ensemble averaging they were successful in finding a whole flux quantum oscillation. Three different kinds of gold loops, fabricated on oxidized Si substrates using an electron-beam lithography process, were used. Their diameter was 2.4 μm, 4.0 μm (circle) and 1.4 μm $\times$ 2.6 μm (rectangular), respectively. In the temperature range around 10 mK an electron phase-coherence length of 12 μm and a thermal diffusion length of 8.7 μm allow the appearance of mesoscopic effects. The analysis of the data of a dc-SQUID magnetometer was connected with a number of problems. First of all background fluctuation of the same order of magnitude as persistent current effects made it difficult to extract signals. Secondly, the temperature dependence was ambiguous and did not show exactly the expected exponential behaviour. Thus, it was not possible to extrapolate the data to zero temperature. Nevertheless, all three gold loops showed an oscillation in the magnetic response with the period $\frac{hc}{e}$. This was the case for the fundamental as well as for the first harmonic signals. However, the amplitude of this oscillatory component corresponds to a persistent current of $(0.3 - 2.0)\frac{ev_F}{L}$. This is more than one order of magnitude larger than predicted by simple theoretical considerations for the diffusion.

Later, in 1993 **D. Mailly, C. Chapelier** and **A. Benoit** [5] reported about persistent currents in semiconductor single loops. Their GaAlAs/GaAs ring had an internal diameter of 2 μm and an external diameter of 3.4 μm. In the temperature range around 15 mK the elastic mean free path was 11 μm, which corresponds to a very weak disorder. The channel number, arising due to the three-dimensional geometry of the ring, was with approximately 4 channels extremely small, too. A modulation of the external magnetic field and a Fourier

transformation lead to power spectrums which clearly show the Aharonov-Bohm oscillation with the period $\frac{hc}{e}$. The high sensitivity of the SQUID magnetometer allowed a clear distinction between noise and signals. An average over several measurements led to a typical current amplitude of 4 ± 2 nA It is important to note that in these measurements the value for the persistent current was in good agreement with the theoretical prediction of $\frac{ev_F}{L} = 5$ nA (using experimental parameters)

Interpretation

The good agreement of the last measurement with theoretical assumptions is interpreted to be due to the fact that the system was in the ballistic regime [6] This regime is defined by the condition that the elastic mean free path for an electron is larger than the circumference of the ring, which means that there is only weak disorder in the system

In the former two measurements the effect of disorder was much stronger A situation in which the circumference of the ring is already larger than the elastic mean free path, but still smaller than the localization length is called diffusive (or metallic) regime. Scientists tried in numerous publications to explain why the persistent current can have such large values in this regime The research mainly concentrates on the effect of elastic and inelastic scatterers and the electron-electron-interaction, and a few examples of different developments shall be mentioned next.

Already **Landauer** and **Büttiker** [7] extended then considerations by an investigation into the effects of inelastic scattering They understood inelastic scattering as a jump between the two upper-most energy levels of the previously mentioned Bloch system This effect of a small but finite temperature is of importance when the flux is increased linearly in time. It results in a non-vanishing time average According to Landauer and Buttinger this behaviour can be explained by the change in the width of the energy gap between the two upper-most levels when travelling through the Brillouin zone and a finite relaxation time

Most of the preceding publications considered situations where the flux is fixed A detailed discussion of the effect of scatterers in the different regimes can

for instance be found in the papers of **Cheung** *et al.* [8]. They mainly found that all forms of disorder reduce the amplitude of the persistent current.

Ambegaokar, Eckern and **Schmidt** [9] stressed the importance of taking a Coulomb electron interaction into consideration They started their considerations with Hartree-Fock approximations and handled the interaction perturbatively, using a diagrammatic technique The authors concluded that such interactions can be used to explain the high values of the persistent current in the experiment However, the results strongly depend on the choice of diagrams that are included into a calculation [10]

Müller-Groeling *et al* [11] have also investigated the effect of Coulomb interaction on the persistent current of one-dimensional, continuous rings at zero temperature They used symmetry arguments and introduced a change of variables to many-particle values. Their discussion and qualitative description led to the result that the Coulomb interaction enhances the persistent current in the presence of impurity scattering

In another paper **Cohen, Richter** and **Berkovits** [12] report about their experience with Hartree-Fock equations for the same situation However, they simplified these equations to ordinary Schrodinger equations and tried to solve them In this way they were able to obtain the result that as soon as a single scatterer is included in the ring, the decay of the Friedel oscillations is suppressed Knowing this, it was possible to invoke an approximate self-consistency and to gain statements regarding the persistent current Cohen *et al* reported that in a ring with a weak delta-scatterer the interaction will not destroy the persistent current If even more scatterers are introduced into the ring, then interaction enhances the average sample persistent current (rather than suppressing it) and introduces a preferred diamagnetic current direction

Numerical investigations with much fewer assumptions were for instance performed by **Kato** and **Yoshioka** First [6], they managed to use the Hartree-Fock approximation for a one-dimensional system of 100 sites and 40 electrons and concluded that the Coulomb interaction between electrons causes a reduction of the persistent current also in the diffusive regime However, one year later the same authors found out that if the other two dimensions are taken into consid-

eration (a system of $20 \times 6 \times 6$ and 300 electrons was used) then the persistent current is enhanced

F. V. Kusmartsev published a series of papers and letters with investigations in the persistent current problem. He used in his considerations tight binding models, mainly the Hubbard model. The on-site Coulomb repulsion of spin fermions is described by an energy U. In most of Kusmartsev's papers this interaction is treated with the help of the Bethe *ansatz*. This method leads to a characteristic set of equations for the coefficients in the chosen wave function, which also include the flux phase. In the limit $U \to \infty$ Kusmartsev was able to solve these equations exactly and to give interesting explanations of his results.

In one of his early works [13] Kusmartsev gave expressions for the ground state total energy of a fixed number of particles, M, on a ring in the previously mentioned limit of strong interaction. They show a periodic dependence as well on the flux threaded by the ring as on the number of up-spin particles. Thinking of a situation where all spins are down at the beginning and the flux is increased from zero, one finds that there exists a certain flux value (and in equidistant steps more values) when it is more favourable for the system that two of the fermions change their spin direction. This leads to a fractional Aharonov-Bohm effect, where the current as a function of the flux has a period $1/M$.

In a later paper [14] Kusmartsev *et al* investigated the fractional Aharonov-Bohm effect further. It is shown analytically for the case of two particles, numerically for three particles and perturbatively for M particles that this effect can exist for any finite value of U. The condition is that $\alpha = tM/UN$ is a small number, where N is the number of sites and t the hopping integral. Furthermore, there is a scaling behaviour of the ground state energy, depending only on α. A thorough analysis of the first order corrections of the Bethe equations in the parameter α reveals that there is even more fine structure in the flux dependence of the energy. Kusmartsev [15] discussed that within certain parameter ranges the conventional Aharonov-Bohm effect can coexist not only with an oscillation with period $1/M$ but also with an $M_\downarrow/M$ oscillatory behaviour. Here, $M_\downarrow$ is the number of down-spin particles.

This Paper on the Persistent Current

The given list of publications is of course far from complete. Especially after the first experimental results were reported in 1990 the number of papers about the persistent-current problem has increased rapidly. This shows that there was and still exists a great interest in this topic. The examples mentioned show furthermore that some questions are the subject of controversial discussion. Although a lot of progress in understanding this phenomenon has been made, some questions remain to be answered. It is therefore reasonable and useful to deal with the persistent-current problem within this master thesis.

The intention of this paper goes in two directions. Firstly, the author makes it possible to gain a deeper insight into the causes of persistent current and its derivation. For this purpose a formalism is developed and the successive steps are explained in some detail. Various exact results have been gained and are discussed. Most of these results were obtained independently of any other publication, but have been compared with other works afterwards.

The above mentioned formalism uses tight-binding models. Throughout the whole paper second quantization and a variational approach is used to evaluate the appearing Hamiltonians. The main task is an analysis of the appearing Hartree-Fock equations. Based on both, tight-binding models and Hartree-Fock approximation, many interesting results are published in the literature [6, 8, 9, 10, 11, 12, 13]. However, their combination, a discrete Hartree-Fock picture, is used very seldom [6].

Secondly, it was the intention to improve the first results by performing more complicated decompositions. The idea was to allow different spin-structures for the ground state, which depend on the flux. For this reason rotations of the spin-quantization axis for each of the sites were introduced. It turned out that this task is quite complicated, and especially an appropriate choice of the wave function was not easy to find. This paper documents the different trials, the concluded results and the reasons for modifications. It does not end with a proper result, but with a suggestion for what is, in the opinion of the author, the best way to manage the proposed spin-structure.

The structure of this thesis is chosen accordingly. It starts with some basic

remarks on the tight-binding models in chapter 1. In chapter 2 the physical background is explained and an expression for the persistent current is derived step by step. However, the model is still simple because no interaction is taken into consideration. This happens in chapter 3, in which it is also explained in detail how the Hartree-Fock calculation is done. The first part ends with expressions for the energy in the Heisenberg model and the standard Hubbard model.

In the second part the notion of rotation is introduced. In chapter 4 some concepts are explained and it is tested in which way the rotation should be included. The last chapter is entitled "Trials of Improvement" and offers solutions for the various problems which appeared in the preceding chapter. The paper finishes with some conclusions.

During the time of research it was necessary to make use of some mathematical techniques. In order not to interrupt the argumentation too often longer explanations of such techniques are occasionally moved to the appendices B to F. This makes it also easier for readers who are familiar with this field, to omit those parts since the main body of the paper is formulated independently of the appendices. Appendix A might be especially helpful. It contains a list of almost all symbols used in this paper.

Chapter 1

The Heisenberg Hamiltonian and its Transformations

1.1 The Heisenberg Spin-Hamiltonian

The Heisenberg Hamiltonian has its greatest importance in the trial to find an explanation of magnetism [16, 17] In this area a mean- or molecular-field theory is apparently not sufficient to describe all existing effects Therefore, Heisenberg introduced a local moment theory He (and independently Dirac) first of all suggested a quantum mechanical exchange interaction to explain the singlet-triplet splitting in the helium spectrum. Two years later, in 1928, he applied this idea to magnetism

Hund's rules allow the possibility to associate with each site of a lattice a certain spin According to these rules, every atom tries to have parallel spins in its outer shell Hence, electrons with a certain spin direction are repelled, others are not This leads, even if there is a considerable electron fluctuation, to a fixed spin of a particular site

The idea to include this electron spin in the wave function has its background in the Pauli exclusion principle Since there is an overlap of the wave functions of neighbouring sites, the exclusion principle implies a correlation between spins of two electrons This can be expressed by a so-called Heisenberg energy which

is proportional to the dot product of the spins

$$\mathcal{H}_{\text{Heis}} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1.1}$$

where $\langle i, j \rangle$ indicates that the sum goes over nearest neighbours only

J is called the exchange integral, which has no classical analogue because it is based on the Pauli exclusion principle It is supposed to be identical for all nearest neighbour pairs, which is of course a simplification The value of J can be calculated from specific heat measurements and spin-wave considerations For instance Hofmann *et al* [18] found for iron and nickel $J \approx 0.01 - 0.02eV$ and for gadolinium $J \approx 0.0002eV$ However, theoretical estimations [19] lead to different values, which shows the weakness of the model.

The origin of mistakes is mainly the assumption of localized magnetic moments, attached to the atomic cores in the material Especially, for elements with high atomic numbers the electrons of the outer shells are unlikely to be localized Here from a physical point of view itinerant electron theories seem to be more favourable, even so, they are much more difficult to handle For 3d transition metals both, the localized and the itinerant theory, have their justification The former explains for instance spin wave phenomena and the temperature dependence of the specific heat, the latter magnetic moments with non-integral numbers of Bohr magnetons per atom

Nevertheless, only the Heisenberg idea of localized magnetic moments and their interaction is used in this work First of all, it is necessary to describe spin operators for spin one-half particles mathematically This can be done with the help of Pauli spin matrices in the form $\mathbf{S}_i = \frac{1}{2}\hbar\boldsymbol{\sigma}$ for site number i The components of these spin matrices are

$$\sigma_x \equiv \sigma(1) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; \sigma_y \equiv \sigma(2) = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } \sigma_z \equiv \sigma(3) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.2}$$

If, furthermore, the ladder operators

$$S_i^{\pm} = S_i^x \pm i S_i^y$$

are introduced, eventually the following set of spin operators

$$S_i^+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, S_i^- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad S_i^z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

can be obtained

It is easy to show that

$$S_i^- S_j^+ + S_i^+ S_j^- = 2S_i^x S_j^x + 2S_i^y S_j^y,$$

which has two consequences. Firstly, it allows the rewriting of the common product of two spin operators

$$\mathbf{S_i S_j} = S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z = \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) + S_i^z S_j^z. \qquad (1.3)$$

Secondly, it shows that the anticommutator of spin operators on the same site is proportional to identity

$$[S_i^+, S_i^-]_+ = \hbar^2 \mathbb{1}_2 \qquad (1.4)$$

1.2 Transformation to Bosons

For angular momentum operators in general, especially if the spin quantum numbers are large, a treatment with matrices might be cumbersome It is often more convenient to work in second quantization. One possibility to replace spin operators is the coupled-boson representation It shall be described here in brevity because it fits into the context. However, it is of little importance for the main body of this paper.

Coupled Boson Representation

The coupled-boson representation was first proposed by Schwinger [20][1] He introduced spinor operators

$$\mathbf{b}^\dagger = \begin{pmatrix} b_1^\dagger & b_2^\dagger \end{pmatrix} \qquad \text{and} \qquad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \qquad (1.5)$$

[1] see also Mattis [21] chap 3 8 or Merzbacher [22] chap 21.2

which consist of two Bose creation and annihilation operators, respectively The latter fulfil the usual commutation relations for bosons

$$[b_i, b_j]_- = [b_i^\dagger, b_j^\dagger]_- = 0, \quad [b_i, b_j^\dagger]_- = \delta_{ij} \tag{1.6}$$

and are well defined if a vacuum state $|0\rangle$ is introduced together with the constraint

$$b_i |0\rangle = 0 \quad \text{or} \quad \langle 0 | b_i^\dagger = 0 \quad \forall i \tag{1.7}$$

Using the Pauli spin matrices (1.2) the representation for a general angular momentum operator (not necessarily half-spin) has the following form

$$\mathrm{S} = \frac{\hbar}{2} \mathrm{b}^\dagger \cdot \boldsymbol{\sigma} \cdot \mathrm{b} \tag{1.8}$$

Proof: It has to be shown that the typical commutation relations for the components of angular momentum operators are fulfilled by S In order to write this in a compact form (S^x, S^y, S^z) is replaced by (S^1, S^2, S^3) and Einstein's sum convention is used

$$\begin{aligned}
S^i S^j - S^j S^i &= \frac{\hbar^2}{4} \left(b_\alpha^\dagger \sigma(i)_{\alpha\beta} b_\beta b_\gamma^\dagger \sigma(j)_{\gamma\delta} b_\delta - b_\gamma^\dagger \sigma(j)_{\gamma\delta} b_\delta b_\alpha^\dagger \sigma(i)_{\alpha\beta} b_\beta \right) \\
&= \frac{\hbar^2}{4} \left(b_\alpha^\dagger \sigma(i)_{\alpha\beta} \delta_{\beta\gamma} \sigma(j)_{\gamma\delta} b_\delta + b_\alpha^\dagger \sigma(i)_{\alpha\beta} b_\gamma^\dagger b_\beta \sigma(j)_{\gamma\delta} b_\delta \right. \\
&\qquad \left. - b_\gamma^\dagger \sigma(j)_{\gamma\delta} \delta_{\delta\alpha} \sigma(i)_{\alpha\beta} b_\beta - b_\gamma^\dagger \sigma(j)_{\gamma\delta} b_\alpha^\dagger b_\delta \sigma(i)_{\alpha\beta} b_\beta \right) \\
&= \frac{\hbar^2}{4} \left(b_\alpha^\dagger \left(\sigma(i) \cdot \sigma(j) \right)_{\alpha\delta} b_\delta - b_\gamma^\dagger \left(\sigma(j) \quad \sigma(i) \right)_{\gamma\beta} b_\beta \right) \\
&= \frac{\hbar^2}{4} \left(b_\alpha^\dagger \left([\sigma(i), \sigma(j)]_- \right)_{\alpha\delta} b_\delta \right) = \frac{\hbar^2}{4} \, 2i \, b_\alpha^\dagger \varepsilon_{ijk} \sigma(k)_{\alpha\delta} b_\delta \\
&= \varepsilon_{ijk} \, i\hbar \, S^k
\end{aligned}$$

□

Having defined the angular momentum in this way, it is also possible to give an expression for the eigenstates in terms of creation operators The result

$$|sm\rangle = \frac{\left(b_1^\dagger\right)^{s+m} \left(b_2^\dagger\right)^{s-m}}{\sqrt{(s+m)!\,(s-m)!}} |0\rangle \tag{1.9}$$

denotes a state with the eigenvalues $\hbar^2 s(s+1)$ and $\hbar m$ of S^2 and S_z, respectively $|0\rangle = |00\rangle$ is again the vacuum state

Proof: It has to be shown that the ladder operators $S^+ = S^x + iS^y$ and $S^- = S^x - iS^y$ rise and lower the m-value correctly and that S^2 gives the correct eigenvalue of $\hbar^2\, s(s+1)$. The former is clear after finding that

$$S^+ = \hbar\, b_1^\dagger b_2, \quad S^- = \hbar\, b_2^\dagger b_1 \quad \text{and} \quad S^z = \frac{\hbar}{2}\left(b_1^\dagger b_1 - b_2^\dagger b_2\right), \tag{1 10}$$

the latter is obvious by showing that

$$\mathrm{S}^2 = \frac{1}{2}\left(S^+S^- + S^-S^+\right) + S_z^2 = \hbar^2\ \mathrm{s(s+1)},$$

where

$$\mathrm{s} = \frac{1}{2}\,\mathrm{b}^\dagger \cdot \mathrm{b} = \frac{1}{2}\left(b_1^\dagger b_1 + b_2^\dagger b_2\right) =: \frac{1}{2}\hat{n}_1 + \frac{1}{2}\hat{n}_2$$

□

Therefore, an interaction of spin operators in the form

$$\mathcal{H} = -J \sum_{\langle i,j\rangle} \mathrm{S}_i\, \mathrm{S}_j + g\mu_B \sum_j \mathrm{B}\ \ \mathrm{S}_j, \tag{1 11}$$

also including an interaction with an external magnetic field B (g and μ_B are constants) can be transformed with the help of (1 8) to an expression with bosonic creation and annihilation operators. Expectation values can be calculated in second quantization, using the eigenstates proposed in (1 9).

Variations

There exist various variations of the above mentioned representation. Most of them have the aim to replace one of the bosonic operators. With the help of quasi-classical arguments it is tried to work with one kind of bosons only. One finds for instance in Merzbacher [22] why a ferromagnetic approximation leads to

$$\mathrm{S}_i\, \mathrm{S}_j = \frac{\hbar^2}{2}\left\{2sb_i^\dagger b_j + 2sb_ib_j^\dagger - 2sb_i^\dagger b_i - 2sb_j^\dagger b_j + 2s^2\right\} \tag{1 12}$$

Another possibility is the Holstein-Primakoff transformation [23], which results in the following representation:

$$S_j^+ = \hbar b_j^\dagger \sqrt{2s}\,\sqrt{1 - \frac{1}{2s}\,b_j^\dagger b_j}, \quad S_j^- = \hbar\sqrt{2s}\,\sqrt{1 - \frac{1}{2s}\,b_j^\dagger b_j}\,b_j, \tag{1 13}$$

$$S_j^z = \hbar\left(b_j^\dagger b_j - s\right).$$

1.3 Transformation to Fermions

For the special case of spin one-half operators it is sometimes more helpful to work with a fermionic representation. One might think of a coupled fermion representation since (1.8) is also valid for fermions. However, there are also ways to manage without a second creation operator. This section introduces the most widely accepted possibility to make a transformation in this direction, the

Jordan-Wigner Transformation

Fermions are characterized by the following anticommutation relations of annihilation operators c_i and creation operators $c_i^\dagger$:

$$[c_i, c_j]_+ = [c_i^\dagger, c_j^\dagger]_+ = 0, \quad [c_i, c_j^\dagger]_+ = \delta_{ij} \tag{1.14}$$

They are well defined with the help of a vacuum state $|0\rangle$, for which holds

$$c_i |0\rangle = 0 \quad \text{or} \quad \langle 0 | c_i^\dagger = 0 \quad \forall i \tag{1.15}$$

The transformation proposed by Jordan and Wigner in 1928 [24][2] makes use of similar properties of spin operators and fermions. It has already been pointed out (1.4) that the anticommutator of spin operators on the same site is

$$[S_i^+, S_i^-]_+ = \hbar^2 \mathbb{1}_2$$

Hence, an identification of spin operators with fermionic operators in the form

$$S_i^+ \equiv \hbar c_i^\dagger, \; S_i^- \equiv \hbar c_i \quad \text{and} \quad S_i^z \equiv \hbar \left(c_i^\dagger c_i - \frac{1}{2} \right)$$

seems to be natural. Unfortunately, it is not that easy. Spin operators for different sites or particles commute with one another

$$[S_i^+, S_j^-]_- = 0 \quad \text{for } i \neq j, \tag{1.16}$$

whereas fermionic operators anticommute. For this reason a phase factor U_i for each site i is necessary to change anticommuting to commuting. U_i should be a unitary operator (as every phase factor), which only contributes a sign to the

[2] a description can for instance be found in Mattis [21] chap. 3.12 and in Tsvelik [25] chap. 18

expressions for the spin operators It is convenient to use the fermionic operators c_i for this purpose. Jordan and Wigner proposed to do that in the following way:

$$\begin{aligned} U_i &= \exp\left[i\pi \sum_{k<i} c_k^\dagger c_k\right] \\ &= \prod_{k<i} \exp\left[i\pi c_k^\dagger c_k\right] = \prod_{k<i} \left(1 - 2c_k^\dagger c_k\right) \end{aligned} \tag{1 17}$$

which holds for one dimension Hence, the spin operators have the form

$$\begin{aligned} S_i^+ &\equiv \hbar c_i^\dagger U_i = \hbar c_i^\dagger \exp\left[i\pi \sum_{k<i} c_k^\dagger c_k\right], \\ S_i^- &\equiv \hbar U_i^* c_i = \hbar \exp\left[-i\pi \sum_{k<i} c_k^\dagger c_k\right] c_i, \\ S_i^z &\equiv \hbar \left(c_i^\dagger U_i U_i^* c_i - \frac{1}{2}\right) = \hbar \left(c_i^\dagger c_i - \frac{1}{2}\right) \end{aligned} \tag{1 18}$$

In order to check that this phase factor has the desired properties, it is sufficient to notice that the operator product $c_k^\dagger c_k$ is an occupation number operator $\hat{n}_k$ An ordering of the sites $i = 1, \ldots, N$ is introduced, and therefore the sum in (1 17) counts the number of occupied sites coming before the site i If this number is even, then $U_i = 1$, otherwise it is -1 In the commutator

$$[S_i^+, S_j^-]_- = \hbar^2 \left(c_i^\dagger U_i U_j^* c_j - U_j^* c_j c_i^\dagger U_i\right),$$

assuming $j < i$, only the sites k with $j \leq k < i$ are important (the rest is counted twice) Owing to the fact that U_i appears in the first summand left to c_j and in the second summand right to c_j, the sum $\sum_{k=j}^{i-1} \hat{n}_k$ differs by 1 in these two cases This gives the required additional phase factor -1 which changes anticommuting to commuting The argumentation for $j > i$ is similar.

By using (1 3), (1 16) and (1 18), the kinetic energy term in the Heisenberg Hamiltonian becomes in one dimension

$$\begin{aligned} \mathcal{H} &= J \sum_{\langle i\,j\rangle} \mathrm{S}_i\, \mathrm{S}_j = J \sum_j \left\{\frac{1}{2}\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right) + S_j^z S_{j+1}^z\right\} \\ &= \hbar^2 J \sum_j \left\{c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + \left(c_j^\dagger c_j - \frac{1}{2}\right)\left(c_{j+1}^\dagger c_{j+1} - \frac{1}{2}\right)\right\} \end{aligned} \tag{1 19}$$

It is clear that in (1 19) the phase factor U_j does not appear any more This is due to the fact that for the sum over the occupation numbers in U_j only the

sites k with $j \leq k < j+1$ are important (the rest is counted twice). However, for $j = k$ either the occupation number operator $\hat{n}_k$ or the fermionic operator $c_j^\dagger$ gives zero owing to the Pauli exclusion principle

Variations

Variations appear if the one-dimensional chain of operators is closed to a ring. This happens when the index $N+1$ is identified with the index number 1. That means physically that periodic boundary conditions are implemented and mathematically that all site indices are understood to be taken (mod N).

In such a situation one has to check the behaviour of the term $S_i^+ S_{i+1}^-$. It does not cause any problems as long as $i \neq N$ However, for $i = N$ the transformation formulas (1 18) lead to

$$\begin{aligned}
\frac{1}{\hbar^2} S_N^+ S_1^- &= c_N^\dagger \exp\left[i\pi \sum_{k<N} c_k^\dagger c_k\right] \exp\left[-i\pi \sum_{k<1} c_k^\dagger c_k\right] c_1 \\
&= c_N^\dagger \exp[i\pi(M-1)]\, c_1 \qquad \text{and} \\
\frac{1}{\hbar^2} S_1^+ S_N^- &= c_1^\dagger \exp\left[i\pi \sum_{k<1} c_k^\dagger c_k\right] \exp\left[-i\pi \sum_{k<N} c_k^\dagger c_k\right] c_N \\
&= c_1^\dagger \exp[-i\pi(M-1)]\, c_N
\end{aligned}$$

Here M is the expectation value of $\sum_{k=1}^{N} c_k^\dagger c_k$ It is equivalent to the number of particles of the system, which is supposed to be fixed

The phase factor $e^{i\pi(M-1)}$ is equal to unity for the case of an odd number of particles However, it gives a minus sign if the number of particles is even [1] To be precise, one therefore has to write instead of (1 19)

$$\begin{aligned}
\mathcal{H} = \hbar^2 J \sum_{j=1}^{N} &\left\{ c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + \left(c_j^\dagger c_j - \frac{1}{2}\right)\left(c_{j+1}^\dagger c_{j+1} - \frac{1}{2}\right)\right\} \\
&+ \left\{ c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right\} \left(e^{i\pi(M-1)} - 1\right) \qquad (1\ 20)
\end{aligned}$$

In such a form the character of the Heisenberg Hamiltonian is preserved and a chain of spins is described The situation is usually called the "a-cyclic" problem [26, 27] [3]

[3] The letter a has its origin in the fact that Lieb *et al* denoted in their paper the operators S_i^+ and S_i^- with the symbols $a_i^\dagger$ and a_i, respectively

On the other hand the additional term proportional to $\left(e^{i\pi(M-1)}-1\right)$ is in the limit of a large number of sites, N, negligible To omit it also means to describe a cyclic problem of real fermions The Hamiltonian

$$\mathcal{H}=\hbar^2 J\sum_{j=1}^{N}\left\{c_j^\dagger c_{j+1}+c_{j+1}^\dagger c_j+\left(c_j^\dagger c_j-\frac{1}{2}\right)\left(c_{j+1}^\dagger c_{j+1}-\frac{1}{2}\right)\right\} \qquad (1\,21)$$

is called "c-cyclic' and is well to distinguish from the previous one.

The main differences are the implied boundary conditions [27] The a-cyclic problem has by construction always periodic boundary conditions In the c-cyclic problem this is only the case for an odd number of particles If the number of particles is even, then the boundary conditions are antiperiodic, how it should be for real fermions.

The reason is that there are the following rules how fermion annihilation and creation operators act on Fock states in second quantization [28]:

$$\begin{aligned} c_{\alpha_r}^\dagger\,|M,\ \ .,n_{\alpha_r},\ \ \rangle &= (-1)^{M_r}\delta_{n_{\alpha_r},0}\,|M+1,\ \ \ ,n_{\alpha_r}+1,\ \ \rangle \\ c_{\alpha_r}\,|M,\ ..,n_{\alpha_r},\ \ \rangle &= (-1)^{M_r}\delta_{n_{\alpha_r},1}\,|M-1,..\ .,n_{\alpha_r}-1,..\rangle, \end{aligned}$$

where

$$M_r=\sum_{i=0}^{r-1}n_{\alpha_i}$$

Hence, it is

$$c_1^\dagger c_N\,|M,0,\ \ .,1\rangle=(-1)^{M-1}\,|M,1,\ \ \ ,0\rangle$$

and vice versa

1.4 Related Hamiltonians

The result of the Jordan-Wigner transformation of the Hubbard Hamiltonian is

$$\begin{aligned}\mathcal{H} &= \hbar^2 J \sum_j \left\{ c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + \left(c_j^\dagger c_j - \frac{1}{2}\right)\left(c_{j+1}^\dagger c_{j+1} - \frac{1}{2}\right)\right\} \\ &= \hbar^2 J \sum_j \left\{ \underbrace{c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j}_{\hat{H}_0} + \underbrace{c_j^\dagger c_j c_{j+1}^\dagger c_{j+1}}_{\hat{V}} - c_j^\dagger c_j \right\}\end{aligned}$$

It consists mainly of two parts $\hat{H}_0$ describes the quantum mechanical hopping of electrons; $\hat{V}$ can be understood as an interaction of different electrons The remaining term is a particle self energy. It is worth noting that the product $c_j^\dagger c_j = \hat{n}_j$ is the occupation number operator in second quantization Summed over all sites j, the total number of particles of the system is obtained In the calculations of this paper this number is supposed to be constant, which allows us to ignore the last term as an unimportant energy shift

In a more general form it is possible [28] to write the Hamiltonian for a combination of the one-particle kinetic energy and a two-particle interaction in second quantization as

$$\mathcal{H} = \sum_{p,q} c_p^\dagger \langle p|\hat{H}_1|q\rangle c_q + \sum_{p,q,r,s} c_p^\dagger c_q^\dagger \langle pq|\hat{H}_2|rs\rangle c_r c_s, \tag{1.22}$$

ignoring many-particle interactions, which are seldom

The equation which follows from the Jordan-Wigner transformation is just a special case of this representation A hopping is only allowed from one site to an adjacent site, which essentially leads to a Kronecker-delta instead of the expectation value of $\hat{H}_1$ Furthermore, the interaction operator $\hat{H}_2$ gives the value V for nearest neighbours only. All other expectation values of $\hat{H}_2$ vanish

The Heisenberg Model

A Hamiltonian of the form

$$\mathcal{H} = -t \sum_k \left(c_k^\dagger c_{k+1} + \text{h c} \right) + V \sum_k \hat{n}_k \hat{n}_{k+1} \tag{1.23}$$

is called in this paper the **Heisenberg model** In this expression the constant in front of the first sum has been renamed to $-t = \hbar^2 J$ and is called "hopping integral", V is a repulsive Coulomb potential, "h c" stands for "hermitian

conjugate". The Heisenberg model works with spinless fermions and includes a hopping and an interaction between nearest neighbours in one dimension.

The Hubbard Model

A further step is not to calculate with spinless fermions but to include the spin of particles into consideration. In this case the interaction is usually simplified even more. Not even the effects of nearest neighbours on a fermion on a certain site are considered. The calculations are reduced to the Coulomb repulsion of two particles which are located on the same site, but have different spin. In the case of spinless fermions this term did not appear because of the Pauli exclusion principle; the spin degeneracy allows such contributions. The Hamiltonian has the form

$$\mathcal{H} = -t \sum_{k} \sum_{\sigma=\uparrow,\downarrow} \left(c^{\dagger}_{k,\sigma} c_{k+1,\sigma} + c^{\dagger}_{k+1,\sigma} c_{k,\sigma} \right) + U \sum_{k} \hat{n}_{k,\uparrow} \hat{n}_{k,\downarrow} \qquad (1.24)$$

Here $c^{\dagger}_{k,\sigma}$ and $c_{k,\sigma}$ are the creation and annihilation operators of a fermion with spin σ on the site k, respectively, $\hat{n}_{k,\sigma}$ is the corresponding occupation number operator.

In either form, (1.23) and (1.24), the Hamiltonian is only an approximation. Nevertheless, such approximations can already lead to interesting and nontrivial results. Unfortunately, even simplifications like this cannot always be solved analytically. Numerical methods or approximations are necessary.

Chapter 2

Rings of Fermions and Bosons

2.1 Heisenberg Model with Spinless Particles

As a first simple example of electronic interactions of charged particles it is possible to use the Heisenberg model. It is the purpose of this section to show how within the Heisenberg model the total energy for a set of particles on a ring can be obtained. This happens first of all in subsection 2.1.1 for only one particle. An expression for the energy of more particles is derived in 2.1.2, and the necessary considerations to minimize this expression are finally explained in 2.1.3. Subsection 2.1.4 adds some remarks on the distribution of the particles.

2.1.1 One Particle on the Ring

We begin our considerations with looking only at the hopping part of the Heisenberg model. That means the Hamiltonian has the following structure

$$\begin{aligned} \mathcal{H} &= \hbar^2 J \sum_{j=1}^{N} \left\{ c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right\} = -t \sum_{j=1}^{N} \left\{ c_j^\dagger c_{j+1} + \text{h.c.} \right\} \\ &= -t \left\{ c_1^\dagger c_2 + c_2^\dagger c_1 + c_2^\dagger c_3 + c_3^\dagger c_2 + \ldots + c_N^\dagger c_{N-1} + c_N^\dagger c_1 + c_1^\dagger c_N \right\}. \end{aligned} \tag{2.1}$$

The variable N gives the number of sites within the system. Because only one dimension is taken into consideration, the system forms a line of adjacent sites, separated by a distance a. Thus, the length of the line is $L = a \cdot N$. One can see from the sign in front of the last two terms that we use the c-cyclic problem, the description with real fermions.

It is also possible to use the expression (2.1) for the case that the operators obey the commutation rules of bosons. More specifically, such a model would describe hard-core bosons. These are particles which behave according to Bose statistics, but only $n_j = 0$ and 1 are allowed as occupation numbers.

However, for a system with only one particle, as examined next, there are no differences between these two descriptions because no commutators appear. In both cases (fermions and bosons) the Heisenberg Hamiltonian annihilates the particle on a certain site and creates a new one on both possible adjacent sites. The sites N and 1 are understood to be adjacent.

The description of the Hamiltonian in terms of annihilation and creation operators implies the usage of second quantization. For this reason, a Fock- or occupation-number representation for the eigenstates is used:

$$|\psi\rangle = \alpha_1 |0.\quad 001\rangle + \alpha_2 |0\ .\ 010\rangle + \quad + \alpha_N |10\ ..00\rangle \tag{2.2}$$

Then the Hamiltonian $\mathcal{H}$ in (2.1) can also be written in matrix representation. Independent of the number of particles the matrix has form shown right.

$$-t \begin{pmatrix} 0 & 1 & & & & 1 \\ 1 & 0 & 1 & & & \\ & 1 & 0 & & 0 & \\ & & & & & \\ & 0 & & \cdot & 1 & \\ & & & & 0 & 1 \\ 1 & & & & 1 & 0 \end{pmatrix} \tag{2.4}$$

The set of eigenvalues of $\mathcal{H}$ is identical with the spectrum of the shown matrix. The latter could be evaluated numerically. However, this seems not to be necessary since the given set of equations for the eigenvalue λ can be solved exactly by assuming that the coefficients are Bloch wave functions,

$$\Longrightarrow \begin{cases} -t(\alpha_2 + \alpha_N) = \lambda\alpha_1 \\ -t(\alpha_1 + \alpha_3) = \lambda\alpha_2 \\ \qquad\qquad\quad \cdot \\ -t(\alpha_{j-1} + \alpha_{j+1}) = \lambda\alpha_j \end{cases}$$

$$\alpha_j = \frac{1}{\sqrt{N}} e^{ikj} \tag{2.3}$$

Because the periodic boundary condition $\alpha_{N+j} = \alpha_j$ must be satisfied for

every j, it turns out that only certain values for k are allowed·

$$k_n = \frac{2\pi}{N} n, \qquad n = 0, 1, \ldots, N-1^1 \tag{2.5}$$

Hence, the eigenvalues are determined by the following equation

$$\begin{aligned} -t\left(e^{ik_n(j-1)} + e^{ik_n(j+1)}\right) &= \lambda_n e^{ik_n j} \\ -t\left(e^{-ik_n} + e^{ik_n}\right) &= \lambda_n. \end{aligned}$$

These numbers λ_n are the eigenvalues of the Hamilton operator $\mathcal{H}$, and therefore the possible energy states for one particle on a ring with N sites are

$$\boxed{E_n = -2t\cos k_n = -2t\cos\left(\frac{2\pi}{N} n\right)} \tag{2.6}$$

2.1.2 Two or More Particles

The case of two particles on the ring must be handled separately for fermions and for bosons. The following calculations concentrate on the former ones. We shall come back to bosons in section 2.3.

The eigenstates of the Hamiltonian $\mathcal{H}$ given in the form (2.1) can be described by two quantum numbers n, m with $n \neq m$. In second quantization the form

$$|\psi\rangle_{n,m} = \sum_{ij} \alpha_{i,j}^{n,m} c_i^\dagger c_j^\dagger |0\rangle \tag{2.7}$$

is appropriate. The properties of the coefficients $\alpha_{i,j}^{n,m}$ are discussed in subsection 2.1.4. At the moment they are just functions of the sites i and j which also depend on the quantum numbers n and m.

The Schrodinger equation $\mathcal{H}|\psi\rangle_{n,m} = E_{n,m}|\psi\rangle_{n,m}$ for this problem can be handled in different ways. One of them is a straight forward usage of the commutation relations

$$\begin{aligned} -\frac{1}{t}\mathcal{H}|\psi\rangle_{n,m} &= \sum_{ijk} \alpha_{i,j}^{n,m}\left(c_k^\dagger c_{k+1} + c_{k+1}^\dagger c_k\right) c_i^\dagger c_j^\dagger |0\rangle \\ &= \sum_{ijk} \alpha_{i,j}^{n,m}\left(c_k^\dagger c_{k+1} c_i^\dagger c_j^\dagger (\delta_{k+1,i} + \delta_{k+1,j}) + c_{k+1}^\dagger c_k c_i^\dagger c_j^\dagger (\delta_{k,i} + \delta_{k,j})\right)|0\rangle \\ &= \sum_{ij} \alpha_{i,j}^{n,m}\left(c_{i-1}^\dagger c_i c_i^\dagger c_j^\dagger + c_{j-1}^\dagger c_j c_i^\dagger c_j^\dagger + c_{i+1}^\dagger c_i c_i^\dagger c_j^\dagger + c_{j+1}^\dagger c_i c_i^\dagger c_j^\dagger\right)|0\rangle \end{aligned}$$

[1] see also discussion in section 2.3

$$
\begin{aligned}
&= \sum_{ij} \alpha_{i,j}^{n,m} \left(c_{i-1}^\dagger c_j^\dagger - c_{j-1}^\dagger c_i^\dagger + c_{i+1}^\dagger c_j^\dagger - c_{j+1}^\dagger c_i^\dagger \right) |0\rangle \\
&= \sum_{ij} \alpha_{i,j}^{n,m} \left(c_{i-1}^\dagger c_j^\dagger + c_i^\dagger c_{j-1}^\dagger + c_{i+1}^\dagger c_j^\dagger + c_i^\dagger c_{j+1}^\dagger \right) |0\rangle \\
&= \sum_{ij} \left(\alpha_{i-1,j}^{n,m} + \alpha_{i,j+1}^{n,m} + \alpha_{i+1,j}^{n,m} + \alpha_{i,j-1}^{n,m} \right) c_i^\dagger c_j^\dagger |0\rangle
\end{aligned}
$$

In the fourth line of this calculation the fact that all terms with $i = j$ disappear due to the Pauli exclusion principle for fermions has been included. In the last line there is a shift of the summation index

A comparison with the right hand side of the Schrodinger equation shows that for all pairs $\{i, j\}$ the equation

$$
-t \left(\alpha_{i-1,j}^{n,m} + \alpha_{i,j+1}^{n,m} + \alpha_{i+1,j}^{n,m} + \alpha_{i,j-1}^{n,m} \right) = E_{n,m} \alpha_{i,j}^{n,m} \tag{2.8}
$$

has to be fulfilled

It is not difficult to see that again Bloch wave functions satisfy this set of equations Actually, the factor $\alpha_{i,j}^{n,m}$, which stands for the wave function of two fermions on the ring, can be factorized, which means that the two fermions can be handled as non-interacting particles

$$
\alpha_i^n \cdot \alpha_j^m \equiv \alpha_{i,j}^{n,m} = \frac{1}{N} \exp\left[\frac{2\pi \mathrm{i}}{N} (ni + mj) \right] = \frac{1}{\sqrt{N}} \mathrm{e}^{\frac{2\pi}{N} ni} \quad \frac{1}{\sqrt{N}} \mathrm{e}^{\frac{2\pi}{N} mj} \tag{2.9}
$$

In this representation the case $n = m$ is not allowed The reason is that $n = m$ leads to parameters which are symmetric in the site index, $\alpha_{i,j}^{n,m} = \alpha_{j,i}^{n,m}$, and hence

$$
\begin{aligned}
|\psi\rangle_{n,m} = \sum_{ij} \alpha_{i,j}^{n,m} c_i^\dagger c_j^\dagger |0\rangle &= \frac{1}{2} \left(\sum_{ij} \alpha_{i,j}^{n,m} c_i^\dagger c_j^\dagger + \sum_{ji} \alpha_{j,i}^{n,m} c_j^\dagger c_i^\dagger \right) |0\rangle \\
&= \frac{1}{2} \left(\sum_{ij} \alpha_{i,j}^{n,m} c_i^\dagger c_j^\dagger - \sum_{ij} \alpha_{i,j}^{n,m} c_i^\dagger c_j^\dagger \right) |0\rangle = 0.
\end{aligned}
$$

That implies that the wave function $|\psi\rangle_{n,n}$ would disappear everywhere

By using Bloch wave functions in the form (2.9) one obtains the following expression for the energy

$$
E_{n,m} = -2t \left(\cos\left(\frac{2\pi}{N} n \right) + \cos\left(\frac{2\pi}{N} m \right) \right) \tag{2.10}
$$

It should not be a great problem to accept the generalization of this expression to the case of M particles on the ring:

$$\boxed{E_{n_1,\ \ldots,n_M} = -2t \sum_{A=1}^{M} \cos\left(\frac{2\pi}{N} n_A\right)} \tag{2.11}$$

2.1.3 Total Energy

The calculated energy in (2.11) still depends on the set of quantum numbers $\{n_i\}_{i=1}^{M}$. In order to obtain the ground state of the system at temperature $T = 0$ this set must be chosen in such a way that the total energy is a minimum. The situation is visualized in figure 2.1.

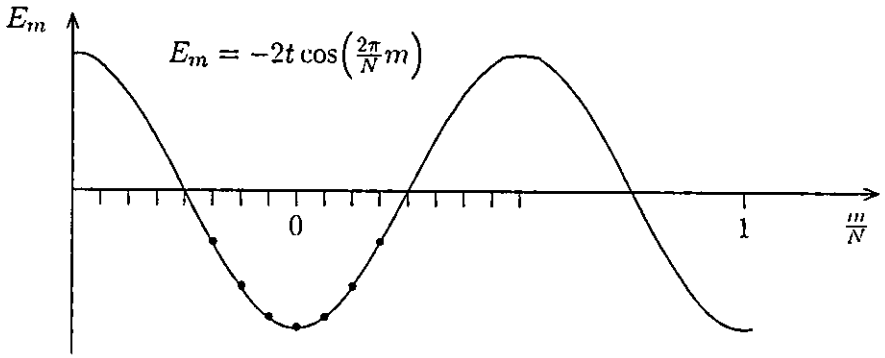


Figure 2.1. *Energy states due to the hopping part of the Heisenberg model. The case of a ring with $N = 16$ sites and $M = 7$ particles is shown. The small ticks on the $x-$axis indicate the different possible m values.*

In the case of spinless fermions each of the indicated points in reciprocal space can be occupied by not more than one particle. The reason for this is the Pauli exclusion principle. For $M = N$, which is referred to *half filling* in the literature, there is only one possibility, which gives a total energy

$$E = -t\left(\sum_{n=0}^{N-1} e^{\frac{2\pi i}{N}n} + \sum_{n=0}^{N-1} e^{-\frac{2\pi i}{N}n}\right) = -t\,\frac{1-e^{\frac{2\pi i}{N}N}}{1-e^{\frac{2\pi i}{N}}} - t\,\frac{1-e^{-\frac{2\pi i}{N}N}}{1-e^{-\frac{2\pi i}{N}}} = 0$$

For a number of particle $M < N$ the lowest energy levels are those which are close to $k = 0 \pmod N$. Hence, the distribution occurs in a way similar to the situation shown in figure 2.1, where dots represent single particles.

For a large number of sizes and a small number of particles, or more precisely for $\frac{M}{N} \ll 1$, the situation is similar to that of free particles. For small x the cos-function can be approximated as being

$$\cos x \approx 1 - \frac{1}{2}x^2,$$

which gives the picture for free fermions on the right hand side

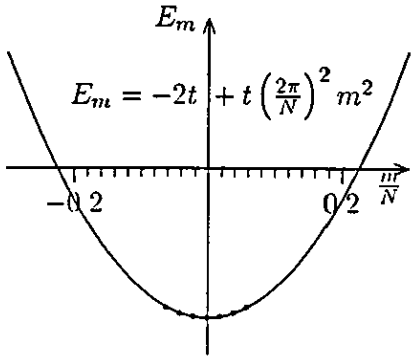


Figure 2.2 *Energy states for a large number of sites ($N = 30$) and a small number of free fermions ($M = 7$)*

In order to calculate the total energy of the system, it is necessary to distinguish between an odd and an even number of particles M.

M even

$$\begin{aligned}
E_{\text{even}} &= -2t \sum_{m=-\frac{M}{2}}^{+\frac{M}{2}-1} \cos\left(\frac{2\pi}{N}m\right) = -t \sum_{m=0}^{M-1} \left\{ \exp\left[\frac{2\pi \mathrm{i}}{N}\left(m - \frac{M}{2}\right)\right] + \text{h c} \right\} \\
&= -t \exp\left[-\frac{\pi \mathrm{i}}{N}M\right] \frac{1 - \exp\left[\frac{2\pi \mathrm{i}}{N}M\right]}{1 - \exp\left[\frac{2\pi \mathrm{i}}{N}\right]} + \text{h c} \\
&= -t \frac{\exp\left[-\frac{\pi \mathrm{i}}{N}M\right] - \exp\left[\frac{\pi \mathrm{i}}{N}M\right]}{1 - \exp\left[\frac{2\pi \mathrm{i}}{N}\right]} \cdot \frac{1 - \exp\left[-\frac{\pi \mathrm{i}}{N}2\right]}{1 - \exp\left[-\frac{2\pi \mathrm{i}}{N}\right]} + \text{h c} \\
&= -t \frac{\cos\left(\frac{\pi}{N}(M-2)\right) - \cos\left(\frac{\pi}{N}(M+2)\right)}{1 - \cos\left(\frac{2\pi}{N}\right)}
\end{aligned}$$

This expression can still be simplified by using some important trigonometric identities

$$\left|\begin{aligned}
\cos(x+y) &= \cos x \cos y - \sin x \sin y \\
\cos(x-y) &= \cos x \cos y + \sin x \sin y \\
\sin 2x &= 2 \sin x \cos x \\
2\sin^2 x &= 1 - \cos 2x
\end{aligned}\right. \qquad (2.12)$$

Hence,

$$E_{\text{even}} = -t \frac{2\sin\left(\frac{\pi}{N}2\right) \sin\left(\frac{\pi}{N}M\right)}{1 - \cos\left(\frac{2\pi}{N}\right)} = -2t \frac{2\sin\left(\frac{\pi}{N}\right)\cos\left(\frac{\pi}{N}\right)}{2\sin^2\left(\frac{\pi}{N}\right)} \sin\left(\frac{\pi}{N}M\right),$$

which gives the final result for the case of an even number of fermions

$$\Longrightarrow \boxed{E_{\text{even}} = -2t\cot\left(\frac{\pi}{N}\right)\sin\left(\frac{\pi}{N}M\right)} \tag{2.13}$$

The calculations for the other case are analogous

$\boxed{M \text{ odd}}$

$$\begin{aligned}
E_{\text{odd}} &= -2t\sum_{m=-\frac{M-1}{2}}^{+\frac{M-1}{2}}\cos\left(\frac{2\pi}{N}m\right) = -t\sum_{m=0}^{M-1}\left\{\exp\left[\frac{2\pi\imath}{N}\left(m-\frac{M-1}{2}\right)\right]+\text{h c}\right\} \\
&= -t\exp\left[-\frac{\pi\imath}{N}(M-1)\right]\frac{1-\exp\left[\frac{2\pi\imath}{N}M\right]}{1-\exp\left[\frac{2\pi\imath}{N}\right]}+\text{h c.} \\
&= -t\frac{\exp\left[-\frac{\pi\imath}{N}(M-1)\right]-\exp\left[\frac{\pi\imath}{N}(M+1)\right]}{1-\exp\left[\frac{2\pi\imath}{N}\right]}\;\frac{1-\exp\left[-\frac{\pi\imath}{N}2\right]}{1-\exp\left[-\frac{2\pi\imath}{N}\right]}+\text{h c} \\
&= -t\frac{2\cos\left(\frac{\pi}{N}(M-1)\right)-2\cos\left(\frac{\pi}{N}(M+1)\right)}{1-\cos\left(\frac{2\pi}{N}\right)} \\
&= -2t\frac{2\sin\left(\frac{\pi}{N}\right)\sin\left(\frac{\pi}{N}M\right)}{2\sin^2\left(\frac{\pi}{N}\right)}
\end{aligned}$$

which gives the final result for the case of an odd number of fermions

$$\Longrightarrow \boxed{E_{\text{odd}} = -2t\frac{1}{\sin\left(\frac{\pi}{N}\right)}\sin\left(\frac{\pi}{N}M\right)} \tag{2.14}$$

A comparison of these two results (2.13) and (2.14) shows that they only differ by a factor of $\cos\left(\frac{\pi}{N}\right)$. This factor appears in the case of an even number of particles due to the fact that one particle is not located symmetrically. For an odd number of particles, all energy levels apart from $m = 0$ are occupied twice in the ground state, because $E_m = E_{-m}$. This is not possible for an even number of fermions, where one particle is left over. However, the importance of this factor $\cos\left(\frac{\pi}{N}\right)$ decreases with a rising number of sites N on the ring. This is understandable with the same argumentation. This parity problem is discussed again in chapter 2.3 after the notion of magnetic flux has been introduced.

2.1.4 Distribution of the Particles

After looking at the behaviour of the energy and therefore the eigenvalues of the Hamiltonian under consideration, it might also be interesting to examine the behaviour of the corresponding wave functions In particular, we are interested in the expectation values of the occupation number operator, which tells us something about the distribution of particles over the possible sites of the ring. Similar to the energy evaluation the calculations were done in several steps.

One particle

In this case the wave function has the form (2 2) which can also be written as

$$|\psi\rangle_n = \sum_{i=1}^{N} \alpha_i^n c_i^\dagger |0\rangle; \qquad {}_n\langle\psi| = \langle 0| \sum_{j=1}^{N} \left(\alpha_j^n\right)^* c_j \tag{2 15}$$

and the desired expectation value is

$$\begin{aligned} {}_n\langle\psi|\hat{n}_k|\psi\rangle_n &= \sum_{i,j} \left(\alpha_j^n\right)^* \alpha_i^n \langle 0|c_j c_k^\dagger c_k c_i^\dagger|0\rangle \\ &= \sum_{i,j} \left(\alpha_j^n\right)^* \alpha_i^n \langle 0|0\rangle \delta_{i,k}\delta_{k,j} = \underline{|\alpha_k^n|^2} \\ &= \left|\frac{1}{\sqrt{N}} e^{\frac{2\pi i}{N} n\, k}\right|^2 = \underline{\frac{1}{N}} \end{aligned} \tag{2 16}$$

Hence, in the case of one particle $|\alpha_k^n|^2$ gives the probability that the particle is located on site k This probability is $1/N$ if Bloch wave functions are used.

Two particles

The wave function for this case, as already proposed in (2 7)

$$|\psi\rangle_{n,m} = \sum_{ij} \alpha_{i,j}^{n,m} c_i^\dagger c_j^\dagger |0\rangle; \qquad {}_{n,m}\langle\psi| = \langle 0| \sum_{st} \left(\alpha_{s,t}^{n,m}\right)^* c_t c_s \tag{2 17}$$

implies the following result

$$
\begin{aligned}
{}_{n,m}\langle\psi\,|\hat{n}_k\,|\,\psi\rangle_{n,m} &= \sum_{i,j,s,t} \alpha_{i,j}^{n,m}\left(\alpha_{s,t}^{n,m}\right)^{*}\langle 0\,|c_l c_s c_k^{\dagger} c_k c_i^{\dagger} c_j^{\dagger}\,|\,0\rangle\,(\delta_{k,i}+\delta_{k,j}) \\
&= \sum_{j,s,t}\left(\alpha_{s,t}^{n,m}\right)^{*}\langle 0\,|c_l c_s c_k^{\dagger} c_j^{\dagger}\,|\,0\rangle\left(\alpha_{k,j}^{n,m}-\alpha_{j,k}^{n,m}\right)(\delta_{s,k}\delta_{l,j}+\delta_{s,j}\delta_{t,k}) \\
&= \sum_{j}\left(\left(\alpha_{k,j}^{n,m}\right)^{*}-\left(\alpha_{j,k}^{n,m}\right)^{*}\right)\left(\alpha_{k,j}^{n,m}-\alpha_{j,k}^{n,m}\right) \\
&= \underline{\sum_{j}\left|\alpha_{k,j}^{n,m}-\alpha_{j,k}^{n,m}\right|^{2}} \qquad (2.18) \\
&= \sum_{j}\left\{\left|\alpha_{k,j}^{n,m}\right|^{2}+\left|\alpha_{j,k}^{n,m}\right|^{2}-2\mathrm{Re}\left(\left(\alpha_{j,k}^{n,m}\right)^{*}\alpha_{k,j}^{n,m}\right)\right\} \\
&= \sum_{j}\left\{\frac{1}{N^2}+\frac{1}{N^2}-0\right\} = \underline{\frac{2}{N}}, \qquad (2\,19)
\end{aligned}
$$

where the last line is again the result for Bloch wave functions in the form (2.9). However, without this assumption the result (2 18) looks differently than expected

This is even more the case when one investigates the expectation value of the operator product $\hat{n}_k\hat{n}_l$ One would expect to obtain $2/N^2$ in the case of Bloch wave functions, because it is the probability[2] of having one particle on site k and the other on site l at the same time Instead, calculations lead to

$$
\begin{aligned}
{}_{n,m}\langle\psi\,|\hat{n}_k\hat{n}_l\,|\,\psi\rangle_{n,m} &= \sum_{i,j,s,t}\alpha_{i,j}^{n,m}\left(\alpha_{s,t}^{n,m}\right)^{*}\langle 0\,|c_l c_s c_k^{\dagger} c_k c_l^{\dagger} c_i^{\dagger} c_j^{\dagger}\,|\,0\rangle\,(\delta_{l,i}+\delta_{l,j}) \\
&= \sum_{j,s,t}\left(\alpha_{s,t}^{n,m}\right)^{*}\langle 0\,|c_l c_s c_k^{\dagger} c_k c_l^{\dagger} c_j^{\dagger}\,|\,0\rangle\left(\alpha_{l,j}^{n,m}-\alpha_{j,l}^{n,m}\right)(\delta_{k,l}+\delta_{k,l}) \\
&= \delta_{k,l}\sum_{j}\left(\left(\alpha_{k,j}^{n,m}\right)^{*}-\left(\alpha_{j,k}^{n,m}\right)^{*}\right)\left(\alpha_{l,j}^{n,m}-\alpha_{j,l}^{n,m}\right) \\
&\qquad -\left(\left(\alpha_{k,l}^{n,m}\right)^{*}-\left(\alpha_{l,k}^{n,m}\right)^{*}\right)\left(\alpha_{l,k}^{n,m}-\alpha_{k,l}^{n,m}\right) \\
&= \underline{\delta_{k,l}\sum_{j}\left|\alpha_{k,j}^{n,m}-\alpha_{j,k}^{n,m}\right|^{2}+\left|\alpha_{k,l}^{n,m}-\alpha_{l,k}^{n,m}\right|^{2}} \qquad (2\,20)
\end{aligned}
$$

The result is consistent with the previous one (2 18), which is just $k=l$ Furthermore, the behaviour for $k\to l$ and for $n=m$ is reasonable However, it is not consistent with the expected value The term

$$
2\mathrm{Re}\left(\left(\alpha_{k,l}^{n,m}\right)^{*}\alpha_{l,k}^{n,m}\right)=\frac{2}{N^2}\cos\left(\frac{2\pi}{N}(n-m)(k-l)\right)
$$

[2]Note that in this context "probability" is not normalized to 1 but to M

also gives a non-trivial contribution for Bloch wave functions.

Characteristics like this lead to the conclusion that even in a representation like (2.9) the two particles do not live independently of each other. The existence of one of them influences the probability distribution of the other one.

Remark: It might well be that such a behaviour is associated with Friedel oscillations in solid state physics. In the appendix of his article on 'The Distribuation of Electrons Round Impurities in Monovalent Metals" [29] Friedel suggested that a spherically symmetrical potential gives rise to an oscillation of the wave function in a sinusoidal form. In one dimension far enough away from a sufficiently fast decreasing potential the electron density behaves like [30]

$$n(x) \propto \frac{\cos(2k_F|x| + \delta)}{|x|},$$

where x is a spatial coordinate, k_F the Fermi momentum and δ is a constant dependent on the structure of the potential. Cohen *et al* [12] also showed in a continuous Hartree-Fock calculation the existence of such density oscillations for one-dimensional rings. However, it needs further investigations to find connections to this effect.

Nevertheless, there is apparently no straight forward interpretation of the physical meaning of values like $\left|\alpha_{i,j}^{n,m}\right|^2$.

M particles

The structure of the wave function for the M-particle case is a canonical generalization of the previous case

$$|\psi\rangle_{n_1 \quad n_M} = \sum_{i_1, \quad i_M} \alpha_{i_1 \quad i_M}^{n_1 \quad n_M} c_{i_1}^\dagger c_{i_2}^\dagger \quad . c_{i_M}^\dagger |0\rangle \tag{2.21}$$

Provided that the coefficients are wave functions of the Bloch type, they have the form

$$\alpha_{i_1 \quad i_M}^{n_1 \quad n_M} = \frac{1}{\sqrt{N}^M} \exp\left[\frac{2\pi \mathrm{i}}{L}\left(n_1 i_1 + n_2 i_2 + \quad n_M i_M\right)\right],$$

where N and M are the number of sites and particles, respectively, and $n_i \neq n_j$ for $i \neq j$ are the quantum numbers.

$$
\begin{aligned}
&{}_{n_1\ \ n_M}\langle\psi\,|\hat{n}_k\,|\psi\rangle_{n_1\ \ n_M} \\
&\quad = \sum_{i_1\ \ i_M}\sum_{j_1\ \ j_M} \alpha^{n_1\ \ n_M}_{i_1\ \ i_M}\left(\alpha^{n_1\ \ n_M}_{j_1\ \ j_M}\right)^{*}\langle 0\,|c_{j_M}\cdots c_{j_1}c^{\dagger}_{k}c_{k}c^{\dagger}_{i_1}\cdots c^{\dagger}_{i_M}\,|0\rangle \\
&\quad = \sum_{A=1}^{M}\sum_{\substack{i_1\ \ i_M\\ j_1\ \ j_M}} \alpha\ \ (\alpha\ )^{*}(-1)^{A-1}\delta_{k,i_A}\underbrace{\langle 0\,|c_{j_M}\cdots c_{j_1}c^{\dagger}_{k}c^{\dagger}_{i_1}\cdots\ \widehat{c^{\dagger}_{i_A}}\cdots c^{\dagger}_{i_M}\,|0\rangle}_{=(-1)^{A-1}\langle 0\,|c_{j_M}\ \ c_{j_1}c^{\dagger}_{i_1}\ \ c^{\dagger}_{k}\ \ c^{\dagger}_{i_M}\,|0\rangle} \\
&\quad = \sum_{A=1}^{M}\sum_{i_1}{}'\sum_{i_M}\sum_{\wp\in\mathcal{P}(M)} \alpha^{n_1\ \ n_M}_{i_1\ \ i_M}\left(\alpha^{n_1\ \ n_M}_{\wp(i_1\ \ i_M)}\right)^{*}\delta_{k,i_A}(-1)^{\operatorname{sgn}\wp} \qquad (2\,22)
\end{aligned}
$$

In the last line the prime at one of the sums indicates that the summation indices should be distinct: $i_k \neq i_l$ for $k \neq l$ However, it is shown in Appendix C that this constraint is not important and can be forgotten

$\mathcal{P}(M)$ is the set of all permutations of the set of numbers $\{1, \quad , M\}$ If Bloch wave functions are again considered, only one of them gives a non-vanishing contribution For $\wp = \mathrm{id}$ the sums above reduce to

$$
\sum_{A=1}^{M}\sum_{i_1\ \ i_M}\left|\alpha^{n_1\ \ n_M}_{i_1\ \ i_M}\right|^{2}\delta_{k,i_A} = \sum_{A=1}^{M}\frac{1}{N^M}\cdot N^{(M-1)} = \frac{M}{N}
$$

For all other permutations exists at least one $x \neq k$ with $\wp^{-1}(x) \neq x$ and in all sums appears the factor

$$
\sum_{i_x=0}^{N-1}\exp\left[\frac{2\pi\mathrm{i}}{N}\left(n_x - n_{\wp^{-1}(x)}\right)i_x\right] = 0
$$

Hence, for M-particle Bloch wave functions the probability to find a particle on a certain site is

$$
{}_{n_1\ \ n_M}\langle\psi\,|\hat{n}_k\,|\psi\rangle_{n_1\ \ n_M} = \underline{\frac{M}{N}} \qquad (2\,23)
$$

It is worth noting that this result does not depend on the site k, nor does it depend on the set of quantum numbers $\{n_1, \quad , n_M\}$

2.2 Magnetic Flux through the Ring

Of special interest is the situation when a ring of fermions is placed inside a magnetic field $\mathbf{B}(\mathbf{r},t)$. Compared to the calculations of the previous chapter a few alterations have to be done in order to describe this situation correctly. However, before a new expression for the total energy can be derived in subsection 2.2.3 some explanations have to be given. Subsection 2.2.1 provides in brevity some general consequences of the existence of a magnetic field. Most of the statements are proven and explained in more detail in appendix B. In 2.2.2 it is shown that it is possible to handle the flux within the Hubbard model in a convenient way.

2.2.1 General Consequences

In general, the vector potential $\mathbf{A}(\mathbf{r},t)$, defined by $\mathbf{B} = \nabla \times \mathbf{A}$, is much more relevant for derivations than the magnetic field itself. For instance, a non-zero vector potential can be taken into consideration by substituting the expression for the momentum in the form

$$\begin{aligned} \hat{\mathbf{p}} &\longrightarrow \hat{\mathbf{p}} - e\mathbf{A} \qquad \text{SI units,} \\ \hat{\mathbf{p}} &\longrightarrow \hat{\mathbf{p}} - \tfrac{e}{c}\mathbf{A} \qquad \text{Gaussian units,} \end{aligned} \tag{2.24}$$

where e is the elementary charge or the charge of an electron and c is the velocity of light [3].

However, in electromagnetism only the fields $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$ are measurable quantities. The scalar potential $\phi(\mathbf{r}.t)$ and the vector potential $\mathbf{A}(\mathbf{r},t)$ are auxiliary fields, which are not uniquely determined. A gauge transformation, that is an alteration of the phase of the fields by a function $\chi(\mathrm{r}\ t)$ without altering the measurable physical quantities, is possible. It has the following form

$$\begin{aligned} \phi &\longrightarrow \phi' = \phi - \tfrac{1}{c}\tfrac{\partial}{\partial t}\chi(\mathbf{r},t) \\ \mathbf{A} &\longrightarrow \mathbf{A}' = \mathbf{A} + \nabla\chi(\mathbf{r},t) \end{aligned} \tag{2.25}$$

With the help of such gauge transformations one can prove the following: If a vector potential is introduced, then the free-particle Hamiltonian in first

[3] Most of the formulas are given in Gaussian units. To get the expressions in the SI-system one mainly has to omit c everywhere.

quantization transforms together with the momentum to

$$\mathcal{H} = \frac{\left(\mathrm{p} - \frac{e}{c}\mathrm{A}\right)^2}{2m} \tag{2 26}$$

In order to keep the Schrödinger equation invariant a simultaneous transformation of the wave function of the form

$$\Psi(\mathbf{r},t) = \psi(\mathbf{r},t)\exp\left[-\frac{ie}{\hbar c}\int^{\mathrm{r}}\mathrm{A}(\mathrm{s})\,\mathrm{ds}\right] \tag{2 27}$$

is necessary [32]. That means, if $\psi(\mathbf{r},t)$ fulfils the Schrodinger equation for a free electron with charge e then $\Psi(\mathbf{r},t)$ does the same for the Hamiltonian (2 26)

The question is how to modify the Heisenberg Hamiltonian, written in the form

$$\mathcal{H} = -t\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}\left\{c^\dagger(\mathbf{r})c(\mathbf{r}') + \mathrm{h\,c.}\right\},$$

accordingly. For the special case that A is not dependent on the coordinates $\mathrm{A}(\mathbf{r},t) = \mathrm{A}(t)$ this is possible with the help of a double Fourier transformation That means that the given Hamiltonian is transformed to momentum representation, then a change of the momentum according to (2 24) is done there, and afterwards the Fourier transformation is applied again This procedure gives for each fermionic operator an additional phase factor which give together

$$\mathcal{H} = -t\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}\left\{c^\dagger(\mathbf{r})\,\mathrm{e}^{\frac{ie}{\hbar c}\mathrm{A}(\mathbf{r}'-\mathbf{r})}c(\mathbf{r}') + \mathrm{h\,c.}\right\}$$

For the more general case that $\mathbf{A}(\mathbf{r},t)$ is also a function of the coordinates, the transformation turns out to be a little bit more difficult and the result[4], known as Peierls substitution [33], is given by

$$\mathcal{H} = -t\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}\left\{c^\dagger(\mathbf{r})\,\mathrm{e}^{\frac{ie}{\hbar c}\int_{\mathrm{r}}^{\mathrm{r}'}\mathrm{A}\,\mathrm{dr}}c(\mathrm{r}') + \mathrm{h\,c}\right\} \tag{2 28}$$

Even so a rigorous prove is not given, the substitution seems to be very reasonable when looking at the previous comments The hopping part represents the kinetic energy of the particles, $c^\dagger(\mathbf{r})c(\mathbf{r}')$ describes a movement of a fermion from site $\mathbf{r}'$ to site $\mathbf{r}$. Equations (2.26) and (2 27) show the consequences of a non-zero

[4] see for instance Fradkin [31], chap 2 2 2

vector potential on the kinetic energy and the wave function in first quantization The Peierls substitution has exactly the same structure, with the only difference that the phase-factor is put into Hamiltonian and not into the wave function

It is furthermore reasonable to state that in interaction terms within the Heisenberg model, which consist of occupation number operators of the form $c^\dagger(\mathbf{r})c(\mathbf{r})$, such a phase factor does not appear Here, no movement is described As a next step the case where the particle moves along a closed path around an area which is threaded by a magnetic field B is considered. Everywhere along the path $\mathbf{B} = 0$, which is called a Aharonov-Bohm situation

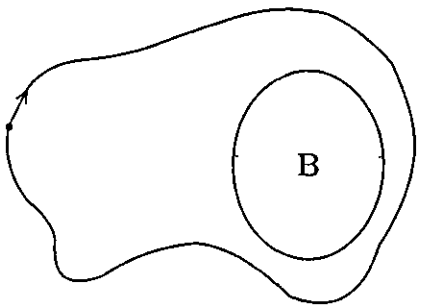


Figure 2 3 *Closed path around an area of nonzero flux*

For such a situation the integral in the exponent of (2.27) has to be taken along a closed path. According to Stoke's theorem it can be transformed in the following way

$$\oint \mathbf{A}(\mathbf{s})\,\mathrm{d}\mathbf{s} = \oint \mathrm{curl}\mathbf{A}\cdot \mathrm{d}^2\mathbf{S} = \oint \mathbf{B}\cdot \mathrm{d}^2\mathbf{S} = \Phi, \tag{2 29}$$

where Φ is the flux of B through the loop.

However, this result is only correct for a simply connected path If the path goes several times along the loop, then one accordingly gets $2\Phi, 3\Phi$ and so on From a physical point of view it should be clear that the wave function $\Psi(\mathbf{r}, t)$ must be single valued, its value must not depend on how often one goes along the loop This can only be fulfilled if the argument of the exponential function in

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}, t)\exp\left[-\frac{ie}{\hbar c}\Phi\right]$$

has the form $-2\pi i n$ with n an integer

Therefore, the constraint of a single valued wave function implies a quantization of the flux through the loop of the form

$$\Phi = n\Phi_0 \qquad \text{with} \qquad \Phi_0 := \frac{2\pi\hbar c}{e} = \frac{hc}{e} \tag{2 30}$$

Φ_0 is called "elementary flux quantum".

2.2.2 Gauge Invariance in the Heisenberg Model

It still remains the task to obtain the spectrum of eigenvalues of the Heisenberg Hamiltonian However, this operator has after including the flux via Peierls substitution (2 28) the form

$$\begin{aligned}\mathcal{H} &= -t \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \left\{ c^{\dagger}(\mathbf{r})\, \mathrm{e}^{\frac{2\pi \mathrm{i}}{\Phi_0} \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{A}\, \mathrm{d}\mathbf{r}} c(\mathbf{r}') + \mathrm{h\,c} \right\} \\ &= -t \Big\{ \mathrm{e}^{\frac{2\pi \mathrm{i}}{\Phi_0}\varphi_{1,2}} c_1^{\dagger} c_2 + \mathrm{e}^{-\frac{2\pi \mathrm{i}}{\Phi_0}\varphi_{1\,2}} c_2^{\dagger} c_1 + \mathrm{e}^{\frac{2\pi \mathrm{i}}{\Phi_0}\varphi_{2\,3}} c_2^{\dagger} c_3 + . \\ &\quad . \quad + \mathrm{e}^{-\frac{2\pi \mathrm{i}}{\Phi_0}\varphi_{N-1,N}} c_N^{\dagger} c_{N-1} + \mathrm{e}^{\frac{2\pi \mathrm{i}}{\Phi_0}\varphi_{N\,1}} c_N^{\dagger} c_1 + \mathrm{e}^{-\frac{2\pi \mathrm{i}}{\Phi_0}\varphi_{N\,1}} c_1^{\dagger} c_N \Big\}\end{aligned} \tag{2 31}$$

where $\varphi_{i,j} = \int_{\text{site } i}^{\text{site } j} \mathbf{A}\, \mathrm{d}\mathbf{r}$ is the necessary gauge field

According to different gauges the phases $\varphi_{i,j}$ can have a different structure. Only the total flux

$$\Phi = \oint \mathbf{A}(\mathrm{s})\, \mathrm{d}\mathbf{s} = \oint \mathrm{curl}\mathbf{A} \cdot \mathrm{d}^2\mathbf{S} = \oint \mathbf{B}\ \ \mathrm{d}^2\mathbf{S}$$

is independent of the gauge A gauge transformation of the form

$$\mathbf{A}' = \mathbf{A} + \nabla\chi$$

leads to the result

$$\varphi'_{i,j} = \int_{\mathrm{r}=\text{site } i}^{\mathrm{r}'=\text{site } j} \mathbf{A}'\, \mathrm{d}\mathbf{r} = \varphi_{i,j} + \chi(\mathbf{r}') - \chi(\mathbf{r})$$

The invariance of the Hamiltonian can be explained (as for instance in Fradkin [31]) as a U(1) symmetry with the local change of phase given by

$$\theta(\mathbf{r}) \equiv -\frac{e}{\hbar c}\chi(\mathrm{i})$$

However, the author wants to give his own proof of the fact that the spectrum of the Hamiltonian under consideration does not depend on the gauge

As a first step in this direction consider the case of four sites arranged in a rectangular shape in the xy-plane. In the z-direction there is a magnetic field

$$\mathbf{B} = B_0 \mathbf{e_z}.$$

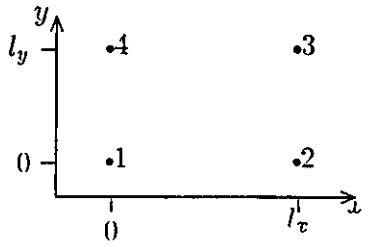


Figure 2.4 *Four sites on a rectangular*

For this case two important gauges are possible.

1st gauge (symmetric gauge)

$$\mathbf{A} = \mathbf{B} \times \mathbf{e_x} = \begin{pmatrix} 0 \\ B_0 x \\ 0 \end{pmatrix}$$

$$\varphi_{2,3} = B_0 l_x l_y$$

$$\varphi_{1,2} = \varphi_{3,4} = \varphi_{4,1} = 0$$

$$-\tfrac{1}{i}H = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & e^{if} & 0 \\ 0 & e^{-if} & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

2nd gauge (Lorentz gauge)

$$\mathbf{A} = \tfrac{1}{2}\mathbf{B} \times \mathbf{r} = \tfrac{1}{2} \begin{pmatrix} -B_0 y \\ B_0 x \\ 0 \end{pmatrix}$$

$$\varphi_{1,2} = \varphi_{4,1} = 0$$

$$\varphi_{2,3} = \varphi_{3,4} = \tfrac{1}{2} B_0 l_x l_y$$

$$-\tfrac{1}{i}H = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & e^{if/2} & 0 \\ 0 & e^{-if/2} & 0 & e^{if/2} \\ 1 & 0 & e^{-if/2} & 0 \end{pmatrix}$$

Here H is the matrix of the Hamiltonian $\mathcal{H}$ for each of the gauges respectively It describes the mapping between Fock states as introduced in (2 2) The constant in the exponent is

$$f = \frac{2\pi}{\Phi_0} B_0 l_x l_y$$

To obtain the spectrum of the $\mathcal{H}$ is equivalent to finding the eigenvalues of the matrix H In a generalization of the two given gauges the determinant

$$\begin{vmatrix} -\lambda & e^{\frac{2\pi i}{\Phi_0}\varphi_{1,2}} & 0 & e^{\frac{2\pi i}{\Phi_0}\varphi_{1,4}} \\ e^{-\frac{2\pi i}{\Phi_0}\varphi_{1,2}} & -\lambda & e^{\frac{2\pi i}{\Phi_0}\varphi_{2,3}} & 0 \\ 0 & e^{-\frac{2\pi i}{\Phi_0}\varphi_{2,3}} & -\lambda & e^{\frac{2\pi i}{\Phi_0}\varphi_{3,4}} \\ e^{-\frac{2\pi i}{\Phi_0}\varphi_{1,4}} & 0 & e^{-\frac{2\pi i}{\Phi_0}\varphi_{3,4}} & -\lambda \end{vmatrix}$$

has to be evaluated After doing this calculation the phase factors only appear

in the combination

$$e^{\frac{2\pi i}{\Phi_0}\varphi_{1,2}} e^{\frac{2\pi i}{\Phi_0}\varphi_{2,3}} e^{\frac{2\pi i}{\Phi_0}\varphi_{3,4}} e^{\frac{2\pi i}{\Phi_0}\varphi_{4,1}} = e^{2\pi i \frac{\Phi}{\Phi_0}}.$$

The characteristic polynomial is

$$0 = \lambda^4 - 4\lambda^2 + 2 - e^{2\pi i \frac{\Phi}{\Phi_0}} - e^{-2\pi i \frac{\Phi}{\Phi_0}}$$

with the solutions

$$\lambda = \pm\sqrt{2 \pm \sqrt{2 + 2\cos\left(2\pi \frac{\Phi}{\Phi_0}\right)}}. \tag{2.32}$$

Hence, it is shown that for the example of a rectangular with four sites the eigenvalues of the Hamiltonian are really independent of the gauge

The next step is to prove the independence in the general case of N sites and an arbitrary gauge. That is, to prove that the determinant of a matrix

$$A = \begin{pmatrix} \lambda & a_1 & 0 & 0 & \cdot & 0 & \frac{1}{a_N} \\ \frac{1}{a_1} & \lambda & a_2 & 0 & & 0 & 0 \\ 0 & \frac{1}{a_2} & \lambda & \ddots & & & \vdots \\ 0 & 0 & & \ddots & & & \\ \cdot & & & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & & & \cdot & \lambda & a_{N-1} \\ a_N & 0 & \cdots & \cdots & 0 & \frac{1}{a_{N-1}} & \lambda \end{pmatrix}$$

only depends on the product $a_1 \cdot a_2 \cdot \ldots \cdot a_N$

The trick is to write the matrix A as a product of two triangular matrices LU, whose determinant can easily be calculated The first, a lower triangular matrix, has only 1's at the diagonal. The second is an upper triangular matrix with nontrivial diagonal elements The easiest way to obtain the result is to start in the upper left corner of A and make their way through the rows of this matrix. The calculations are shown here up to $N = 5$, but it is easy to see how they have to continue For convenience, symbols for the following chain fractions are introduced

$$\lambda_1 = \lambda, \quad \lambda_2 = \lambda - \frac{1}{\lambda} = \lambda - \frac{1}{\lambda_1}, \quad \lambda_3 = \lambda - \frac{1}{\lambda - \frac{1}{\lambda}} = \lambda - \frac{1}{\lambda_2},$$

Then it is

$$A = LU \iff \begin{matrix} & U \\ L & A \end{matrix} \qquad \begin{pmatrix} \lambda_1 & a_1 & 0 & 0 & \frac{1}{a_5} \\ 0 & \lambda_2 & a_2 & 0 & -\frac{1}{a_1 a_5}\frac{1}{\lambda_1} \\ 0 & 0 & \lambda_3 & a_3 & \frac{1}{a_1 a_2 a_5}\frac{1}{\lambda_1\lambda_2} \\ 0 & 0 & 0 & \lambda_4 & a_4 - \odot \\ 0 & 0 & 0 & 0 & \lambda_5 - \oplus \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ \frac{1}{a_1}\frac{1}{\lambda_1} & 1 & 0 & 0 & 0 \\ 0 & \frac{1}{a_2}\frac{1}{\lambda_2} & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{a_3}\frac{1}{\lambda_3} & 1 & 0 \\ \frac{a_5}{\lambda_1} & -\frac{a_1 a_5}{\lambda_1\lambda_2} & \frac{a_1 a_2 a_5}{\lambda_1\lambda_2\lambda_3} & \frac{1}{a_4}\frac{1}{\lambda_4} - \otimes & 1 \end{pmatrix} \qquad \begin{pmatrix} \lambda & a_1 & 0 & 0 & \frac{1}{a_5} \\ \frac{1}{a_1} & \lambda & a_2 & 0 & 0 \\ 0 & \frac{1}{a_2} & \lambda & a_3 & 0 \\ 0 & 0 & \frac{1}{a_3} & \lambda & a_4 \\ a_5 & 0 & 0 & \frac{1}{a_4} & \lambda \end{pmatrix}$$

where

$$\odot = \frac{1}{a_1 a_2 a_3 a_5}\frac{1}{\lambda_1\lambda_2\lambda_3} \qquad \otimes = \frac{a_1 a_2 a_3 a_5}{\lambda_1\lambda_2\lambda_3\lambda_4}$$

$$\oplus = \frac{1}{\lambda_1} + \frac{1}{\lambda_1^2\lambda_2} + \frac{1}{\lambda_1^2\lambda_2^2\lambda_3} + \frac{1}{\lambda_1^2\lambda_2^2\lambda_3^2\lambda_4} - \frac{a_1 a_2 a_3 a_4 a_5}{\lambda_1\lambda_2\lambda_3\lambda_1} - \frac{1}{a_1 a_2 a_3 a_4 a_5 \lambda_1\lambda_2\lambda_3\lambda_4}$$

The rest of the argumentation is trivial

$$\det A = \det L \cdot \det U = \lambda_1 \cdot \lambda_2 \quad \lambda_3 \quad \lambda_4 \quad (\lambda_5 - \oplus)$$

and therefore the matrix elements $a_1, \quad ., a_5$ appear in the characteristic polynomial only in the form $a_1 a_2 a_3 a_1 a_5$ That is what we wanted to prove. □

2.2.3 Change of Total Energy

Having obtained this result, it is possible to choose a convenient gauge for the calculation of the spectrum of the Heisenberg Hamiltonian.
The only constraint given is

$$\sum_{i=1}^{N} \varphi_{i,i+1} = \Phi$$

which leads to the simplest choice for A being in such a way, that

$$\varphi_{i,i+1} = \frac{\Phi}{N}, \quad i = 1, .. \ N \qquad (2\,33)$$

or, in other words, the matrix of $\mathcal{H}$ has the shown form.

$$\begin{pmatrix} 0 & e^{if} & & & e^{-if} \\ e^{-if} & 0 & e^{if} & 0 & \\ & \ddots & \ddots & & \\ & & & & \\ & 0 & & 0 & e^{if} \\ e^{if} & & & e^{-if} & 0 \end{pmatrix}$$

where $f = \frac{2\pi}{N}\frac{\Phi}{\Phi_0}$

In the same way as in the case of no magnetic flux in chapter 2 1 1 it is again reasonable to assume that the coefficients are Bloch wave functions

$$\alpha_j = \frac{1}{\sqrt{N}} e^{ikj} \qquad (2\,34)$$

$$\Longrightarrow \begin{cases} -t\,(e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\alpha_2 + e^{-\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\alpha_N) = \lambda\alpha_1 \\ -t\,(e^{-\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\alpha_1 + e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\alpha_3) = \lambda\alpha_2 \\ \vdots \qquad\qquad \cdot \\ -t\,(e^{-\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\alpha_{j-1} + e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\alpha_{j+1}) = \lambda\alpha_j \end{cases}$$

Owing to the constraint of single valued wave functions, the possible wave-vectors are quantized

$$k_m = \frac{2\pi}{N} m \qquad m = 0, 1, \quad , N-1$$

and hence, the eigenvalues are determined by the following equation

$$\begin{aligned} -t\left(e^{-\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}} \ e^{ik_m(j-1)} + e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}} \cdot e^{ik_m(j+1)}\right) &= \lambda_m e^{ik_m j} \\ -t\left(e^{-\frac{2\pi i}{N}\left(m+\frac{\Phi}{\Phi_0}\right)} + e^{\frac{2\pi i}{N}\left(m+\frac{\Phi}{\Phi_0}\right)}\right) &= \lambda_m \end{aligned}$$

These numbers λ_m are the eigenvalues of the Hamilton operator $\mathcal{H}$ and therefore the possible energy states for one particle on a ring with N sites and trapped

magnetic flux Φ are.

$$\boxed{E_m = -2t\cos\left(\frac{2\pi}{N}\left(m+\frac{\Phi}{\Phi_0}\right)\right)} \tag{2 35}$$

Having obtained this result, the next task is to find the total energy for a system of M particles For these particles the quantum numbers $m = 0, \quad , N-1$ are possible For every fixed m there is a characteristic dependence of the energy on the magnetic flux Φ trapped through the ring

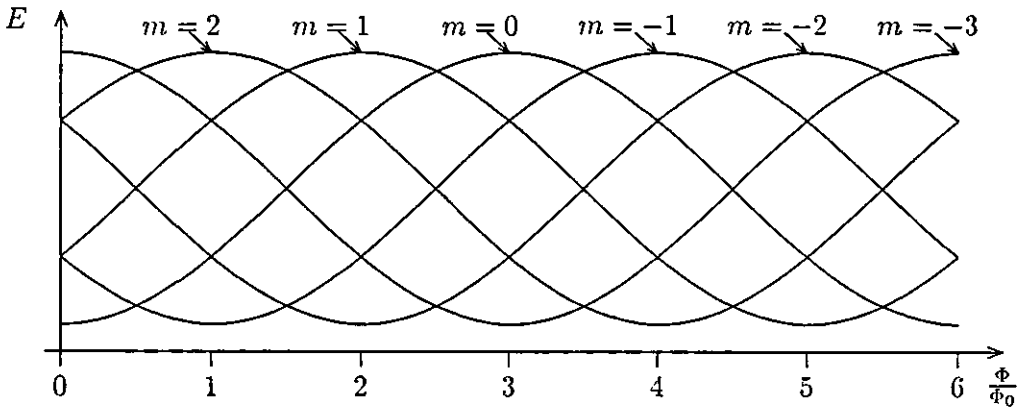
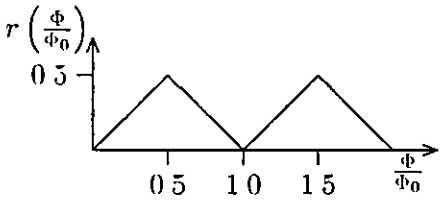


Figure 2.5 *The energy dependence on the flux Φ for the different possible m-values is shown In this picture the number of sites is $N = 6$*

This situation is shown in figure 2.5, where only for a better visualization a relatively small number of sites is chosen One can see that the picture repeats periodically Obviously, it is only necessary to make calculations for the case $0 \leq \Phi/\Phi_0 < \frac{1}{2}$, because for the rest of the possible values of the flux Φ the picture, and therefore the total energy, is the same.

Hence, it is reasonable to restrict an arbitrary value of Φ within this interval (which is an analogue to the first Brillouin zone) by a function like in figure 2 6,



$$r\left(\frac{\Phi}{\Phi_0}\right) = \left|\frac{\Phi}{\Phi_0} - \left[\frac{\Phi}{\Phi_0}+\frac{1}{2}\right]\right| \tag{2 36}$$

Figure 2 6 *Restriction of trapped flux onto a sufficient interval*

where $[z]$ stands for the largest integer which is $\leq z$

Furthermore, it can be seen from figure 2 5 that for $0 \leq \Phi/\Phi_0 < \frac{1}{2}$ the sites will be occupied by fermions in the order $m = 0, -1, 1, -2, 2, -3$ Hence, for the calculation of the total energy the same kind of sums as in chapter 2 1 3 are used:

$\boxed{M \text{ even}}$

$$
\begin{aligned}
E_{\text{even}} &= -2t \sum_{m=-\frac{M}{2}}^{+\frac{M}{2}-1} \cos\left(\frac{2\pi}{N}\left(m + \frac{\Phi}{\Phi_0}\right)\right) \\
&= -t \exp\left[\frac{2\pi \mathrm{i}}{N}\frac{\Phi}{\Phi_0}\right] \exp\left[-\frac{\pi \mathrm{i}}{N} M\right] \sum_{m=0}^{M-1} \exp\left[\frac{2\pi \mathrm{i}}{N} m\right] + \text{h c} \\
&= -t \exp\left[\frac{2\pi \mathrm{i}}{N}\frac{\Phi}{\Phi_0}\right] \frac{\exp\left[-\frac{\pi \mathrm{i}}{N} M\right] - \exp\left[\frac{\pi \mathrm{i}}{N} M\right]}{1 - \exp\left[\frac{2\pi \mathrm{i}}{N}\right]} \; \frac{1 - \exp\left[-\frac{\pi \mathrm{i}}{N} 2\right]}{1 - \exp\left[-\frac{2\pi \mathrm{i}}{N}\right]} + \text{h c} \\
&= -t \frac{\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0} - \frac{\pi}{N} M\right) - \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0} + \frac{\pi}{N} M\right)}{1 - \cos\left(\frac{2\pi}{N}\right)} - \\
&\quad - t \frac{-\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0} - \frac{\pi}{N}(M+2)\right) + \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0} + \frac{\pi}{N}(M-2)\right)}{1 - \cos\left(\frac{2\pi}{N}\right)} \\
&= -t \frac{2\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\left(\frac{\pi}{N} M\right) - 2\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0} - \frac{2\pi}{N}\right)\sin\left(\frac{\pi}{N} M\right)}{1 - \cos\left(\frac{2\pi}{N}\right)} \\
&= -2t \frac{\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\left[1 - \cos\left(\frac{2\pi}{N}\right)\right] + \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\left(\frac{2\pi}{N}\right)}{2\sin^2\left(\frac{\pi}{N}\right)} \sin\left(\frac{\pi}{N} M\right) \\
&= -2t \frac{\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin^2\left(\frac{\pi}{N}\right) + \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\left(\frac{\pi}{N}\right)\cos\left(\frac{\pi}{N}\right)}{\sin^2\left(\frac{\pi}{N}\right)} \sin\left(\frac{\pi}{N} M\right) \\
&= -2t \frac{\cos\left(\frac{\pi}{N} - \frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)}{\sin\left(\frac{\pi}{N}\right)} \sin\left(\frac{\pi}{N} M\right) \\
&= -2t \left[\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) + \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cot\left(\frac{\pi}{N}\right)\right] \sin\left(\frac{\pi}{N} M\right)
\end{aligned}
$$

For these calculations the trigonometric identities (2 12) were used several times The final result for the case of an even number of fermions with flux is

$$
\Longrightarrow \boxed{E_{\text{even}} = -2t \frac{\sin\left(\frac{\pi}{N} M\right)}{\sin\left(\frac{\pi}{N}\right)} \cos\left(\frac{\pi}{N} - \frac{2\pi}{N} r\left(\frac{\Phi}{\Phi_0}\right)\right)} \qquad (2\ 37)
$$

The calculations for the other case are analogous:

$$\boxed{M \text{ odd}}$$

$$\begin{aligned}
E_{\text{odd}} &= -2t \sum_{m=-\frac{M-1}{2}}^{+\frac{M-1}{2}} \cos\left(\frac{2\pi}{N}\left(m+\frac{\Phi}{\Phi_0}\right)\right) \\
&= -t\exp\left[\frac{2\pi \mathrm{i}}{N}\frac{\Phi}{\Phi_0}\right]\exp\left[-\frac{\pi \mathrm{i}}{N}(M-1)\right]\sum_{m=0}^{M-1}\exp\left[\frac{2\pi \mathrm{i}}{N}m\right] + \text{h c.} \\
&= -t\exp\left[\frac{2\pi \mathrm{i}}{N}\frac{\Phi}{\Phi_0}\right]\frac{\exp\left[-\frac{\pi \mathrm{i}}{N}(M-1)\right]-\exp\left[\frac{\pi \mathrm{i}}{N}(M+1)\right]}{1-\exp\left[\frac{2\pi \mathrm{i}}{N}\right]}\cdot\frac{1}{1} + \text{h c} \\
&= -t\frac{\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}-\frac{\pi}{N}(M-1)\right)-\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}+\frac{\pi}{N}(M+1)\right)}{1-\cos\left(\frac{2\pi}{N}\right)} - \\
&\quad \ldots - t\frac{-\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}-\frac{\pi}{N}(M+1)\right)+\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}+\frac{\pi}{N}(M-1)\right)}{1-\cos\left(\frac{2\pi}{N}\right)} \\
&= -t\frac{2\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\left(\frac{\pi}{N}(M-1)\right)-2\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\left(\frac{\pi}{N}(M+1)\right)}{1-\cos\left(\frac{2\pi}{N}\right)} \\
&= -2t\frac{\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\left(\frac{\pi}{N}M\right)\sin\left(\frac{\pi}{N}\right)}{2\sin^2\left(\frac{\pi}{N}\right)},
\end{aligned}$$

which gives the final result for this case of an odd number of fermions with flux

$$\Longrightarrow \boxed{E_{\text{odd}} = -2t\frac{\sin\left(\frac{\pi}{N}M\right)}{\sin\left(\frac{\pi}{N}\right)}\cos\left(\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right)} \qquad (2\,38)$$

It is necessary to stress again that these calculations were made for the case $0 \leq \Phi/\Phi_0 < \frac{1}{2}$. Only at the end the argumentation above was used to reduce all other cases to this one, using the function (2.36). The total energy is therefore a periodic function in Φ.

2.3 The Parity Effect

It is worth comparing the obtained expressions for the total energy with included flux dependence (2.37) and (2.38) with former results for situations without flux, (2.13) and (2.14). Such a comparison shows that in both cases, for an even and for an odd number of particles, the flux changes the argument of a trigonometric

function in the numerator of the formula for the total energy

$$\begin{array}{lrcl} \text{even.} & \cos\left(\frac{\pi}{N}\right) & \longrightarrow & \cos\left(\frac{\pi}{N} - \frac{2\pi}{N} r \left(\frac{\Phi}{\Phi_0}\right)\right) \\ \text{odd.} & \cos(0) & \longrightarrow & \cos\left(0 - \frac{2\pi}{N} r \left(\frac{\Phi}{\Phi_0}\right)\right) \end{array} \qquad (2\ 39)$$

Furthermore, it confirms that $\Phi = 0$ gives the former results, that the two calculations are consistent.

The actual dependence of the total energy of a ring of fermions on the trapped magnetic flux Φ can be drawn. According to formula (2.37) and (2 38) the shape of the graph should mainly depend on whether an even or an odd number of particles is assumed

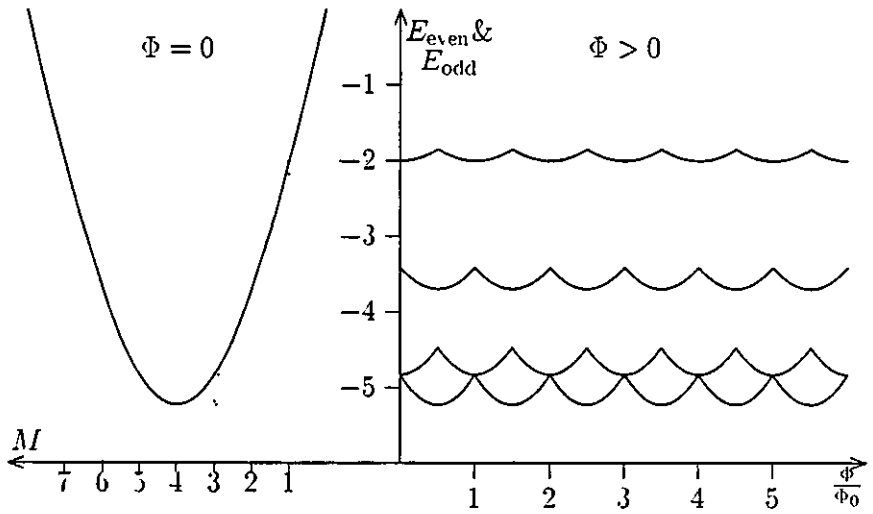


Figure 2 7 *The dependence of the total energy of a ring with $N = 8$ sites on the flux for $t = 1$ has the predicted periodicity (right) On the left hand side the ratio $-2t \sin\left(\frac{\pi}{N}M\right) / \sin\left(\frac{\pi}{N}\right)$ is calculated for different M-values, which gives the energy for zero flux apart from the factor $\cos\left(\frac{\pi}{N}\right)$ for an even particle number.*

Indeed, one can see in figure 2 7 that there is a periodicity of the flux dependence of the total energy The shape of the periodicity depends on whether the number of particles is even or odd

This difference between an even and an odd number of particles. which is described by the additional term $\frac{\pi}{N}$ in the cosine has already been mentioned briefly in section 2.1 3. After the effect of the flux has been evaluated, a more detailed explanation using statistical arguments is possible It is based on a publication of Kusmartsev [27]

One Fermion

Starting with one fermion, the following situation has to be considered. There is a ring with N sites The particle, which might be located on a certain site j_0 at time t_0 is free to move around the ring However, every time it reaches the site j_0 the situation is the same as for the time t_0 This obvious statement is included in the mathematical description of the situation by forcing periodic boundary conditions and single valued wave functions

The movement of the particle is connected with kinetic energy and a one-dimensional wave vector k The dispersion relation between them is of the form $E(k) = -2t\cos(k)$ (2 6). The possible k-values are quantized in the form $k_m = \frac{2\pi}{N}m$ (2 5) owing to the introduced periodic boundary conditions, and the ground state energy refers to $k = 0$ as long as there is no magnetic flux

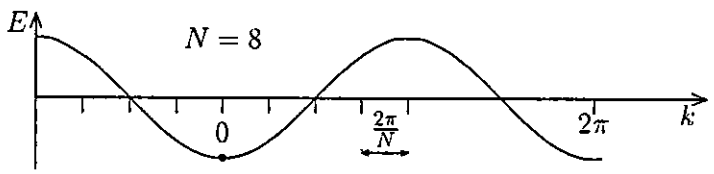


Figure 2.8 *Dispersion relation with* $M = 1$ *fermion and* $\Phi = 0$

If there is a flux trapped through the ring then the dispersion relation changes to $E_m = -2t\cos\left(\frac{2\pi}{N}\left(m + \frac{\Phi}{\Phi_0}\right)\right)$ (2 35) This means that the flux has the effect of adding momentum to the particle or, so to say, of moving it along the graph of the dispersion relation The choice of m which minimizes the total energy

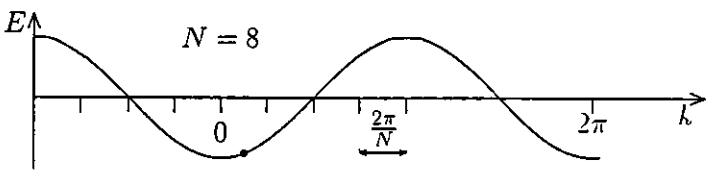


Figure 2 9: *Dispersion relation with* $M = 1$ *fermion and* $\Phi > 0$

depends now on the flux It is $m = 0$ for $\frac{\Phi}{\Phi_0} < \frac{1}{2}$, but as soon as an increasing flux passes this boundary the system will jump to $m = -1$ for the ground state. This was the physical reason for the introduced restriction-function (2 36).

Two Fermions

The situation becomes much more interesting when a second particle is added. If one of the two particles, called particle A, is assumed to be fixed on a certain site and the other one, B, moves around the ring, then the situation occurs that B has to pass A. Because of the fact that the particles are supposed to be fermions and because of their special anticommutation relations, this process of passing implies a minus sign in the wave function. In other words, the journey of one particle around the ring leads to an additional phase factor of $e^{\pi i}$. The boundary conditions are not any more periodic, but antiperiodic.

Something very similar occurs when an external magnetic flux is taken into consideration. The movement of a particle once around a loop trapped by a magnetic flux leads also to a phase factor, which has according to formula (2.27) the form $e^{2\pi i\frac{\Phi}{\Phi_0}}$. This analogy helps to understand the problem. Particle B experience the existence of particle A in the form of an internal flux of magnitude $\frac{\Phi_0}{2}$, called **statistical flux.**

An external magnetic flux changes the argument of the cosine in the expression of the total energy by $\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)$. Similarly, the mentioned internal flux causes the term $\frac{\pi}{N}$ in the cosine. Hence, the internal flux has also the effect of moving particles along the graph of the dispersion relation. This is important for the following reason: Formally, the total energy for a two particle system is minimized by choosing for the wave vectors $k_A = \frac{2\pi}{N}\ \frac{1}{2}$ and $k_B = \frac{2\pi}{N}\ \left(-\frac{1}{2}\right)$.

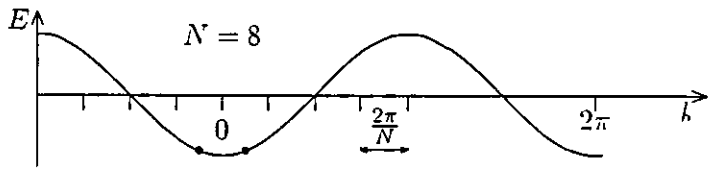


Figure 2.10: *Dispersion relation without parity effect*

However, a quantum number which is a half-odd integer implies that the α-factor of the wave function is antiperiodic.

$$\alpha_{j+N} = \frac{1}{\sqrt{N}}e^{\frac{2\pi i}{N}\frac{1}{2}(j+N)} = \frac{1}{\sqrt{N}}e^{i\pi}e^{\frac{2\pi i}{N}\frac{1}{2}j} = -\alpha_j$$

Additionally, the c-cyclic Hamiltonian used for these calculations shows an antiperiodicity as explained in 1.3. Together, the situation is periodic in contrary

to the considerations above.

To make this periodicity antiperiodic one has to use integer quantum numbers. This is exactly what is done when all particles are moved along the graph of the dispersion relation by an amount of $\frac{\pi}{N}$. The statistical flux ensures that an antiperiodicity exits ! It justifies the calculations that have been done with the result that the total energy of two particles on the ring with external magnetic flux is (2 37)

$$E_{\text{tot}} = -2t\frac{\sin\left(\frac{\pi}{N}2\right)}{\sin\left(\frac{\pi}{N}\right)} \cdot \cos\left(\frac{\pi}{N} - \frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right).$$

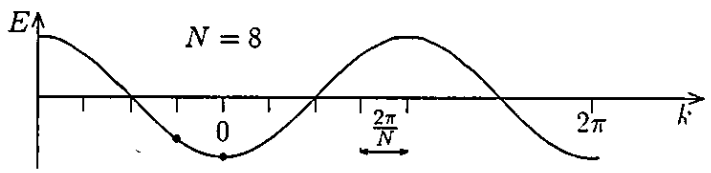


Figure 2.11: *Dispersion relation with parity effect*

An Arbitrary Number of Fermions

For an arbitrary number M of fermions each particle has to pass $M-1$ others in order to move once around the ring Hence, the phase factor connected with this movement is $e^{\pi i(M-1)} = (-1)^{M-1}$ The general expression of the total energy might therefore be written in the following way

$$E_{\text{tot}} = -2t\frac{\sin\left(\frac{\pi}{N}M\right)}{\sin\left(\frac{\pi}{N}\right)} \cdot \cos\left(\frac{\pi}{N}(M-1) - \frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)$$

However, this is in most cases not the ground state energy, but one of the exited states To obtain the former, it is necessary to find out which sites in momentum space should be occupied Then the right expression for the ground state energy is given by

$$E_{\text{ground}} = -2t\frac{\sin\left(\frac{\pi}{N}M\right)}{\sin\left(\frac{\pi}{N}\right)} \cdot \cos\left(\frac{\pi}{N}((M-1) \bmod 2) - \frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right). \qquad (2\,40)$$

In this formula all possible effects are included. The argumentation which leads to this result is called the "parity effect".

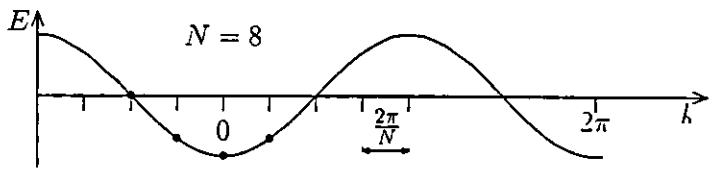


Figure 2.12 *Dispersion relation with $M = 4$ fermions and $\Phi > 0$*

Bosons

After presenting these arguments the result for the case that the particles under consideration are bosons instead of fermions can be predicted. Then commutation relations as given in (1.6) do not lead to a factor -1 when one particle passes another one. In other words, the many-body wave function is symmetric with respect to the exchange of two particles.

This means that for hardcore bosons, that is for bosons with allowed occupation numbers 0 and 1, the situation is *a priori* for every M the same as that for an odd number of fermions. Since, the shift of $\frac{\pi}{N}$ does not appear, the picture for the flux dependence of the total energy does not have two different shapes. There is no parity effect in this case.

The previous calculations for fermions are in essence also valid for bosons. However, in the case of an even number of particles there is of course a difference. It is based on the fact that here the previously mentioned situation appears that the ground state is formed by half-integer quantum numbers. That means that compared to an even number of fermions all particles are moved by $\frac{1}{2}\left(\frac{2\pi}{N}\right)$, what exactly annihilates the $\frac{\pi}{N}$ in the cosine. Hence, for hardcore bosons the ground

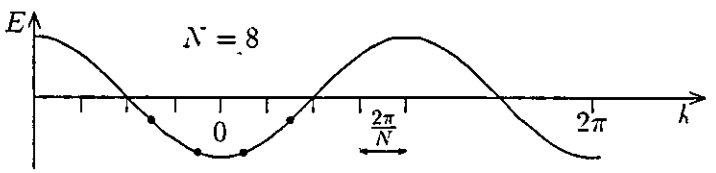


Figure 2.13: *Dispersion relation with $M = 4$ bosons and $\Phi = 0$*

state energy has always the form

$$E_{\text{boson}} = -2t\frac{\sin\left(\frac{\pi}{N}M\right)}{\sin\left(\frac{\pi}{N}\right)} \cdot \cos\left(\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right). \qquad (2.41)$$

2.4 Persistent Current

After the expression for the total energy E of the electron ring has been derived, it does not cause much more effort to obtain the value of the persistent current I. It is nothing other than the derivative of the total energy with respect to the flux through the ring,

$$I = -c\frac{\partial E}{\partial \Phi} \tag{2.42}$$

There are several possible explanations of this fact. The author would like to present two of them, one which uses macroscopic quantities to describe the situation and another one which starts from a microscopic point of view.

Macroscopic Explanation

The ring under consideration is placed in a homogeneous magnetic field B. Consequently, there is a flux $\Phi = \mathrm{B} \cdot \mathrm{S}$ threaded by the ring. Here S is a normal vector to the plane of the ring with a length proportional to the area enclosed by the circle.

The flux gives rise to a current I inside the ring. The dependence on the flux $I = I(\Phi)$ is *a priori* unknown. Whatever the current might be, its existence causes a magnetic moment m connected to the ring and parallel to S.

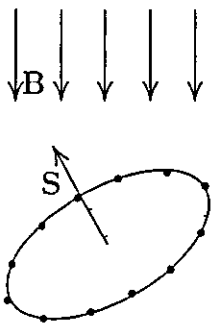


Figure 2.14 *Ring with 12 sites in a plane with a normal vector* S, *threaded by a magnetic field* B.

Its value is for the special case of a circular current density easily calculated to be

$$\mathrm{m} = \frac{1}{2c}\int \mathrm{d}^3 r\, \mathrm{r} \times \mathrm{j} = \frac{1}{2c} r \cdot 2\pi r \;\; I \;\; \mathrm{n} = \frac{1}{c} I \;\; \mathrm{S} \tag{2.43}$$

Such a magnetic moment inside a magnetic field posses a certain potential energy, which is minimal if the moment is aligned parallel to the field lines. Thus, the part of the energy of the ring which is connected to magnetic effects has the form

$$E_{\mathrm{magn}} = -\mathrm{m} \;\; \mathrm{B} = -\frac{1}{c} I \mathrm{S} \cdot \mathrm{B} = -\frac{1}{c} I \Phi \tag{2.44}$$

In a thermodynamic description $\mathbf{m}$ and B are independent variables The same is therefore true for the pair (I, Φ) and the persistent current becomes

$$I(\Phi) = -c \left(\frac{\partial E_{\text{magn}}}{\partial \Phi} \right)_I$$

□

Microscopic Explanation

Usually in the literature [3, 7, 8] the current is calculated by looking at its cause: the movement of electrons The energy dependence for the mth particle, as given in (2 35), can in the limit $N \gg M$ be assumed to be quadratic in the wave vector, $E_m = \frac{\hbar^2 k^2}{2m_{\text{eff}}}$. The unknown effective mass m_{eff} vanishes again if the velocity $v_m = \frac{\hbar k}{m_{\text{eff}}}$ is expressed as

$$v_m = \frac{1}{\hbar} \frac{\partial E_m}{\partial k} \quad \left(= \frac{\partial \omega}{\partial k} \Rightarrow \text{group velocity} \right) \tag{2 45}$$

On the other hand, the wave vector k is determined by the flux. The quantum number is only important for a reduction to the first Brillouin zone according to (2 36) and is taken into account again when switching to the total energy. However, one has to be careful with dimensionalities The unit of length has in all previous calculations been the distance between two sites on the ring, called a. In order to have a wave vector with the dimensionality 1/length, thus a has to be included.

$$\begin{aligned} v_m &= \frac{1}{\hbar} \frac{\partial E_m}{\partial \Phi} \frac{\partial \Phi}{\partial k} = \frac{1}{\hbar} \frac{\partial E_m}{\partial \Phi} \frac{1}{\frac{\partial k}{\partial \Phi}} \\ &= \frac{1}{\hbar} \frac{\partial E_m}{\partial \Phi} \frac{1}{\frac{2\pi}{aN} \frac{1}{\Phi_0}} = \frac{1}{\hbar} \frac{\partial E_m}{\partial \Phi} \frac{aN}{2\pi} \frac{hc}{e} = aN \frac{c}{e} \frac{\partial E_m}{\partial \Phi} \end{aligned} \tag{2 46}$$

The actual current is the common effect of all participating particles It can be calculated from

$$I = -e \sum_{m=1}^{M} \frac{v_m}{aN} = -c \sum_m \frac{\partial E_m}{\partial \Phi} = -c \frac{\partial E}{\partial \Phi},$$

where E is now the total energy of the many particle system □

Expressions for the Current

For the derivatives it is again necessary to distinguish between an odd and an even number of particles Starting with the expressions (2 37) and (2 38) for the total energy, we obtain after a short calculation.

$$I_{\text{even}} = \mp\frac{2te}{N\hbar}\frac{\sin\left(\frac{\pi}{N}M\right)}{\sin\left(\frac{\pi}{N}\right)}\cdot\sin\left(\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)-\frac{\pi}{N}\right) \qquad (2\,47)$$

$$I_{\text{odd}} = \mp\frac{2te}{N\hbar}\frac{\sin\left(\frac{\pi}{N}M\right)}{\sin\left(\frac{\pi}{N}\right)}\sin\left(\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right) \qquad (2\,48)$$

Apparently, there is an oscillation in the current-flux dependence This is in agreement with predictions by Buttinger, Imry and Landauer [2], with experimental results [3, 4, 5] and numerous other publications [8, 11, 12, 27] Nevertheless, it is worth discussing these expressions for the persistent current a bit more.

First of all, a remark on the sign is necessary The two different possibilities are caused by the derivative of the function $r(x)$, which restricts the flux onto a sufficient interval It is shown in figure 2 6 on page 42 that this function has a saw-tooth shape due to which the derivative has sometimes positive and sometimes negative values Instead of putting this fact into a sophisticated mathematical description, it is more convenient to show the figure 2 15. For large values of N the sin-function can well be approximated by straight lines

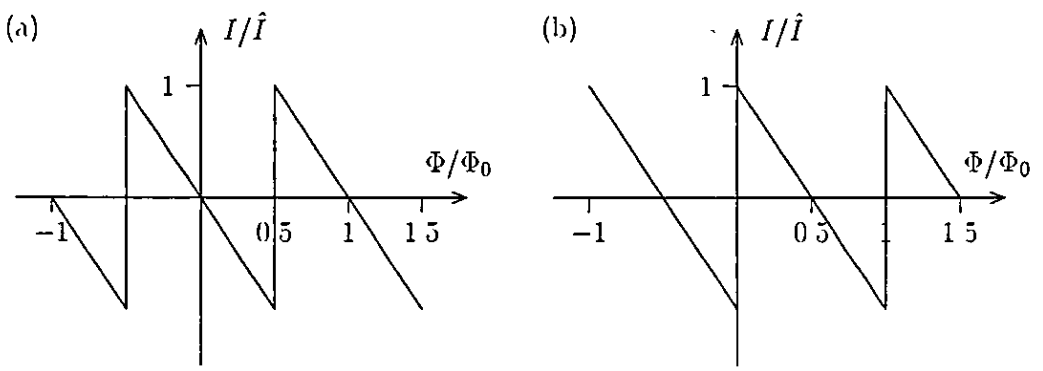


Figure 2.15 *Dependence of the persistent current on the trapped flux for (a) an odd number of particles and (b) an even number of particles $\hat{I}$ is the amplitude of the current*

The Amplitude

In many papers the amplitude of the oscillating current is compared with $\hat{I} = \frac{ev_F}{L}$, where v_F is the Fermi velocity and $L = aN$ is the circumference of the ring For this reason the results will now be transformed accordingly

In the case of an odd number of particles the maximum value for the current is connected to $\Phi/\Phi_0 = \frac{1}{2}$ The resulting sin-function at the end of (2 48) therefore cancels with $\sin\left(\frac{\pi}{N}\right)$ in the denominator The same can be done for an even number of particles and $\Phi = 0$

The velocity v_F for a particle at the Fermi edge ($m = \frac{M}{2}$) can be evaluated from its energy with the help of a derivative as above

$$v_F = -\frac{1}{\hbar}\frac{\partial}{\partial k} 2t\cos\left(\frac{\pi M}{N}\right) = \frac{2ta}{\hbar}\sin\left(\frac{\pi M}{N}\right) \Longrightarrow \quad \hat{I} = \frac{2te}{N\hbar}\sin\left(\frac{\pi M}{N}\right) = \frac{ev_F}{L}$$

Hence, the current can also be expressed in the following way

$$I_{\text{even}} \approx \mp\frac{ev_F}{L}\sin\left(\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right) - \frac{\pi}{N}\right) \frac{1}{\sin\left(\frac{\pi}{N}\right)} \tag{2 49}$$

$$I_{\text{odd}} \approx \mp\frac{ev_F}{L}\sin\left(\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right) \frac{1}{\sin\left(\frac{\pi}{N}\right)} \tag{2 50}$$

This result for the order of magnitude of the persistent current indicates that almost only the upper-most particle, the electron which has the energy of the Fermi edge, contributes to the current This surprising fact has its origin in different signs of the currents for the several lower lying particles, which effectively cancel each other [2, 7, 35]

Period Halving

One can clearly see in figure 2 15 that the period of the oscillation of the persistent current is one flux quantum $\Phi_0 = \frac{hc}{e}$. This is also what is obtained in experiments, provided that measurements were performed on single metallic loops For instance Chandrasekhar *et al* [4] were able to confirm this result by using a single, isolated gold loop However, first experimental results were published by Lévy *et al* [3]. They reported about an oscillation with a period half the flux quantum

The reason for the period halving is the fact that these scientists measured the effect of 10^7 copper rings simultaneously. The kind of averaging connected to such a large number of rings is discussed by various authors [3, 8, 36, 37]

Already in 1987 Cheung *et al.* [8] pointed out that one has to distinguish between a grand canonical and a canonical ensemble average. In the first case the chemical potential is kept fixed for each ring and the number of electrons varies with the flux Under such circumstances the average over different values for the chemical potential gives zero

In the second case of a canonical ensemble the number of particles is maintained, no matter what the value of the flux through the ring is This is exactly the situation we have investigated so far. Here the average has to be performed over different numbers of particles for the different rings.

If the same amplitude of the current is assumed for every particle number and if there are as many rings with an odd number of electrons as with an even number of electrons, then the average can simply be found The figure on the right hand side shows the period halving

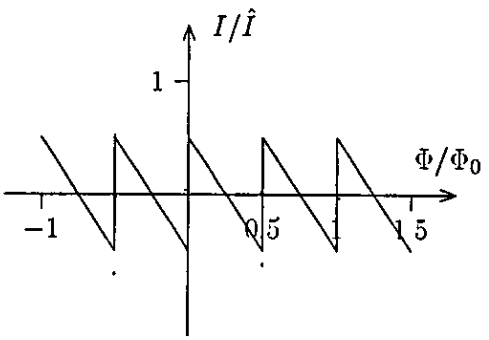


Figure 2.16 *Persistent current per ring (solid line) when averaged over a canonical ensemble of rings with an odd and an even number of particles respectively (dotted lines)*

Furthermore, one can see nicely in this figure that the averaging is also connected with an amplitude halving, with a decrease of the maximum of the persistent current

Loss and Goldbart [37] discussed this averaging process in more detail They assumed that the number of particles of a certain ring is Poisson distributed around a mean value λ. Then the probability for the ring to have M conduction electrons is $e^{-\lambda}\frac{\lambda^M}{M!}$ The sin-functions in (2 48) and (2 47) are linearised, which

allows to write them in the following form:

$$I(M) \approx X \cdot M \cdot \begin{cases} \left(\frac{2\Phi}{\Phi_0}\right) & \text{for } M \text{ odd} \\ \left(\frac{2\Phi}{\Phi_0} - 1\right) & \text{for } M \text{ even} \end{cases},$$

where X is some constant which does not depend on Φ and M, and the flux is for simplicity supposed to be within the interval $0 \leq \frac{\Phi}{\Phi_0} \leq \frac{1}{2}$.

Therefore, the expectation value of the function $I(M)$ is

$$\begin{aligned} \langle I \rangle_{\text{Poisson}} &= X\,\mathrm{e}^{-\lambda}\left(1\frac{\lambda^1}{1!} + 3\frac{\lambda^3}{3!} + . \quad + (2k+1)\frac{\lambda^{(2k+1)}}{(2k+1)!} + \quad\right)\left(\frac{2\Phi}{\Phi_0}\right) \\ &\quad + X\,\mathrm{e}^{-\lambda}\left(0\frac{\lambda^0}{0!} + 2\frac{\lambda^2}{2!} + . \;. + (2k)\frac{\lambda^{(2k)}}{(2k)!} + \quad\right)\left(\frac{2\Phi}{\Phi_0} - 1\right) \\ &= X\,\mathrm{e}^{-\lambda}\left[\frac{\lambda}{2}\left(\mathrm{e}^{\lambda} + \mathrm{e}^{-\lambda}\right)\left(\frac{2\Phi}{\Phi_0}\right) + \frac{\lambda}{2}\left(\mathrm{e}^{\lambda} - \mathrm{e}^{-\lambda}\right)\left(\frac{2\Phi}{\Phi_0} - 1\right)\right] \\ &= \frac{1}{2}X\lambda\left[2\left(\frac{2\Phi}{\Phi_0}\right) - 1 + \mathrm{e}^{-2\lambda}\right] \\ &\approx \frac{1}{2}\hat{I}(\lambda)\left(\frac{2\Phi}{\Phi_0/2} - 1\right) \end{aligned} \tag{2.51}$$

In the last line the term $\mathrm{e}^{-2\lambda}$ has been neglected because the mean number of particles is assumed to be large. The fact that the constant X goes together with λ means that the amplitude of the averaged current is that which corresponds to a ring with the mean number of particles; or better to say, it is half of that value as the fraction in front of the current indicates.

What is important about the calculation is that in the end Φ_0 is replaced by $\Phi_0/2$. This confirms that within the interval $0 \leq \frac{\Phi}{\Phi_0} \leq \frac{1}{2}$ the graph of the current versus the flux is steeper than before by a factor of 2. One can also check for the other intervals that the result of the Poisson average is exactly the same as already shown in figure 2.16 (if $I/\hat{I}$ is understood to be $\langle I \rangle / \hat{I}(\lambda)$). Thus, it is only natural that Lévy *et al.* discovered a half flux quantum periodicity.

Chapter 3

Interacting Fermions

3.1 Hartree-Fock Equations

There are mainly two possible ways for the derivation of the Hartree-Fock (HF) equations. One is well explained in the textbook of Kittel [38][1]. Here the one-particle solutions $\varphi_j(\mathrm{x})$ of the Hamiltonian are combined to field operators

$$\Psi(\mathrm{x}) = \sum_j c_j \varphi_j(\mathrm{x}) \quad \text{and} \quad \Psi^+(\mathrm{x}) = \sum_j c_j^\dagger \varphi_j^*(\mathrm{x}),$$

and the Hamiltonian is expressed in these operators. A study of the equation of motion $i\hbar\dot{\Psi} = -[\mathcal{H}, \Psi]_-$ leads then to the desired set of equations.

The other approach, which can f e be found in the books of Merzbacher [22], Nolting [28] or Fulde [39], uses variational methods. The Hamiltonian $\mathcal{H}$ under consideration is the sum of a single particle kinetic energy $\hat{H}_0$ and a two-particle interaction $\hat{V}$. The trial wave function for the variation is in this approach chosen to be a symmetrized product of M single particle wave functions. In second quantization this symmetrization happens automatically, in the continuous case a Slater-determinant form must be used:

$$|HF\rangle = \frac{1}{\sqrt{M!}} \sum_{p \in P(M)} (-1)^{\mathrm{sgn}\, p} \left(|\varphi_{\alpha_1}^{p(1)}\rangle\, |\varphi_{\alpha_2}^{p(2)}\rangle \quad \ldots \quad |\varphi_{\alpha_M}^{p(M)}\rangle \right).$$

With this trial wave function an expectation value of the Hamiltonian can be

[1] In a Green's function notation it can also be found in the book of Kadanoff and Baym [40]

derived. If all permutations are handled correctly, the result is

$$\langle HF|\mathcal{H}|HF\rangle = \sum_{\mu=1}^{M} \langle\varphi_{\alpha_\mu}^{(1)}|\hat{H}_0^{(1)}|\varphi_{\alpha_\mu}^{(1)}\rangle + \frac{1}{2}\sum_{\mu,\nu}^{\mu\neq\nu} \Big\{\langle\varphi_{\alpha_\nu}^{(1)}\varphi_{\alpha_\mu}^{(2)}|\hat{V}^{(1,2)}|\varphi_{\alpha_\nu}^{(1)}\varphi_{\alpha_\mu}^{(2)}\rangle - \langle\varphi_{\alpha_\nu}^{(1)}\varphi_{\alpha_\mu}^{(2)}|\hat{V}^{(1,2)}|\varphi_{\alpha_\nu}^{(2)}\varphi_{\alpha_\mu}^{(1)}\rangle\Big\},$$

where $\hat{H}_0^{(1)}$ is the part of $\hat{H}_0$ that acts on particle 1 and $\hat{V}^{(1,2)}$ describes the interaction of particles 1 and 2. In the interaction the first term is called "direct" and the second "exchange" term

By introducing unities at appropriate positions, it is also possible to rewrite this expression in position representation If the spin is separated from the quantum numbers α_j and the Hamiltonian is supposed to be spin independent, one obtains

$$\langle HF|\mathcal{H}|HF\rangle = \sum_{\mu\sigma}\int \mathrm{d}^3r\,\varphi_{\mu\sigma}^*(\mathbf{r})H_0(\mathbf{r})\varphi_{\mu\sigma}(\mathbf{r}) + \frac{1}{2}\sum_{\mu\sigma,\nu\sigma'}^{(\mu\sigma)\neq(\nu\sigma')}\iint \mathrm{d}^3r\mathrm{d}^3r' * \\ * \varphi_{\mu\sigma}^*(\mathbf{r})\varphi_{\nu\sigma'}^*(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\Big(\underbrace{\varphi_{\mu\sigma}(\mathbf{r})\varphi_{\nu\sigma'}(\mathbf{r}')}_{\text{direct}} - \underbrace{\delta_{\sigma,\sigma'}\varphi_{\mu\sigma'}(\mathbf{r}')\varphi_{\nu\sigma}(\mathbf{r})}_{\text{exchange}}\Big) \tag{3.1}$$

The variation principle[2] uses the fact that, no matter which kind of trial function is used, the expectation value of the Hamiltonian gives always an upper boundary of the ground state energy

$$\frac{\langle HF|\mathcal{H}|HF\rangle}{\langle HF|HF\rangle} = E \geq E_0 \tag{3.2}$$

In order to come the ground state energy as close as possible it is reasonable to minimize the left hand side.

$$\begin{aligned} 0 &\overset{!}{=} \delta\left(\frac{\langle HF|\mathcal{H}|HF\rangle}{\langle HF|HF\rangle}\right) \\ &= \langle HF|HF\rangle^{-2}\left(\langle HF|HF\rangle\ \delta\langle HF|\mathcal{H}|HF\rangle - \langle HF|\mathcal{H}|HF\rangle\ \delta\langle HF|HF\rangle\right) \\ &= \delta\langle HF|\mathcal{H}|HF\rangle - E\cdot\delta\langle HF|HF\rangle \\ &= \delta\langle HF|\mathcal{H}-E|HF\rangle, \end{aligned} \tag{3.3}$$

where a proper normalization of $|HF\rangle$ has been assumed

[2] also called Ritz method

Eventually, this procedure is equivalent to a minimization of $\langle HF|\mathcal{H}|HF\rangle$ together with normalization conditions introduced via a Lagrange multiplier $\lambda = E$ It is also common to take the normalization of each single particle wave function into account with the help of such multipliers

$$\delta\left(\langle HF|\mathcal{H}|HF\rangle - \sum_{\mu=1}^{M} \lambda_{\mu\sigma}\langle\varphi_{\alpha_\mu}^{(\mu)}|\varphi_{\alpha_\mu}^{(\mu)}\rangle\right) \stackrel{!}{=} 0 \tag{3.4}$$

Applied to the expectation value in integral notation (3.1), the variation principle gives the well-known **Hartree-Fock equations:**

$$\begin{aligned}\lambda_{\mu\sigma}\varphi_{\mu\sigma}(\mathbf{r}) &= \left(H_0(\mathbf{r}) + \sum_{\nu\sigma'}^{(\mu\sigma)\neq(\nu\sigma')} \int \mathrm{d}^3r'\, \varphi^*_{\nu\sigma'}(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\varphi_{\nu\sigma'}(\mathbf{r}')\right)\varphi_{\mu\sigma}(\mathbf{r}) \\ &\quad - \sum_{\nu}^{\nu\neq\mu} \int \mathrm{d}^3r'\, \varphi^*_{\nu\sigma}(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\varphi_{\mu\sigma'}(\mathbf{r}')\varphi_{\nu\sigma}(\mathbf{r})\end{aligned} \tag{3.5}$$

When looking at this formula, it becomes clear why it is also called **self-consistent field equation.** On the right hand side we have wave functions with primed arguments and without. Once the wave functions are known, it is possible to evaluate the integrals, which leave only unprimed terms The latter form a matrix equation, which can be solved (at least with numerical methods) The procedure should, therefore, be like this:

- Start with an assumption for the single-particle wave functions.
- Calculate the integrals with these functions
- Solve the matrix equations with the integrals as coefficients
- Use the gained wave functions again for the integral evaluation and continue

According to this procedure each particle moves within the field of the rest of the particles The iteration stops when the new wave functions are equal to these which were used for the integrals In this case one can speak of self-consistency

It is clear that such an iteration can only be performed by a computer Even so, a numerical investigation was not planned to be used for the present work, Hartree-Fock like calculations have been started This happened mainly to get a deeper insight into the structure of the problem and not in the first place to achieve exact results.

Remark: One also finds in the literature [28] another equation with the name Hartree-Fock approximation It is a similar mean-field approximation, but in this case for a product of two operators $\hat{A}\hat{B}$. Such a product can be rewritten in the form

$$\hat{A}\hat{B} = \left(\hat{A} - \langle\hat{A}\rangle\right)\left(\hat{B} - \langle\hat{B}\rangle\right) + \hat{A}\langle\hat{B}\rangle + \hat{B}\langle\hat{A}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle$$

The approximation is based on the assumption that close to self-consistency fluctuations around the expectation value can be neglected. Hence,

$$\hat{A}\hat{B} \approx \hat{A}\langle\hat{B}\rangle + \hat{B}\langle\hat{A}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle, \tag{3 6}$$

which reduces in an elegant way the operator product to a linear problem This approximation, which is for the special case of the Hubbard model and its product of occupation number operators called Stoner model, allows in a similar way as above to perform an iteration. Although it is not used in this particular way within this work, we shall see similar structures when using the Hubbard-Stratanovic decomposition.

3.2 The α-problem

As a first step into an investigation of interactions between different particles on the ring, an ensemble of spinless fermions is considered. An appropriate Hamiltonian in this context is the above mentioned Heisenberg operator (1.23)

$$\mathcal{H} = -t\sum_k \left(c_k^\dagger c_{k+1} + c_{k+1}^\dagger c_k\right) + V\sum_k \hat{n}_k\hat{n}_{k+1}.$$

It is the aim to find the corresponding eigenfunctions and eigenvalues The latter, that means the energies of the system, are of particular interest because they enable us to obtain statements on the persistent current

Unfortunately, the Hartree-Fock equations (3 5) cannot be used directly to solve this task This is not only because they form an iterative approach to the problem. The fact that they have so far only been formulated for the continuous case is an even bigger limitation However, in the situation under consideration the space is a discrete lattice in one dimension For this reason the variation is done again by hand With the wave functions introduced in 3 2 1 an expectation

value of the Hamiltonian can be obtained (3 2 2), and the derivative in 3 2 4 leads to Hartree-Fock equations which can be solved (3.2 5).

3.2.1 The Variational Wave Functions

In the previous chapter the case $V \equiv 0$ has been investigated The many-body wave function was formulated in second quantization in a way that several (M) fermions were created at the same time on different sites Each of the possibilities was weighted with a factor, which depended on a set of quantum numbers All together, as for instance in section 2 1 4, we used the form

$$|\psi\rangle_{n_1 \quad n_M} = \sum_{i_1, \quad ,i_M} \alpha_{i_1}^{n_1 \quad n_M} {}_{i_M} c_{i_1}^\dagger c_{i_2}^\dagger \quad c_{i_M}^\dagger |0\rangle,$$

where N and M are the number of sites and particles, respectively

However, we got the result that Bloch wave functions are solutions and that the coefficients can, therefore, be written as

$$\alpha_{i_1 \quad i_M}^{n_1 \quad n_M} = N^{-M/2} \exp\left[\frac{2\pi \imath}{N}(n_1 i_1 + n_2 i_2 + \quad n_M i_M)\right]$$

This knowledge allows to represent the wave-function as

$$|\psi\rangle_{n_1 \quad n_M} = \prod_{s=1}^{M} \left(\sum_{i_s=1}^{N} \alpha_{i_s}^{n_s} c_{i_s}^\dagger \right) |0\rangle \tag{3 7}$$

with the splitted coefficients

$$\alpha_{i_s}^{n_s} = \frac{1}{\sqrt{N}} \exp\left[\frac{2\pi \imath}{N} n_s \quad i_s\right]$$

Such a representation is essentially a reduction of the complicated many particle problem to a problem of M separate particles Each of them is described by the functional dependence of $\alpha_{i_s}^{n_s}$ on the site number i_s, determined by the quantum number n_s A normalization for the single particle, $\sum_{i_s=1}^{N} |\alpha_{i_s}^{n_s}|^2 = 1$, as well as for the complete wave function, ${}_{n_1 \quad n_M}\langle\psi|\psi\rangle_{n_1 \quad n_M} = 1$, is given

The *ansatz* for the following calculations is that the variational wave function can also for the case $V \neq 0$ be handled in a way as if M separated particles were moving along the ring. That is, the variational wave function has the form (3 7) with unknown coefficients $\alpha_{i_s}^{n_s}$ [3]

[3] It is common to tackle the many-particle problem within the Hubbard model in such a way

3.2.2 Expectation Value

With the help of the variational wave function an expectation value for the Heisenberg Hamiltonian can be evaluated. This has to be done carefully for both involved parts. However, the steps are very similar to those in section 2.1.4. Especially, sums over all possible permutations of M particles appear again.

Hopping Part

$$
\begin{aligned}
&{}_{n_1\ \ n_M}\langle\psi|\hat{H}_0|\psi\rangle_{n_1\ \ n_M} \\
&= -t\sum_k \sum_{\substack{i_1 \\ j_1}} \cdots \sum_{\substack{i_M \\ j_M}} \alpha_{j_1}^{n_1 *}\cdots\alpha_{j_M}^{n_M *}\alpha_{i_1}^{n_1}\ \cdot\alpha_{i_M}^{n_M}\ \cdots \\
&\qquad\qquad \cdot\ \ \langle 0|c_{j_M}\cdot\ \ c_{j_1}\left(c_k^\dagger c_{k+1}+c_{k+1}^\dagger c_k\right)c_{i_1}^\dagger\cdots c_{i_M}^\dagger|0\rangle \\
&= \cdot\quad \sum_{A=1}^{M}\Big\{\langle 0|c_{j_M}\cdot\ \cdot c_{j_1}c_k^\dagger c_{k+1}c_{i_1}^\dagger\cdot\ \cdot c_{i_M}^\dagger|0\rangle\delta_{i_A,k+1} \\
&\qquad\qquad +\langle 0|c_{j_M}\quad c_{j_1}c_k^\dagger c_{k-1}c_{i_1}^\dagger\quad c_{i_M}^\dagger|0\rangle\delta_{i_A,k-1}\Big\} \\
&= \cdot\ \cdot\sum_{A=1}^{M}\Big\{\langle 0|c_{j_M}\cdot\ \ c_{j_1}c_{i_1}^\dagger\cdots c_{i_A-1}\widehat{c_{i_A}^\dagger}\cdot\ \ c_{i_M}^\dagger|0\rangle\,\delta_{i_A-1,k} \\
&\qquad\qquad +\langle 0|c_{j_M}\cdot\ \ c_{j_1}c_{i_1}^\dagger\cdot\ \cdot\widehat{c_{i_A}^\dagger}c_{i_A+1}^\dagger\cdots c_{i_M}^\dagger|0\rangle\,\delta_{i_A+1,k}\Big\} \\
&= -t\sum_{A=1}^{M}\sum_{\substack{i_1 \\ j_1}}\cdots\sum_{\substack{i_M \\ j_M}}\alpha_{j_1}^{n_1 *}\quad\alpha_{j_M}^{n_M *}\alpha_{i_1}^{n_1}\ \cdot\left(\alpha_{i_A+1}^{n_A}+\alpha_{i_A-1}^{n_A}\right)\ \cdot\ \alpha_{i_M}^{n_M}\langle 0|c_{j_M}\quad\cdot c_{j_1}c_{i_1}^\dagger\cdots c_{i_M}^\dagger|0\rangle \\
&= -t\sum_{A=1}^{M}\sum_{j_1}\sum_{j_M}\sum_{\wp\in\mathcal{P}(M)}(-1)^{\operatorname{sgn}\wp}\alpha_{j_1}^{n_1 *}\quad\alpha_{j_M}^{n_M *}\alpha_{j_1}^{n_{\wp(1)}}\quad\left(\alpha_{j_A+1}^{n_{\wp(A)}}+\alpha_{j_A-1}^{n_{\wp(A)}}\right)\quad\alpha_{j_M}^{n_{\wp(M)}}
\end{aligned}
$$

Interaction Part

$$
\begin{aligned}
&{}_{n_1\ \ n_M}\langle\psi|\hat{V}|\psi\rangle_{n_1\ \ n_M} \\
&\quad = V\sum_k\sum_{\substack{i_1 \\ j_1}}\cdots\sum_{\substack{i_M \\ j_M}}\alpha_{j_1}^{n_1 *}\cdots\alpha_{j_M}^{n_M *}\alpha_{i_1}^{n_1}\ \cdot\alpha_{i_M}^{n_M} \\
&\qquad\cdot\langle 0|c_{j_M}\cdot\ \ c_{j_1}c_k^\dagger c_k c_{k+1}^\dagger c_{k+1}c_{i_1}^\dagger\quad c_{i_M}^\dagger|0\rangle
\end{aligned}
$$

For instance Tasaki used in his review articles [43] for expressions like $\sum_{i_s=1}^{N}\alpha_{i_s}^{n_s}c_{i_s}^\dagger$ the index free notation $C^\dagger\left(\alpha^{(n_s)}\right)$

$$= \cdot \sum_{\substack{A\,B=1\\A\neq B}}^{M} \langle 0|c_{j_M}\cdots c_{j_1}c^\dagger_{i_1} \cdot c^\dagger_k c_k c^\dagger_{i_A} c^\dagger_{k+1}c_{k+1}c^\dagger_{i_B} \cdot c^\dagger_{i_M}|0\rangle \delta_{k,i_A}\delta_{k+1,i_B}$$

$$= \cdot \sum_{\substack{A\,B=1\\A\neq B}}^{M} \langle 0|c_{j_M}\cdot\cdot c_{j_1}c^\dagger_{i_1} \cdot c^\dagger_{i_M}|0\rangle \delta_{k,i_A}\delta_{i_B,i_A+1}$$

$$= \sum_{\substack{A\,B=1\\A\neq B}}^{M} \sum_{j_1} \sum_{j_M} \sum_{p\in\mathcal{P}(M)} (-1)^{\mathrm{sgn}p}\alpha^{n_1*}_{j_1}\cdots\alpha^{n_M*}_{j_M}\alpha^{n_{p(1)}}_{j_1}\cdot\cdot\alpha^{n_{p(M)}}_{j_M}\delta_{j_B,j_A+1}$$

Normalization

$${}_{n_1\ \ n_M}\langle\psi|\psi\rangle_{n_1\ \ n_M} = \sum_{j_1\ \ j_M}\sum_{p\in\mathcal{P}(M)}(-1)^{\mathrm{sgn}p}\alpha^{n_1*}_{j_1}\ \ \alpha^{n_M*}_{j_M}\alpha^{n_{p(1)}}_{j_1}\cdot\cdot\ \alpha^{n_{p(M)}}_{j_M}$$

That is nothing other than a Slater determinant

3.2.3 Remark on Lagrange Multipliers

The next step within a Ritz procedure is to take derivatives with respect to one of the parameters of the variational wave function. However, from experience the author would like to interpolate a brief remark One might feel tempted to simplify the expression for the expectation values above by using normalization conditions like $\sum_{i=1}^{N}|\alpha_i^{n_s}|^2 = 1$

For instance, for a two-particle Hubbard model with the Hamiltonian

$$\mathcal{H} = -t\sum_k\sum_{\sigma=\uparrow,\downarrow}\left(c^\dagger_{k,\sigma}c_{k+1,\sigma} + c^\dagger_{k+1,\sigma}c_{k,\sigma}\right) + U\sum_k \hat{n}_{k,\uparrow}\hat{n}_{k,\downarrow}$$

and a wave function

$$|\psi\rangle = \sum_{i,j}\alpha_i\beta_j c^\dagger_{i,\uparrow}c^\dagger_{j,\downarrow}|0\rangle$$

one finds the expectation value for the hopping part to be

$$\langle\psi|\hat{H}_0|\psi\rangle = -t\sum_{i,j}\left(\alpha_{i+1}\beta_j\alpha^*_i\beta^*_j + \alpha_i\beta_{j+1}\alpha^*_i\beta^*_j\right) + \text{h c}\,,$$

where h.c. has here the consequence that $i+1$ is replaced by $i-1$ A normalization for the single particle means that $\sum_i \alpha_i\alpha^*_i = 1$ and for β respectively. This leads to

$$\langle\psi|\hat{H}_0|\psi\rangle = -t\sum_i\left\{\alpha^*_i\left(\alpha_{i+1}+\alpha_{i-1}\right) + \beta^*_i\left(\beta_{i+1}+\beta_{i-1}\right)\right\}$$

and together with the interaction part to

$$\langle\psi|\mathcal{H}|\psi\rangle = -t\sum_i \left\{\alpha_i^*\left(\alpha_{i+1}+\alpha_{i-1}\right)+\beta_i^*\left(\beta_{i+1}+\beta_{i-1}\right)\right\}+U\sum_i|\alpha_i\beta_i|^2\,.$$

A derivative with respect to one of the coefficients, say α_k^*, with a normalization condition for the many particle wave function included via a Lagrange multiplier λ leads to the following set of equations [4]

$$\begin{aligned} t\left(\alpha_{k+1}+\alpha_{k-1}\right) &= \left[U|\beta_k|^2-\lambda\right]\alpha_k, \\ t\left(\beta_{k+1}+\beta_{k-1}\right) &= \left[U|\alpha_k|^2-\lambda\right]\beta_k \end{aligned} \tag{3 8}$$

On the other hand, if the normalization condition for the single particle is not used at the beginning, the equations after the derivative have a form which contains an additional exchange term

$$\begin{aligned} t\left(\alpha_{k+1}+\alpha_{k-1}\right) &= \left[U|\beta_k|^2-t\textstyle\sum_i\left(\beta_{i+1}+\beta_{i-1}\right)\beta_i^*-\lambda\right]\alpha_k, \\ t\left(\beta_{k+1}+\beta_{k-1}\right) &= \left[U|\alpha_k|^2-t\textstyle\sum_i\left(\beta_{i+1}+\beta_{i-1}\right)\beta_i^*-\lambda\right]\beta_k \end{aligned} \tag{3 9}$$

The second possibility 3 9 is of course the more correct one In the version 3 8 a normalization was used which is also included in the constraint via Lagrange multipliers However, constraints coupled with the help of Lagrange multipliers should not be used before the derivative is done

3.2.4 Derivatives and Simplifications

After this interpolation it is the right moment to perform the derivatives In the variational wave function of the form (3 7) the free parameters are the coefficients $\alpha_{i_c}^{n_s}$. They appear in every term of the expectation value in this way as well as in the complex conjugate form

Arbitrary, for derivatives the complex conjugate coefficient $\alpha_x^{n_c*}$ for a certain site x and connected with a certain quantum number n_c has been chosen The quantum number, of course, has to be within the set $\{n_s\}_{s=1}^{M}$ which determines the many-particle wave function

[4] An equalization of α_k and β_k has the consequence of a nonlinear Schrodinger equation of the form $-t\alpha_{k+1}-t\alpha_{k-1}+U\alpha_k^3=\lambda\alpha_k$, which has been studied intensively and with exact solutions by Dhillon and Kusmartsev [41]

However, a variational method with $M \times N$ parameters leads two $M \times N$ equations of the form

$$0 \overset{!}{=} \frac{\partial}{\partial \alpha_x^{n_c *}} \left({}_{n_1 \ \ n_M}\langle \psi | \mathcal{H} | \psi \rangle_{n_1 \ \ n_M} - \lambda_{n_1 \ \ n_M} \langle \psi | \psi \rangle_{n_1 \ \ n_M} \right) \tag{3 10}$$

Furthermore, a derivative with respect to the Lagrange multiplier reproduces the normalization condition All these equations have to be fulfilled at the same time This implies that if within the general notation with an arbitrary x and n_c a result for λ can be found, then this result must be independent of x and n_c.

Another remark is connected to the simplifications which are according to the previous section only possible after the derivative Encouraged by the solutions for non-interacting particles, which were Bloch wave functions, we suppose not only a normality

$$\sum_{j=1}^{N} \alpha_j^{n_s} \alpha_j^{n_s *} = 1 \quad \forall n_s, \tag{3 11}$$

but also an orthogonality for different quantum numbers

$$\sum_{j=1}^{N} \alpha_j^{n_s} \alpha_j^{n_t *} = 0 \quad \forall n_s \neq n_t \tag{3 12}$$

The latter condition does not necessarily have to hold It is already a rigorous assumption that the many-particle problem can be separated in different factors for the several particles To demand also orthogonality of these factors is even less justified Nevertheless, as long as solutions can be found which obey them, constraints can be formulated

Hopping Part

$$\begin{aligned}
&\frac{\partial}{\partial \alpha_x^{n_C *}} \left({}_{n_1 \ \ n_M}\langle \psi | \hat{H}_0 | \psi \rangle_{n_1 \ \ n_M} \right) \\
&= -t \sum_{\lambda=1}^{M} \sum_{\wp} (-1)^{\operatorname{sgn}\wp} \sum_{j_1 \ \ j_M}^{j_C = x} \alpha_{j_1}^{n_1 *} \cdots \widehat{\alpha_{j_C}^{n_c *}} \cdots \alpha_{j_M}^{n_M *} \alpha_{j_1}^{n_{\wp(1)}} \cdot \left(\alpha_{j_A+1}^{n_{\wp(\lambda)}} + \alpha_{j_A-1}^{n_{\wp(A)}} \right) \cdots \alpha_{j_M}^{n_{\wp(M)}} \\
&= \underbrace{-t \sum_{\substack{\lambda=1 \\ A \neq C}}^{M} \sum_{j_A} \alpha_{j_A}^{n_A *} \left(\alpha_{j_A+1}^{n_A} + \alpha_{j_A-1}^{n_A} \right) \alpha_x^{n_C}}_{\wp = \mathrm{id},\, A \neq C} + \underbrace{t \sum_{\substack{\lambda=1 \\ A \neq C}}^{M} \sum_{j_A} \alpha_{j_A}^{n_A *} \left(\alpha_{j_A+1}^{n_C} + \alpha_{j_A-1}^{n_C} \right) \alpha_x^{n_A}}_{\wp(A)=C,\, \wp(C)=A,\, A \neq C} \\
&\quad \underbrace{-t \left(\alpha_{x+1}^{n_C} + \alpha_{x-1}^{n_C} \right)}_{\wp = \mathrm{id},\, A = C}
\end{aligned}$$

Interaction Part

$$\frac{\partial}{\partial\alpha_x^{n_c*}}\left({}_{n_1\ \ n_M}\langle\psi|\hat{V}|\psi\rangle_{n_1\ \ n_M}\right)$$

$$= V\sum_{\substack{A\\A\neq B}}^{M}\sum_{\substack{B=1\\A\neq B}}^{M}\sum_{p\in\mathcal{P}(M)}(-1)^{\mathrm{sgn}p}\sum_{j_1\ \ j_M}^{j_c=x}\delta_{j_B,j_A+1}\alpha_{j_1}^{n_1*}\quad\widehat{\alpha_{j_c}^{n_c*}}\quad\alpha_{j_M}^{n_M*}\alpha_{j_1}^{n_{p(1)}}\cdots\alpha_{j_M}^{n_{p(M)}}$$

$$= V\sum_{\substack{A\\A\neq B}}^{\substack{A\neq C\\B\neq C}}\sum_{j_A,j_B}^{j_B=j_A+1}\alpha_{j_A}^{n_A*}\alpha_{j_B}^{n_B*}\left\{\alpha_{j_A}^{n_A}\alpha_{j_B}^{n_B}\alpha_x^{n_C}-\alpha_{j_A}^{n_A}\alpha_{j_B}^{n_C}\alpha_x^{n_B}-\alpha_{j_A}^{n_B}\alpha_{j_B}^{n_A}\alpha_x^{n_C}\right.$$

$$\left.+\alpha_{j_A}^{n_B}\alpha_{j_B}^{n_C}\alpha_x^{n_A}+\alpha_{j_A}^{n_C}\alpha_{j_B}^{n_A}\alpha_x^{n_B}-\alpha_{j_A}^{n_C}\alpha_{j_B}^{n_B}\alpha_x^{n_A}\right\}$$

$$+\ V\sum_{\substack{A\\A\neq B}}^{B=C}\sum_{\substack{j_A\\j_A+1=x}}\alpha_{j_A}^{n_A*}\left\{\alpha_{j_A}^{n_A}\alpha_x^{n_C}-\alpha_{j_A}^{n_C}\alpha_x^{n_A}\right\}+V\sum_{\substack{A\\A\neq B}}^{A=C}\sum_{\substack{j_B\\j_B=x+1}}\alpha_{j_B}^{n_B*}\left\{\alpha_{j_B}^{n_B}\alpha_x^{n_C}-\alpha_{j_B}^{n_C}\alpha_x^{n_B}\right\}$$

Normalization

$$\frac{\partial}{\partial\alpha_x^{n_c*}}\left({}_{n_1\ \ n_M}\langle\psi|\psi\rangle_{n_1\ \ n_M}\right)$$

$$= \sum_{p\in\mathcal{P}(M)}(-1)^{\mathrm{sgn}p}\sum_{j_1\ \ j_M}^{j_c=x}\alpha_{j_1}^{n_1*}\cdots\widehat{\alpha_{j_c}^{n_c*}}\cdots\alpha_{j_M}^{n_M*}\alpha_{j_1}^{n_{p(1)}}\quad\alpha_{j_M}^{n_{p(M)}}$$

$$= \alpha_x^{n_c}$$

If all these terms are put together in the variational formula (3 10), a set of equations for the coefficients $\alpha_{i_s}^{n_s}$ is obtained The problem to find proper solutions is called in this work the **α-problem**

$$-\ t\sum_{\substack{A\\A\neq C}}^{M}\sum_{\substack{A=1\\A\neq C}}^{M}\sum_j\alpha_j^{n_A*}\left(\alpha_{j+1}^{n_A}+\alpha_{j-1}^{n_A}\right)\alpha_x^{n_C}+t\sum_{\substack{A\\A\neq C}}^{M}\sum_{\substack{A=1\\A\neq C}}^{M}\sum_j\alpha_j^{n_A*}\left(\alpha_{j+1}^{n_C}+\alpha_{j-1}^{n_C}\right)\alpha_x^{n_A}$$

$$-\ t\left(\alpha_{x+1}^{n_C}+\alpha_{x-1}^{n_C}\right)$$

$$+\ V\sum_{\substack{A\\A\neq B}}^{\substack{A\neq C\\B\neq C}}\sum_{\substack{A=1\\A\neq B}}^{\substack{A\neq C\\B\neq C}}\sum_j\alpha_j^{n_A*}\alpha_{j+1}^{n_B*}\left\{\left(\alpha_j^{n_A}\alpha_{j+1}^{n_B}-\alpha_j^{n_B}\alpha_{j+1}^{n_A}\right)\alpha_x^{n_C}\right.$$

$$\left.+\left(\alpha_j^{n_C}\alpha_{j+1}^{n_A}-\alpha_j^{n_A}\alpha_{j+1}^{n_C}\right)\alpha_x^{n_B}+\left(\alpha_j^{n_B}\alpha_{j+1}^{n_C}-\alpha_j^{n_C}\alpha_{j+1}^{n_B}\right)\alpha_x^{n_A}\right\}$$

$$+\ V\sum_{\substack{A\\A\neq C}}^{M}\sum_{\substack{A=1\\A\neq C}}^{M}\left\{\left(\alpha_{x-1}^{n_A*}\alpha_{x-1}^{n_A}+\alpha_{x+1}^{n_A*}\alpha_{x+1}^{n_A}\right)\alpha_x^{n_C}-\left(\alpha_{x-1}^{n_A*}\alpha_{x-1}^{n_C}+\alpha_{x+1}^{n_A*}\alpha_{x+1}^{n_C}\right)\alpha_x^{n_A}\right\}$$

$$= \lambda\alpha_x^{n_C} \qquad (3\ 13)$$

If this result is compared with the original self-consistent field equation how it was derived in (3.5) one finds the same structure Both equations consist of a direct part and an exchange part. What was former an integral over space is in the discrete version a sum over the lattice sites The former quantum numbers $(\mu\sigma)$ and $(\nu\sigma)$ are now n_C and n_A, accordingly

3.2.5 Solutions

The α-problem looks like a quite complicated task. However, it turns out that the solution is simple. Even so an interaction is now included, **Bloch wave functions** still fulfil the given set of equations In order to prove this, $\alpha_{i_s}^{n_s}$ is set to be

$$\alpha_{i_s}^{n_s} = \frac{1}{\sqrt{N}} \exp\left[\frac{2\pi \mathrm{i}}{N} n_s \cdot i_s\right],$$

and the whole equation is divided by $\alpha_x^{n_c}$ Hence, an expression for λ is obtained As already mentioned above, the solution is correct if this expression does neither depend on x nor on n_c This would show that no matter with respect to which parameter the derivative is done, the equations are always the same

Proof: The independence of x and n_c can be shown for each of the parts in (3 13) separately. In the hopping part the direct terms

$$\begin{cases} -t \sum\limits_{\substack{A=1 \\ A\neq C}}^{M} \frac{1}{N} \sum\limits_{j} e^{-\frac{2\pi \mathrm{i}}{N} n_A j} \left(e^{\frac{2\pi \mathrm{i}}{N} n_A (j+1)} + e^{\frac{2\pi \mathrm{i}}{N} n_A (j-1)}\right) & \text{and} \\ -t \left(e^{\frac{2\pi \mathrm{i}}{N} n_C} + e^{-\frac{2\pi \mathrm{i}}{N} n_C}\right) \end{cases}$$

can be combined to one sum which runs over all used quantum numbers·

$$= -t \sum_{A=1}^{M} \left(e^{\frac{2\pi \mathrm{i}}{N} n_A} + e^{-\frac{2\pi \mathrm{i}}{N} n_A}\right) \tag{3 14}$$

The remaining exchange term in the hopping part essentially contains a common factor

$$\sum_{j=1}^{N} e^{\frac{2\pi \mathrm{i}}{N}(n_C - n_A) j} = \sum_{j=0}^{N-1} e^{\frac{2\pi \mathrm{i}}{N} n j} = \frac{1 - e^{\frac{2\pi \mathrm{i}}{N} n N}}{1 - e^{\frac{2\pi \mathrm{i}}{N} n}} = 0 \quad \text{with } n = n_C - n_A \neq 0 \tag{3 15}$$

The behaviour of the pure kinetic energy part is not surprising because Bloch wave functions are solutions for the free particle case Much more surprising is the independence of x and n_C for the interaction part

Here many of the terms vanish because of a similar geometric row effect as used in (3 15). Two sums reduce to unimportant constants due to the characteristic of Bloch wave functions that $|\alpha_j^n|^2 = 1/N$ The only three remaining terms are

$$\begin{cases} -V \sum\limits_{\substack{A\neq C \\ B\neq C}}^{\substack{A\neq B}} \frac{1}{N^2} \sum\limits_{j} e^{-\frac{2\pi i}{N} n_A j} e^{-\frac{2\pi i}{N} n_B (j+1)} e^{\frac{2\pi i}{N} n_B j} e^{\frac{2\pi i}{N} n_A (j+1)}, \\ -V \sum\limits_{\substack{A=1 \\ A\neq C}}^{M} \frac{1}{N} e^{-\frac{2\pi i}{N} n_A (x-1)} e^{\frac{2\pi i}{N} n_C (x-1)} e^{\frac{2\pi i}{N} (n_A - n_C) x} \quad \text{and} \\ -V \sum\limits_{\substack{A=1 \\ A\neq C}}^{M} \frac{1}{N} e^{-\frac{2\pi i}{N} n_A (x+1)} e^{\frac{2\pi i}{N} n_C (x+1)} e^{\frac{2\pi i}{N} (n_A - n_C) x} \end{cases}$$

which can be combined again to a sum over all quantum numbers

$$= -\frac{V}{N} \sum_{A\neq B} e^{-\frac{2\pi i}{N}(n_A - n_B)} \tag{3 16}$$

This finishes the proof □

3.3 Energy in the Heisenberg Model

After having shown that Bloch wave functions are solutions of the Hartree-Fock equations, it is now possible to use them for the calculation of the energy of the interacting system Here it is important to notice that the following calculation of the expectation value of the Hamiltonian will only give an upper boundary of the ground state How close it is to the real value depends on the quality of the choice of the variational wave function

We continue the calculation of the expectation value in subsection 3 2 2

Hopping Part

$$\begin{aligned} {}_{n_1 \ \ n_M}\langle \psi | \hat{H}_0 | \psi \rangle_{n_1 \ \ n_M} \\ &= -t \sum_{A=1}^{M} \sum_{j_1} \sum_{j_M} \sum_{\wp \in P(M)} (-1)^{\operatorname{sgn}\wp} \alpha_{j_1}^{n_1 *} \cdot \alpha_{j_M}^{n_M *} \alpha_{j_1}^{n_{\wp(1)}} \underbrace{\left(\alpha_{j_A}^{n_{\wp(A)}} + \alpha_{j_A}^{n_{\wp(A)}} \right)}_{= \alpha_{j_A}^{n_{\wp(A)}} \left(e^{\frac{2\pi i}{N} n_{\wp(1)}} + e^{-\frac{2\pi i}{N} n_{\wp(1)}} \right)} \alpha_{j_M}^{n_{\wp(M)}} \\ &= -2t \sum_{A=1}^{M} \cos\left(\frac{2\pi}{N} n_A \right) \end{aligned}$$

This is exactly the formula (2 11) of the previous chapter

Interaction Part

$$
\begin{aligned}
&{}_{n_1\ \ n_M}\langle\psi|\hat{V}|\psi\rangle_{n_1\ \ n_M} \\
&= V\sum_{\substack{A,B=1\\A\neq B}}^{M}\sum_{j_1}\cdots\sum_{j_M}\sum_{\wp\in\mathcal{P}(M)}(-1)^{\operatorname{sgn}\wp}\alpha_{j_1}^{n_1*}\cdots\alpha_{j_M}^{n_M*}\alpha_{j_1}^{n_{\wp(1)}}\cdots\alpha_{j_M}^{n_{\wp(M)}}\delta_{j_B,j_A+1}\cdots
\end{aligned}
$$

1st case: $\wp = \mathrm{id}$

$$
= V\sum_{\substack{A,B=1\\A\neq B}}^{M}\sum_{j_1}\cdots\sum_{j_M}\delta_{j_B,j_A+1} = \frac{V}{N}M(M-1)
$$

2nd case: $\wp(A) = B$, $\wp(B) = A$

$$
\begin{aligned}
&= -V\sum_{\substack{A,B=1\\A\neq B}}^{M}\frac{1}{N^2}\sum_{j}e^{-\frac{2\pi i}{N}n_A j}e^{-\frac{2\pi i}{N}n_B(j+1)}e^{\frac{2\pi i}{N}n_B j}e^{\frac{2\pi i}{N}n_A(j+1)} \\
&= -\frac{V}{N}\sum_{\substack{A,B=1\\A\neq B}}^{M}e^{\frac{2\pi i}{N}(n_A-n_B)} = -\frac{V}{N}\frac{1}{2}\left\{\sum_{\substack{A,B=1\\A\neq B}}^{M}e^{\frac{2\pi i}{N}(n_A-n_B)}+\sum_{\substack{A,B=1\\A\neq B}}^{M}e^{\frac{2\pi i}{N}(n_B-n_A)}\right\} \\
&= -\frac{V}{N}\sum_{\substack{A,B=1\\A\neq B}}^{M}\cos\left(\frac{2\pi}{N}(n_A-n_B)\right)
\end{aligned}
$$

All other possible permutations lead to zero sums.

Together

$$
\boxed{{}_{n_1\ \ n_M}\langle\psi|\mathcal{H}|\psi\rangle_{n_1\ \ n_M} = -2t\sum_{A=1}^{M}\cos\left(\frac{2\pi}{N}n_A\right)+\frac{V}{N}\sum_{A,B=1}^{M}\left[1-\cos\left(\frac{2\pi}{N}(n_A-n_B)\right)\right]}
\tag{3.17}
$$

From this result one can see nicely the structure of the two contributions to the energy. The hopping part is a pure one-particle effect. The total kinetic energy is simply the sum of single particle energies, determined by quantum numbers n_A. The interaction on the other hand is a two-particle effect. It is a sum over all pairs of quantum numbers, which is equivalent to a sum over all pairs of particles. Each summand depends only on the difference of these two numbers. The explicit value of a single quantum number is of no importance.

By the way, the result is of course the same as the value which was evaluated for λ above. The Lagrange multiplier is nothing else than the ground state energy of the many-particle system, because all equations consist only of terms of same order in the parameters.

Evaluation of the Sums

As already in section 2.1.3 and 2.2.3 it is now the task to evaluate the sums for the ground state. For this it is necessary to find out which quantum numbers $n_1, \ldots n_M$ are chosen in order to minimize the total energy.

The situation is similar to that of non-interacting particles, which is the reason for presenting almost the same figure again.

As one can see from this figure 3.1 and as already discussed before, the kinetic

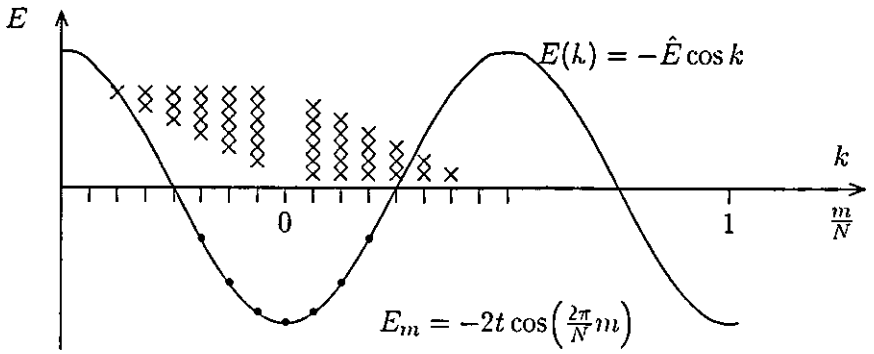


Figure 3.1: *Energy states due to the hopping (dots) and the interacting (crosses) part of the Heisenberg model for $N = 16$ and $M = 7$. The number of crosses above a certain point in momentum space indicates the weight of the corresponding energy in the interaction*

energy

$$E_{\text{hopp}} = -2t \sum_{i=1}^{M} \cos\left(\frac{2\pi}{N} n_i\right)$$

leads to the effect that small k-values are preferred. This is because the cosine has its minimum for $k = 0$.

The interaction part, if a constant energy shift is ignored, has the structure

$$E_{\text{int}} = -\frac{V}{N} \sum_{A,B=1}^{M} \cos\left(\frac{2\pi}{N}(n_A - n_B)\right)$$

This is the same functional dependence as before, apart from the fact that instead of the quantum numbers itself only differences of quantum numbers appear in the argument.

For that reason the interaction tends to keep particles close together in reciprocal space. As a distance of zero is not allowed due to Pauli exclusion, the best possibility is to occupy a block of adjacent sites in momentum space. For

the case of 7 particles all appearing differences are shown in figure 3.1 They are indicated by crosses in the same picture as the hopping energy because they contribute to the total energy with the same cosine dependence It can be seen that such a block is the best possibility to concentrate crosses around $k = 0$.

Since a minimization with respect to the kinetic energy also leads to the result that a block of adjacent sites in reciprocal space is occupied, there is no competition between hopping and interaction. Therefore, the results (2.13), (2 14) or (2.37), (2 38) for the hopping part can be used without alteration

For the interaction part the double sum has to be evaluated

M odd

$$\sum_{k,l=-\frac{M-1}{2}}^{\frac{M-1}{2}} \cos\left(\frac{2\pi}{N}(k-l)\right) = \left(\sum_{k=-\frac{M-1}{2}}^{\frac{M-1}{2}} \cos\left(\frac{2\pi}{N}k\right)\right)^2 + \left(\sum_{k=-\frac{M-1}{2}}^{\frac{M-1}{2}} \sin\left(\frac{2\pi}{N}k\right)\right)^2$$

$$\text{and} \sum_{k=-\frac{M-1}{2}}^{\frac{M-1}{2}} \cos\left(\frac{2\pi}{N}k\right) = \frac{\sin\left(\frac{\pi}{N}M\right)}{\sin\left(\frac{\pi}{N}\right)} \quad \text{(see (2 14))},$$

$$\sum_{k=-\frac{M-1}{2}}^{\frac{M-1}{2}} \sin\left(\frac{2\pi}{N}k\right) = 0 \quad \text{(sin is an odd function)}$$

M even

$$\sum_{k,l=-\frac{M}{2}}^{\frac{M}{2}-1} \cos\left(\frac{2\pi}{N}(k-l)\right) = \left(\sum_{k=-\frac{M}{2}}^{\frac{M}{2}-1} \cos\left(\frac{2\pi}{N}k\right)\right)^2 + \left(\sum_{k=-\frac{M}{2}}^{\frac{M}{2}-1} \sin\left(\frac{2\pi}{N}k\right)\right)^2$$

$$\text{and} \sum_{k=-\frac{M}{2}}^{\frac{M}{2}-1} \cos\left(\frac{2\pi}{N}k\right) = \frac{\sin\left(\frac{\pi}{N}M\right)}{\sin\left(\frac{\pi}{N}\right)} \cdot \cos\left(\frac{\pi}{N}\right) \quad \text{(see (2 13))},$$

$$\sum_{k=-\frac{M}{2}}^{\frac{M}{2}-1} \sin\left(\frac{2\pi}{N}k\right) = -\sin\left(\frac{\pi}{N}M\right) \quad \text{(sin is an odd function)}$$

$$\Rightarrow \sum_{k,l=-\frac{M}{2}}^{\frac{M}{2}-1} \cos\left(\frac{2\pi}{N}(k-l)\right) = \frac{\sin^2\left(\frac{\pi}{N}M\right)}{\sin^2\left(\frac{\pi}{N}\right)}\left\{\cos^2\left(\frac{\pi}{N}\right) + \sin^2\left(\frac{\pi}{N}\right)\right\} = \frac{\sin^2\left(\frac{\pi}{N}M\right)}{\sin^2\left(\frac{\pi}{N}\right)}$$

Furthermore, a flux through the ring can again be taken into consideration It has been explained that this causes a change in the momentum operator and influences, therefore, only the kinetic energy

Hence, we have all together

$$\boxed{E_{\text{even}} = -2t\,\frac{\sin\left(\frac{\pi}{N}M\right)}{\sin\left(\frac{\pi}{N}\right)}\cdot\cos\left(\frac{\pi}{N}-\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right)+\frac{V}{N}\left\{M^2-\frac{\sin^2\left(\frac{\pi}{N}M\right)}{\sin^2\left(\frac{\pi}{N}\right)}\right\}} \tag{3 18}$$

and

$$\boxed{E_{\text{odd}} = -2t\,\frac{\sin\left(\frac{\pi}{N}M\right)}{\sin\left(\frac{\pi}{N}\right)}\cos\left(\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right)+\frac{V}{N}\left\{M^2-\frac{\sin^2\left(\frac{\pi}{N}M\right)}{\sin^2\left(\frac{\pi}{N}\right)}\right\}} \tag{3 19}$$

The form of the solution implies the surprising result that the persistent current is not influenced by the interaction. Apparently, in a model of spinless fermions the persistent current is only determined by the hopping part of the Hamiltonian

3.4 Energy in the Hubbard Model

In the Hubbard model most of the calculations are analogous to the Heisenberg model The main difference comes from the fact that the particles possess a spin. This has already an effect on the variational wave function. For this reason $S_\uparrow$ and $S_\downarrow$ are introduced as the set of quantum numbers that represent up-spin and down-spin fermions, respectively. The number of elements in $S_\uparrow$ ($S_\downarrow$) is called $M_\uparrow$ ($M_\downarrow$) At the moment these numbers are supposed to be conserved, and their sum $M = M_\uparrow + M_\downarrow$ is again the total number of particles

With the help of this notation it is possible to express an arbitrary state as

$$|\psi\rangle_{S_\uparrow,S_\downarrow} = \prod_{n\in S_\uparrow}\left(\sum_{i_n=1}^{N}\beta_{i_n}^{n}c_{i_n,\uparrow}^{\dagger}\right)\prod_{m\in S_\downarrow}\left(\sum_{i_m=1}^{N}\beta_{i_m}^{m}c_{i_m,\downarrow}^{\dagger}\right)|0\rangle \tag{3 20}$$

It has to be mentioned that another assumption is included in this notation To write down the coefficients without an index for the spin implies that the single particle wave function for up- and down-spin particles might be the same. That is, that two particles might have exactly the same behaviour apart from the fact that their spin projections point in different directions This assumption is reasonable because it is in accord with the Pauli exclusion principle and because of the fact that no spin direction is preferred

The Hamiltonian with included flux

$$\mathcal{H} = -t \sum_{k} \sum_{\sigma=\uparrow,\downarrow} \left(c^{\dagger}_{k,\sigma} c_{k+1,\sigma} e^{\frac{2\pi i}{\Lambda} \frac{\Phi}{\Phi_0}} + c^{\dagger}_{k+1,\sigma} c_{k,\sigma} e^{-\frac{2\pi i}{N} \frac{\Phi}{\Phi_0}} \right) + U \sum_{k} \hat{n}_{k,\uparrow} \hat{n}_{k,\downarrow} \qquad (3\,21)$$

shall again be investigated in its different parts

Hopping Part

$$\hat{H}_0 = -t \sum_{k} \left(c^{\dagger}_{k,\uparrow} c_{k+1,\uparrow} e^{\frac{2\pi i}{\Lambda} \frac{\Phi}{\Phi_0}} + c^{\dagger}_{k,\downarrow} c_{k+1,\downarrow} e^{\frac{2\pi i}{N} \frac{\Phi}{\Phi_0}} + \text{h c} \right)$$

$$_{S_\uparrow,S_\downarrow}\langle \psi | \hat{H}_0 | \psi \rangle_{S_\uparrow,S_\downarrow}$$

$$= -t \Bigg(\sum_{A=1}^{M_\uparrow} \sum_{j_1} \sum_{j_{M_\uparrow}} \sum_{\wp \in \mathcal{P}(M_\uparrow)} (-1)^{\operatorname{sgn}\wp} \beta^{n_1 *}_{j_1} \cdots \beta^{n_{M_\uparrow} *}_{j_{M_\uparrow}} \cdot$$

$$\beta^{n_{\wp(1)}}_{j_1} \cdots \left(\beta^{n_{\wp(A)}}_{j_A+1} e^{\frac{2\pi i}{N} \frac{\Phi}{\Phi_0}} + \beta^{n_{\wp(A)}}_{j_A-1} e^{-\frac{2\pi i}{\Lambda} \frac{\Phi}{\Phi_0}} \right) \cdots \beta^{n_{\wp(M_\uparrow)}}_{j_{M_\uparrow}} \Bigg) *$$

$$* \left(\sum_{j_1} \sum_{j_{M_\downarrow}} \sum_{\wp \in \mathcal{P}(M_\downarrow)} (-1)^{\operatorname{sgn}\wp} \beta^{m_1 *}_{j_1} \cdots \beta^{m_{M_\downarrow} *}_{j_{M_\downarrow}} \beta^{m_{\wp(1)}}_{j_1} \cdots \beta^{m_{\wp(M_\downarrow)}}_{j_{M_\downarrow}} \right)$$

$$-t \Bigg(\sum_{A=1}^{M_\downarrow} \sum_{j_1} \sum_{j_{M_\downarrow}} \sum_{\wp \in \mathcal{P}(M_\downarrow)} (-1)^{\operatorname{sgn}\wp} \beta^{m_1 *}_{j_1} \cdots \beta^{m_{M_\downarrow} *}_{j_{M_\downarrow}} \cdot$$

$$\beta^{m_{\wp(1)}}_{j_1} \cdots \left(\beta^{m_{\wp(A)}}_{j_A+1} e^{\frac{2\pi i}{N} \frac{\Phi}{\Phi_0}} + \beta^{m_{\wp(A)}}_{j_A-1} e^{-\frac{2\pi i}{N} \frac{\Phi}{\Phi_0}} \right) \cdots \beta^{m_{\wp(M_\downarrow)}}_{j_{M_\downarrow}} \Bigg) *$$

$$* \left(\sum_{j_1} \sum_{j_{M_\uparrow}} \sum_{\wp \in \mathcal{P}(M_\uparrow)} (-1)^{\operatorname{sgn}\wp} \beta^{n_1 *}_{j_1} \cdots \beta^{n_{M_\uparrow} *}_{j_{M_\uparrow}} \beta^{n_{\wp(1)}}_{j_1} \cdots \beta^{n_{\wp(M_\uparrow)}}_{j_{M_\uparrow}} \right)$$

take the derivative with an $n_C \in S_\uparrow$

$$\frac{\partial}{\partial \beta^{n_C *}_{\tau}} \left(_{S_\uparrow,S_\downarrow}\langle \psi | \hat{H}_0 | \psi \rangle_{S_\uparrow,S_\downarrow} \right)$$

$$= -t \sum_{\substack{n \in S_\uparrow \\ n \neq n_c}} \sum_{j=1}^{N} \beta^{n *}_{j} \left(\beta^{n}_{j+1} e^{\frac{2\pi i}{N} \frac{\Phi}{\Phi_0}} + \beta^{n}_{j-1} e^{-\frac{2\pi i}{N} \frac{\Phi}{\Phi_0}} \right) \beta^{n_C}_{\tau}$$

$$-t \left(\beta^{n_C}_{x+1} e^{\frac{2\pi i}{\Lambda} \frac{\Phi}{\Phi_0}} + \beta^{n_C}_{x-1} e^{-\frac{2\pi i}{\Lambda} \frac{\Phi}{\Phi_0}} \right)$$

$$+t \sum_{\substack{n \in S_\uparrow \\ n \neq n_c}} \sum_{j=1}^{N} \beta^{n *}_{j} \left(\beta^{n_C}_{j+1} e^{\frac{2\pi i}{\Lambda} \frac{\Phi}{\Phi_0}} + \beta^{n_C}_{j-1} e^{-\frac{2\pi i}{\Lambda} \frac{\Phi}{\Phi_0}} \right) \beta^{n}_{\tau}$$

$$-t \sum_{m \in S_\downarrow} \sum_{j=1}^{N} \beta^{m *}_{j} \left(\beta^{m}_{j+1} e^{\frac{2\pi i}{N} \frac{\Phi}{\Phi_0}} + \beta^{m}_{j-1} e^{-\frac{2\pi i}{\Lambda} \frac{\Phi}{\Phi_0}} \right) \beta^{n_C}_{\tau}$$

Interaction Part

$$\hat{\Gamma} = U \sum_k c^\dagger_{k,\uparrow} c_{k,\uparrow} c^\dagger_{k,\downarrow} c_{k,\downarrow}$$

$$
\begin{aligned}
&{}_{S_\uparrow,S_\downarrow}\langle\psi|\hat{\Gamma}|\psi\rangle_{S_\uparrow,S_\downarrow} \\
&= U \sum_{A=1}^{M_\uparrow} \sum_{j_1} \sum_{j_{M_\uparrow}} \sum_{\wp\in\mathcal{P}(M_\uparrow)} (-1)^{\mathrm{sgn}\wp} \beta^{n_1 *}_{j_1} \cdots \beta^{n_{M_\uparrow} *}_{j_{M_\uparrow}} \beta^{n_{\wp(1)}}_{j_1} \cdots \beta^{n_{\wp(M_\uparrow)}}_{j_{M_\uparrow}} * \\
&\quad * \sum_{B=1}^{M_\downarrow} \sum_{i_1} \sum_{i_{M_\downarrow}} \sum_{\varsigma\in\mathcal{P}(M_\downarrow)} (-1)^{\mathrm{sgn}\varsigma} \beta^{m_1 *}_{i_1} \cdots \beta^{m_{M_\downarrow} *}_{i_{M_\downarrow}} \beta^{m_{\varsigma(1)}}_{i_1} \cdots \beta^{m_{\varsigma(M_\downarrow)}}_{i_{M_\uparrow}} \quad \delta_{j_A,i_B}
\end{aligned}
$$

take the derivative with an $n_C \in S_\uparrow$

$$
\begin{aligned}
&\frac{\partial}{\partial \beta^{n_C *}_x} \left({}_{S_\uparrow,S_\downarrow}\langle\psi|\hat{V}|\psi\rangle_{S_\uparrow,S_\downarrow} \right) \\
&= U \sum_{\substack{A=1 \\ A\neq C}}^{M_\uparrow} \sum_{B=1}^{M_\downarrow} \sum_{j=1}^{N} \left\{ \underbrace{\beta^{n_A *}_j \beta^{n_A}_j \beta^{n_C}_x}_{\wp=\mathrm{id},\, A\neq C} + \underbrace{\beta^{n_A *}_j \beta^{n_C}_j \beta^{n_A}_x}_{\wp(A)=C,\, \wp(C)=A} \right\} |\beta^{m_B}_j|^2 + U \sum_{B=1}^{M_\downarrow} \underbrace{\beta^{n_C}_x |\beta^{m_B}_x|^2}_{\wp=\mathrm{id},\, A=C}
\end{aligned}
$$

The β-problem

summarizes the results for the derivative of the two parts For convenience it is written here without the flux dependence.

$$
\begin{aligned}
&- t \sum_{\substack{n\in S_\uparrow \\ n\neq n_c}} \sum_{j=1}^{N} \beta^{n *}_j \left(\beta^n_{j+1} + \beta^n_{j-1} \right) \beta^{n_C}_x - t \left(\beta^{n_C}_{x+1} + \beta^{n_C}_{x-1} \right) \\
&+ t \sum_{\substack{n\in S_\uparrow \\ n\neq n_c}} \sum_{j=1}^{N} \beta^{n *}_j \left(\beta^{n_C}_{j+1} + \beta^{n_C}_{j-1} \right) \beta^n_x - t \sum_{m\in S_\downarrow} \sum_{j=1}^{N} \beta^{m *}_j \left(\beta^m_{j+1} + \beta^m_{j-1} \right) \beta^{n_C}_x \\
&+ U \sum_{\substack{n\in S_\uparrow \\ n\neq n_c}} \sum_{m\in S_\downarrow} \sum_{j=1}^{N} \left\{ \beta^{n *}_j \beta^n_j \beta^{n_C}_x + \beta^{n *}_j \beta^{n_C}_j \beta^n_x \right\} |\beta^m_j|^2 + U \sum_{m\in S_\downarrow} \beta^{n_C}_x |\beta^m_x|^2 \\
&= \lambda \beta^{n_C}_x
\end{aligned}
\tag{3 22}
$$

The structure of this set of equations is similar to the α-problem of the Heisenberg Hamiltonian The interaction is in an even more simple form because up- and down-spin fermions are treated independently As above, the task is again to find expressions for the coefficients β in such a way that each equation is fulfilled This is the case if λ does not depend on the derivative parameters x and n_c That

Bloch Wave Functions are Solution

$$\beta_{i_n}^n = \frac{1}{\sqrt{N}} \exp\left[\frac{2\pi \mathrm{i}}{N} n \cdot \imath_n\right].$$

is briefly shown in the following

Proof:

$$\left.\begin{array}{l} -t \sum\limits_{\substack{n\in S_\uparrow \\ n\neq n_c}} \frac{1}{N} \sum\limits_j e^{-\frac{2\pi \mathrm{i}}{N} n j} \left(e^{\frac{2\pi \mathrm{i}}{N} n(j+1)} + e^{\frac{2\pi \mathrm{i}}{N} n(j-1)}\right) \\ -t \left(e^{\frac{2\pi \mathrm{i}}{N} n_C} + e^{-\frac{2\pi \mathrm{i}}{N} n_C}\right) \\ -t \sum\limits_{m\in S_\downarrow} \sum\limits_j e^{-\frac{2\pi \mathrm{i}}{N} m j} \left(e^{\frac{2\pi \mathrm{i}}{N} m(j+1)} + e^{\frac{2\pi \mathrm{i}}{N} m(j-1)}\right) \end{array}\right\} = -t \sum_{n\in S_\uparrow \cup S_\downarrow} \left(e^{\frac{2\pi \mathrm{i}}{N} n} + e^{-\frac{2\pi \mathrm{i}}{N} n}\right)$$

$$+t \sum_{\substack{n\in S_\uparrow \\ n\neq n_c}} \frac{1}{N} \sum_j e^{\frac{2\pi \mathrm{i}}{N}(n_C - n)(j-x)} \left(e^{\frac{2\pi \mathrm{i}}{N} n_C} + e^{-\frac{2\pi \mathrm{i}}{N} n_C}\right) = 0$$

$$U \sum_{\substack{n\in S_\uparrow \\ n\neq n_c}} \sum_{m\in S_\downarrow} \sum_{j=1}^{N} \frac{1}{N^2} + U \sum_{m\in S_\downarrow} \frac{1}{N} = U \sum_{n\in S_\uparrow} \sum_{m\in S_\downarrow} \frac{1}{N} = U \frac{M_\uparrow \cdot M_\downarrow}{N}$$

$$U \sum_{\substack{n\in S_\uparrow \\ n\neq n_c}} \sum_{m\in S_\downarrow} \sum_{j=1}^{N} \frac{1}{N^2} e^{\frac{2\pi \mathrm{i}}{N}(j-x)(n_C - n)} = 0$$

□

The Energy

$$\boxed{E = -2t \sum_{n\in S_\uparrow \cup S_\downarrow} \cos\left(\frac{2\pi}{N}\left(n - r\left(\frac{\Phi}{\Phi_0}\right)\right)\right) + U \frac{M_\uparrow \cdot M_\downarrow}{N}} \qquad (3\ 23)$$

consists of a logical kinetic and a surprising interaction part. The former is logical because it describes the independent filling of the energy levels according to the cos-dependence with up- and down-spin particles This is a generalization of the situation in the Heisenberg model The later surprises because the expression does not depend at all on the chosen set of quantum numbers Only the up-spin and down-spin number of particles is of importance The fact that these numbers are kept fixed in the calculations is probably the reason for the constant potential energy.

Thus, in order to achieve a minimal energy value one only has to look at the kinetic energy part. There are four possible situations (K is an integer).

$$E_{M=4K} = -4t\frac{\sin\left(\frac{\pi}{N}\frac{M}{2}\right)}{\sin\left(\frac{\pi}{N}\right)}\cdot\cos\left(\frac{\pi}{N}-\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right)+U\frac{M_\uparrow\cdot M_\downarrow}{N}$$

$$E_{M=4K+1} = -2t\left[\frac{\sin\left(\frac{\pi}{N}\frac{M-1}{2}\right)}{\sin\left(\frac{\pi}{N}\right)}\cos\left(\frac{\pi}{N}-\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right)+\right.$$

$$\left.\ldots+\frac{\sin\left(\frac{\pi}{N}\frac{M+1}{2}\right)}{\sin\left(\frac{\pi}{N}\right)}\cos\left(\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right)\right]+U\frac{M_\uparrow\ M_\downarrow}{N}$$

$$E_{M=4K+2} = -4t\frac{\sin\left(\frac{\pi}{N}\frac{M}{2}\right)}{\sin\left(\frac{\pi}{N}\right)}\cdot\cos\left(\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right)+U\frac{M_\uparrow\cdot M_\downarrow}{N}$$

$$E_{M=4K-1} = -2t\left[\frac{\sin\left(\frac{\pi}{N}\frac{M+1}{2}\right)}{\sin\left(\frac{\pi}{N}\right)}\cos\left(\frac{\pi}{N}-\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right)+\right.$$

$$\left.\ldots+\frac{\sin\left(\frac{\pi}{N}\frac{M-1}{2}\right)}{\sin\left(\frac{\pi}{N}\right)}\cos\left(\frac{2\pi}{N}r\left(\frac{\Phi}{\Phi_0}\right)\right)\right]+U\frac{M_\uparrow\cdot M_\downarrow}{N}$$

From these four energy expressions it is possible to evaluate the persistent current by using $I=-c\dfrac{\partial E}{\partial\Phi}$. The result will be a combination of the derivations for the Heisenberg model for an odd and an even number of particles in section 2.4. Of particular interest are the cases $M=4K+1$ and $M=4K-1$ because here $M_\uparrow$ is even and $M_\downarrow$ is odd (or vice versa). Similarly to the previous discussion about an ensemble-average and the figure 2.16, the combination leads in these cases to a quasi half-flux periodicity of the current [5]. However, Loss and Goldbart [37] pointed out that the average over all particle numbers is still the same as in the case of spinless fermions. For large N one obtains in the linear approximation[6]

$$\langle I\rangle_{\text{Poisson}}=\frac{1}{2}\hat{I}(\lambda)\left[\frac{2\Phi}{\Phi_0/2}-1+\mathrm{e}^{-\lambda}\sin\lambda\left(1+\frac{1}{\lambda}\right)\right], \qquad (3.24)$$

where λ is here the mean value of the Poisson distribution and is assumed to be large. Because the last summand is negligible, this is exactly the same as (2.51).

It should also be mentioned that a fractional $1/M$ or $M_\uparrow/M$ Aharonov-Bohm effect as found by Kusmartsev *et al.* [13, 14, 15] with the help of the Bethe *ansatz*, does not appear within this context. Especially in the limit of strong interaction the obtained result is apparently not in good agreement with these and other publications.

---

[5] Weisz *et al* [42] found that the period is again a full flux-quantum in the presence of disorder.

[6] The result differs slightly from what Loss and Goldbart [37] have obtain.

3.5 However, ...

..one should bear in mind that the Hartree-Fock method only gives an upper boundary for the ground state energy Even if all Hartree-Fock equations are fulfilled, the discrepancy between the gained energy and the real value for the ground state does not have to vanish This is only the case if the variational wave function has the structure of a proper eigenfunction of the Hamiltonian

Therefore, one should not be too happy about exact solutions of the Hartree-Fock equations found. On the contrary, it is well-known [43] that in general $\hat{H}_0$ and $\hat{V}$ cannot be diagonalized simultaneously

The eigenfuntions of the hopping Hamiltonian $\hat{H}_0$ are plane waves - this is correct. However, as soon as two particles with different spins are involved Bloch wave functions are not eigenfunctions of the operator $\sum_k \hat{n}_{k,\uparrow}\hat{n}_{k,\downarrow}$. It can easily be seen that in such a two-particle situation, the double-sum is reduced to a single sum

$$\sum_{k=1}^{N} \hat{n}_{k,\uparrow}\hat{n}_{k,\downarrow} \sum_{i=1}^{N}\sum_{j=1}^{N} \beta_i^n \beta_j^m c_{i,\uparrow}^\dagger c_{j,\downarrow}^\dagger |0\rangle = \sum_{k=1}^{N} \beta_k^n \beta_k^m c_{k,\uparrow}^\dagger c_{k,\downarrow}^\dagger |0\rangle \qquad (3\,25)$$

because the Hamiltonian gives in most of the cases zero

The proper eigenstates of the interaction Hamiltonian are of the form

$$\left(\prod_{i\in\{1,\ ,N\}} c_{i,\uparrow}^\dagger\right)\left(\prod_{j\in\{1,\ ,N\}} c_{j,\downarrow}^\dagger\right)|0\rangle, \qquad (3\,26)$$

and, since $\hat{V}$ is not linear, the same is not necessarily true for linear combinations. In contrast to the wave-like solutions of the hopping Hamiltonian, such states are sometimes calls "particle-like" or "localized" solutions Apparently, there is a competition in the Hubbard model between these two possibilities In the limit $t \gg U$ the first becomes more likely, the limit $t \ll U$ favours the second one Such behaviour is the reason why it is so interesting to study this model Of course, all these remarks are equally valid for the Heisenberg model.

The task for rest of this work is to apply a couple of techniques to the Hubbard model in order to obtain a better approximation for the ground state energy and to understand the behaviour of this system better.

Chapter 4

The Notion of Rotation

In order to improve previous results, two techniques shall be used next. On the one hand the interaction should be simplified by applying a so-called Hubbard-Stratonovic decomposition (sect. 4.2). In order to do this it is necessary to rewrite the problem in the exponential form of a partition function (sect. 4.1). On the other hand it is also useful to introduce rotations of the spin-quantization axis of each site (sect. 4.3). In a different context but also for the Hubbard model a spin-space reference frame has been introduced by H. J. Schulz [44]. Therefore, it is convenient to follow the first couple of steps in his paper. This is done at the beginning of section 4.4. New ideas are developed soon in order to find a more appropriate description of our particular situation. The playing with the rotations leads in section 4.5 even to a change in the order of the techniques proposed.

4.1 The Partition Function

An ordinary time evolution operator (TEO) and its trace have in the case of a time-independent Hamiltonian the form

$$U(t_b, t_a) = \exp\left[-\frac{1}{\hbar}(t_b - t_a)\mathcal{H}\right] \qquad Z_{\mathrm{TEO}} = \mathrm{Tr}\left(\exp\left[-\frac{1}{\hbar}(t_b - t_a)\mathcal{H}\right]\right) \tag{4.1}$$

It is possible to evaluate such expressions with the help of path integrals. If the Hamiltonian is expressed in fermionic creation and annihilation operators it is for this purpose necessary to introduce Grassmann numbers Ψ and Ψ^*. Its

components $\xi_{1,\uparrow}, \xi_{1,\downarrow}, \ldots, \xi_{N,\downarrow}$ have two indices: one for the site position and one for the spin projection. They satisfy the eigenvalue equations $c_{k,\sigma}|\Psi\rangle = \xi_{k,\sigma}|\Psi\rangle$ and $\langle\Psi|c^{\dagger}_{k,\sigma} = \langle\Psi|\xi^{*}_{k,\sigma}$ and therefore anticommute with one another. Then the trace of the time evolution operator, called time generating function, can be written as

$$Z_{\mathrm{TEO}} = \int \mathcal{D}\Psi^{*}\mathcal{D}\Psi \, \exp\left[\mathrm{i}\int_{t_a}^{t_b} \mathrm{d}t \left(\Psi^{*}\mathrm{i}\frac{\partial}{\partial t}\Psi - \frac{1}{\hbar}\mathcal{H}(\Psi^{*},\Psi)\right)\right] \tag{4.2}$$

A thorough explanation of the formalism behind these remarks is given in appendix D

In thermodynamics of finite temperature all properties of a system are determined by the partition function In the grand canonical case this has the form

$$Z = \mathrm{Tr}\left(\exp\left[-\frac{1}{k_B T}(\mathcal{H} - \mu\mathcal{N})\right]\right), \tag{4.3}$$

where μ is the chemical potential, $\mathcal{N}$ the particle-number operator and k_B is Boltzmann's constant There is a striking similarity between this expression and the form of the time generating function in (4 1) If in the latter $t - t_a$ is replaced according to

$$\tau = \mathrm{i}(t - t_a) \xrightarrow[t\to t_b]{} \frac{\hbar}{k_B T} = \hbar\beta \tag{4.4}$$

one ends up with the partition function Such a pure imaginary time is called Matsubara time, and the proposed transformation implies without additional effort a path integral form for Z. In analogy to (4 2) it is

$$Z = \int \mathcal{D}\Psi^{*}\mathcal{D}\Psi \, \exp\left[-\int_0^{\hbar\beta} \mathrm{d}\tau \left(\Psi^{*}\left(\frac{\partial}{\partial\tau} - \frac{\mu}{\hbar}\right)\Psi + \frac{1}{\hbar}\mathcal{H}(\Psi^{*},\Psi)\right)\right], \tag{4.5}$$

where products like $\Psi^{*}\cdot\Psi$ are understood as vector products $\sum_{k=1}^{N}\sum_{\sigma=\uparrow,\downarrow}\xi^{*}_{k,\sigma}\xi_{k\,\sigma}$

The concrete Hamiltonian under consideration is the Hubbard model with included flux contribution To write it in terms of Grassmann numbers it has to be brought in a normal ordered form (all annihilation operators are standing to the right of all creation operators) Afterwards one just has to replace any fermionic operator by the corresponding Grassmann number

$$\mathcal{H}(\Psi^{*},\Psi) = -t\sum_{k=1}^{N}\sum_{\sigma=\uparrow,\downarrow}\left(\xi^{*}_{k,\sigma}\xi_{k+1,\sigma}\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}} + \xi^{*}_{k+1,\sigma}\xi_{k,\sigma}\mathrm{e}^{-\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}\right)$$

$$+U\sum_{k=1}^{N}\xi^*_{k,\uparrow}\xi^*_{k,\downarrow}\xi_{k,\downarrow}\xi_{k,\uparrow}. \tag{4.6}$$

It is sometimes convenient to introduce the term "action" for the exponent of the partition function. If the action S is the sum of the two terms

$$S_0 = \int_0^{\hbar\beta} \mathrm{d}\tau \sum_{k=1}^{N}\sum_{\sigma=\uparrow,\downarrow}\left\{\xi^*_{k,\sigma}\left(\hbar\partial_\tau - \mu\right)\xi_{k,\sigma} - t\left(\xi^*_{k,\sigma}\xi_{k+1,\sigma}\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}} + \right.\right.$$

$$\left.\left. + \xi^*_{k+1,\sigma}\xi_{k,\sigma}\mathrm{e}^{-\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}\right)\right\}$$

$$S_{\mathrm{int}} = U\int_0^{\hbar\beta}\mathrm{d}\tau\sum_{k=1}^{N}\xi^*_{k,\uparrow}\xi^*_{k,\downarrow}\xi_{k,\downarrow}\xi_{k,\uparrow}$$

then the partition function has the form

$$Z = \int \mathcal{D}\Psi^*\mathcal{D}\Psi\,\mathrm{e}^{-(S_0+S_{\mathrm{int}})/\hbar} \tag{4.7}$$

4.2 Hubbard-Stratonovic Decomposition

Unfortunately, the action for the interaction S_{int} consists of products of four Grassmann numbers, $\xi^*_{k,\uparrow}\xi^*_{k,\downarrow}\xi_{k,\downarrow}\xi_{k,\uparrow}$. These nonlinearities lead to difficulties in its treatment. The Hubbard-Stratonovic decomposition is a good possibility to reduce this term to a second-order expression. There are different ways to do this.

We shall follow the advice of Schulz [44], because he and before him already Hamann [45] claim that only their choice reproduces in a saddle-point approximation the results of Hartree-Fock calculations. Therefore, two new operators have to be introduced

$$\hat{n}_k = c^\dagger_{k,\uparrow}c_{k,\uparrow} + c^\dagger_{k,\downarrow}c_{k,\downarrow} \quad \text{and} \quad \hat{s}_k = c^\dagger_{k,\uparrow}c_{k,\uparrow} - c^\dagger_{k,\downarrow}c_{k,\downarrow} \tag{4.8}$$

$\hat{n}_k$ counts the number of particles on a certain site and therefore represents the charge degree of freedom. $\hat{s}_k$ gives the total spin projection on the z-axis at the same site, hence, it is related to the spin degree of freedom. In the following, the related Grassmann numbers are represented by the same symbols as the operators, but the hat is omitted. Then the above mentioned product of Grassmann numbers becomes

$$\xi^*_{k,\uparrow}\xi^*_{k,\downarrow}\xi_{k,\downarrow}\xi_{k,\uparrow} = \frac{1}{4}\left(n_k^2 - s_k^2\right) \tag{4.9}$$

Accordingly, the interaction part of the partition function changes and one obtains

$$Z = \int \mathcal{D}\Psi^* \mathcal{D}\Psi \, \exp\left[-\frac{S_0}{\hbar} - \frac{U}{4\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \sum_{k=1}^{N} \left(n_k^2 - s_k^2\right)\right] \tag{4.10}$$

If one forgets for a moment about all integrations and summations in the partition function, then the interaction is essentially expressed by a quadratic form in the exponent. Expressions like this can be modified with the help of the well-known Gaussian identity (σ is a parameter)

$$\int_{-\infty}^{+\infty} \mathrm{d}x \, \mathrm{e}^{-x^2/\sigma^2} = \sqrt{\pi\sigma^2} \quad \Longleftrightarrow_{x=a-\Delta} \quad \mathrm{e}^{a^2/\sigma^2} = \frac{1}{\sqrt{\pi\sigma^2}} \int_{-\infty}^{+\infty} \mathrm{d}\Delta \, \mathrm{e}^{-\left(\Delta^2 - 2a\Delta\right)/\sigma^2}. \tag{4.11}$$

Stratonovic first suggested this trick and Hubbard applied it to the partition function, which is the reason that it carries now the name of both. Hubbard-Stratonovic decomposition [46]

In principle, it is just necessary to find an appropriate choice for a^2/σ^2 in the case that the exponent has the form

$$E = \exp\left[-\frac{U}{4\hbar}\left(n_k^2 - s_k^2\right)\right]$$

and afterwards one can apply the Gaussian identity. One possibility is to set respectively

$$(a_c, \sigma_c^2) = \left(\frac{\mathrm{i}}{2} U n_k, \hbar U\right) \quad \text{and} \quad (a_s, \sigma_s^2) = \left(\frac{1}{2} U s_k, \hbar U\right)$$

and to obtain

$$E = \frac{1}{\pi\hbar U} \iint \mathrm{d}\Delta_c \mathrm{d}\Delta_s \exp\left[-\frac{1}{U\hbar}\left(\Delta_c^2 + \Delta_s^2\right) + \frac{1}{\hbar}\Delta_c n_k + \frac{1}{\hbar}\Delta_s s_k\right] \tag{4.12}$$

This choice is convenient because it brings U in the denominator One can easily see that it leads to integration variables which have the dimensionality of an energy

However, things are slightly more difficult mainly because of the integration over Matsubara time To avoid any problems with this, the interval $[0, \hbar\beta]$ is divided into N_τ segments of length $\Delta_\tau = \frac{\hbar\beta}{N_\tau}$, and at the end the limit $N_\tau \to \infty$ is taken. [39]

$$
\begin{aligned}
e^{-S/\hbar} &= \lim_{N_\tau\to\infty} \exp\left[-\frac{S_0}{\hbar} - \frac{1}{\hbar}\sum_{k=1}^{N}\sum_{j=1}^{N_\tau}\Delta_\tau\frac{U}{4}\left(n_k^2 - s_k^2\right)\right] \\
&= \lim_{N_\tau\to\infty}\int\left(\prod_{k=1}^{N}\prod_{j=1}^{N_\tau}\frac{1}{\pi\hbar U}\Delta_\tau \mathrm{d}\Delta_c(k,\tau_j)\mathrm{d}\Delta_s(k,\tau_j)\right) * \\
&\qquad . \quad * \exp\left[-\frac{S_0}{\hbar} + \frac{1}{\hbar}\sum_{k=1}^{N}\sum_{j=1}^{N_\tau}\Delta_\tau\left\{-\frac{1}{U}\left(\Delta_c^2+\Delta_s^2\right) + \mathrm{i}\Delta_c n_k + \Delta_s s_k\right\}\right] \\
&= \int \mathcal{D}^2\Delta_{c,s}(k,\tau)\exp\left[-\frac{1}{\hbar}\left(S_0 + \int_0^{\hbar\beta}\sum_{k=1}^{N}\left\{\frac{1}{U}\left(\Delta_c^2+\Delta_s^2\right) - \mathrm{i}\Delta_c n_k - \Delta_s s_k\right\}\right)\right]
\end{aligned}
\tag{4.13}
$$

where

$$
\mathcal{D}^2\Delta_{c,s}(k,\tau) = \prod_{k=1}^{N}\lim_{N_\tau\to\infty}\prod_{j=1}^{N_\tau}\left(\frac{\mathrm{d}\Delta_c(k,\tau_j=\frac{\hbar\beta}{N_\tau}j)\mathrm{d}\Delta_s(k,\tau_j)}{N_\tau}\ \frac{\beta}{\pi U}\right) \tag{4.14}
$$

is a dimensionless integration symbol which is called "functional differential". The arguments k and τ indicate the dependences of the integration variables Δ_c and Δ_s. Because of the name of this kind of integrals, the whole procedure also has the name functional-integral method [39]

From a physical point of view such kind of decompositions provide possibilities for an approximation of the partition function The interaction between fermions disappears, and the particles move instead in the fictitious fields Δ_c and Δ_s Those fields might depend on the position in space and temperature Provided that they are chosen properly, they have the same effect on the particles as an interaction would have Then the functional-integral method is exact. The more the fictitious fields are only approximations the less correctly are interactions described.

By the way, the idea of moving particles in a mean field is exactly the same as in the Hartree-Fock approximation and has especially the same structure as the Stoner model (3.6)

Remark: The charge interaction part will essentially lead to terms like $\mathrm{i}\Delta_c M$ and causes a problem of dealing with complex quantities In order to get the complete Hamiltonian hermitian it is therefore necessary to deal with imaginary mean fields, which is not very convenient In an attempt to avoid such difficulties

one could try to alter the Hubbard-Stratonovic decomposition. In order to do this, the fictitious field Δ_c has to be split into one part and its complex conjugate at the beginning of this transformation. A treatment of the form

$$\begin{aligned}\exp\left[-\frac{U}{4\hbar}n_k^2\right] &= \frac{1}{\pi\hbar U}\int \mathrm{d}\Delta_c \exp\left[-\frac{1}{U\hbar}\Delta_c\Delta_c^* + \mathrm{i}\Delta_c\xi_k^*\xi_k - \mathrm{i}\Delta_c^*\xi_k^*\xi_k\right] \\ &= \frac{1}{\pi\hbar U}\int \mathrm{d}\Delta_c \exp\left[-\frac{1}{U\hbar}|\Delta_c|^2 + \underbrace{2\mathrm{Re}(\mathrm{i}\Delta_c)}_{\Delta_c'}\xi_k^*\xi_k\right] \qquad (4.15)\end{aligned}$$

at least proves that it is also possible to calculate with real terms. However, it turned out that this form of notation is even more inconvenient for further calculations.

4.3 Spin-rotation Invariance

The main point of the paper of Schulz [44] is that the expression for the action should be rotational invariant. The reason is the *a priori* rotational invariance of the Hubbard model That means that if the spin quantization axis for the whole system is rotated in a certain way, then the Hubbard Hamiltonian remains unchanged [1]

Proof: The statement is obviously fulfilled for the hopping part, provided that every site is rotated by the same angle Then a rotation and a backward-rotation cancel each other. Otherwise the kinetic energy part is not rotational invariant and such statements for the whole Hamiltonian are only true in the limit $\frac{U}{t} \gg 1$

For the interaction part one should note that a spin operator for a certain site can also be represented in the form [31]

$$S_k = \frac{\hbar}{2}c_{k,\alpha}^\dagger \sigma_{\alpha\beta} c_{k\beta}, \qquad (4.16)$$

where σ is the set of Pauli spin matrices defined in (1.2) and it is summed automatically over $\alpha, \beta \in \{\uparrow, \downarrow\}$. The proof is equivalent to the one for the corresponding coupled boson representation (1.8) A straight forward calculation

[1] In recent papers [47] Zhang and others pointed out that the Hubbard model posses an approximate SO(5) symmetry This feature can be used to unify antiferromagnetism and d-wave superconductivity

leads with the help of the relation $\sum_i \sigma(i)_{\alpha,\beta}\sigma(i)_{\gamma,\delta} = 2\delta_{\alpha,\delta}\delta_{\beta,\gamma} - \delta_{\alpha,\beta}\delta_{\gamma,\delta}$ to the surprising result that the square of the operator S_k has the form

$$S_k^2 = \frac{3}{4}\hbar^2 (\hat{n}_{k,\uparrow} + \hat{n}_{k,\downarrow})^2 - 3\hbar^2 \hat{n}_{k,\uparrow}\hat{n}_{k,\downarrow} \tag{4 17}$$

Summed over all sites, this can be used to express the interaction of the Hubbard model in the following way.

$$\hat{V} = U \sum_{k=1}^{N} \hat{n}_{k,\uparrow}\hat{n}_{k,\downarrow} = \frac{M^2 U}{4} - \frac{U}{3\hbar^2} \sum_{k=1}^{N} S_k^2, \tag{4 18}$$

which shows the claimed SU(2) symmetry more explicit □

On the other hand the spin term $\hat{s}_k$ in (4 9) shows no rotation invariance A spin projection does of course depend on the direction of the spin-quantization axis Nevertheless, the Hubbard-Stratonovic decomposition (4 13) can still be exact because the invariance is ensured for the sum of the charge and the spin term This indicates a strong spin-charge interaction However, as soon as approximations are performed this interaction is perturbed and the spin-rotation invariance destroyed [48]. In this sense it might be more appropriate to use (4 17) instead of (4 9).

Schulz [44] suggests another way by introducing a spin-space reference frame that varies in time and space He states that "The fluctuations of the orientation of the reference frame then allow for a rather natural inclusion of spin-rotation invariance "

That means that the spin quantization axis is allowed to differ from site to site The axis on a certain site must of course be the same for both fermions sitting on this site. However, for the Hamiltonian it is not necessary that the spin directions of electrons on different sites have something to do with one another Nevertheless, if arbitrary spin-quantization axes are allowed the pictorial explanation of the kinetic energy term as a hopping of electrons will get lost. Furthermore, it is not clear any more why only $c^\dagger_{k,\uparrow}c_{k+1,\uparrow}$ appears in the Hamiltonian and not for instance $c^\dagger_{k,\uparrow}c_{k+1,\downarrow}$, because the axis are now independent from one another The only reason for the favour of the first kind of operators could be that the angle differs from one site to a neighbouring site only slightly, and the electron can overcome this change

The unit vector in the direction of the new spin quantization axis on a certain site k is described by a pair of polar angles, $\Omega_k = \Omega_k(\theta, \zeta)$ θ is the angle between the spin axis and the z-axis; ζ is the angle between the projection of the spin axis on the xy-plane and the x-axis[2] The rotation itself is performed by a matrix of the form

$$\hat{R}_k(\theta,\zeta) = \begin{pmatrix} \cos\left(\frac{1}{2}\theta\right) & -e^{-i\zeta}\sin\left(\frac{1}{2}\theta\right) \\ e^{i\zeta}\sin\left(\frac{1}{2}\theta\right) & \cos\left(\frac{1}{2}\theta\right) \end{pmatrix} \tag{4 19}$$

It is a unitary transformation ($\hat{R}_k \cdot \hat{R}_k^+ = \mathbb{1}$) with the desired property

$$\hat{R}_k(\theta,\zeta)\sigma_z\hat{R}_k^+(\theta,\zeta) = \Omega_k \quad \sigma.$$

Example: If the spin quantization axis should be the bisector of the angle formed by the x-axis and the y-axis, then $\theta = \frac{\pi}{2}$ and $\zeta = \frac{\pi}{4}$, and one obtains

$$\left(\frac{1}{\sqrt{2}}\right)^2 \begin{pmatrix} 1 & -\frac{1}{\sqrt{2}}(1-i) \\ \frac{1}{\sqrt{2}}(1+i) & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{\sqrt{2}}(1-i) \\ -\frac{1}{\sqrt{2}}(1+i) & 1 \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1-i \\ 1+i & 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\sigma_x + \frac{1}{\sqrt{2}}\sigma_y$$

as wanted. □

A proper explanation why the rotation can be written in the form above is given in appendix E. It is based on the properties of Euler angles

With the help of such matrices one can introduce new spinor variables in the form

$$\tilde{\xi}_k \equiv \begin{pmatrix} \tilde{\xi}_{k,\uparrow} \\ \tilde{\xi}_{k,\downarrow} \end{pmatrix} = \hat{R}_k^+(\theta,\zeta) \begin{pmatrix} \xi_{k,\uparrow} \\ \xi_{k,\downarrow} \end{pmatrix} \quad \Longleftrightarrow \quad \hat{R}_k(\theta,\zeta) \begin{pmatrix} \tilde{\xi}_{k,\uparrow} \\ \tilde{\xi}_{k,\downarrow} \end{pmatrix} = \begin{pmatrix} \xi_{k,\uparrow} \\ \xi_{k,\downarrow} \end{pmatrix} \tag{4 20}$$

Here it is implied that a Grassmann number without a spin index denotes a spinor with two spin components Nevertheless, the rotation $\hat{R}_k(\theta,\zeta)$ is a unitary change of the spin-quantization axis and not in the first place a rotation of spinors This remark is related to the fact that

$$\hat{R}_k^+(2\pi,\zeta) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \end{pmatrix} \neq \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

[2]Its usually denoted by φ, but in this paper φ is reserved for the flux

It is worth studying the anticommutation relations of these new Grassmann numbers. They can be reduced quickly to those of the normal (not rotated) Grassmann numbers $\xi_{j,\eta}$ and $\xi^*_{j,\eta}$ For instance $\tilde{\xi}_{k,\sigma}$ and $\tilde{\xi}_{k',\sigma'}$ always anticommute, because both are linear combinations of numbers $\xi_{j,\eta}$ without the use of conjugate numbers $\xi^*_{j,\eta}$ It is only slightly more difficult for combinations of conjugate and non-conjugate numbers. With the help of Einstein's sum convention one can write

$$\begin{aligned}\left[\tilde{\xi}_{k,\sigma}, \tilde{\xi}^*_{k',\sigma'}\right]_+ &= \left[\left(\hat{R}^+_k\right)_{\sigma,\eta} \xi_{k,\eta}, \xi^*_{k',\eta'} \left(\hat{R}_{k'}\right)_{\eta',\sigma'}\right]_+ = \left(\hat{R}^+_k\right)_{\sigma,\eta} \left(\hat{R}_{k'}\right)_{\eta',\sigma'} \delta_{k\,k'}\delta_{\eta,\eta'} \\ &= \delta_{k,k'} \left(\hat{R}^+_k\right)_{\sigma,\eta} \left(\hat{R}_k\right)_{\eta,\sigma'} = \delta_{k,k'}\delta_{\sigma,\sigma'}, \qquad (4\,21)\end{aligned}$$

At the end of this calculation the fact that the rotation matrix $\hat{R}_k$ is unitary has been used Provided that this is the case, rotated Grassmann numbers obey exactly the same anticommutation relations as all other Grassmann numbers

The aim for the rest of this chapter is to transform the action of our problem accordingly and to draw conclusions That means that every contribution to the action has to be expressed in terms of the rotated Grassmann numbers $\tilde{\xi}_{k,\sigma}$ instead of the "normal" Grassmann numbers $\xi_{k,\sigma}$. Only the phase factor for the magnetic flux is not effected by the change of the spin quantization axis

The problem is that we have to apply now two transformations at the same time One of them is the Hubbard-Stratonovic decomposition, the other is the introduction of a spin-space reference frame Which of them should be applied first? We shall try both possibilities and will see that they lead to different results. To begin with we follow the way of Schulz [44]

4.4 Rotation First

4.4.1 Derivation of the Action

Rotation

As discussed above, already the splitting of the interaction part into a term for the charge degree of freedom and one for the spin degree of freedom leads to expressions which are not rotational invariant. Therefore, a spin-space reference frame is introduced by using the transformation (4.20). The effect on the action is the appearance of *rotated* Grassmann numbers together with the rotation matrices

However, because of the spin-rotation invariance of the interaction part it does not matter whether $\xi^*_{k,\uparrow}\xi^*_{k,\downarrow}\xi_{k,\downarrow}\xi_{k,\uparrow}$ is expressed in normal or rotated Grassmann numbers. Provided that the splitting in a charge and a spin part is done after the rotation, there will not appear any rotation matrices in the interaction

The action becomes

$$\begin{aligned} S_0 &= \int_0^{\hbar\beta} \mathrm{d}\tau \sum_{k=1}^{N} \left\{ \tilde{\xi}^*_k \left(\hbar\partial_\tau - \mu + \hat{R}^+_k (\partial_\tau \hat{R}_k) \right) \tilde{\xi}_k \right. \\ &\qquad \left. - t \left(\tilde{\xi}^*_k \hat{R}^+_k \hat{R}_{k+1} \tilde{\xi}_{k+1} \mathrm{e}^{\frac{2\pi \mathrm{i}}{N} \frac{\Phi}{\Phi_0}} + \tilde{\xi}^*_{k+1} \hat{R}^+_{k+1} \hat{R}_k \tilde{\xi}_k \mathrm{e}^{-\frac{2\pi \mathrm{i}}{N} \frac{\Phi}{\Phi_0}} \right) \right\} \\ S_{\mathrm{int}} &= \frac{U}{4} \int_0^{\hbar\beta} \mathrm{d}\tau \sum_{k=1}^{N} \left\{ \left(\tilde{\xi}^*_k \tilde{\xi}_k \right)^2 - \left(\tilde{\xi}^*_k \sigma_z \tilde{\xi}_k \right)^2 \right\} = \frac{U}{4} \int_0^{\hbar\beta} \mathrm{d}\tau \sum_{k=1}^{N} \left\{ \tilde{n}^2_k - \tilde{s}^2_k \right\}, \quad (4.22) \end{aligned}$$

where the spinor notation is used and charge and spin numbers are altered self-explanatory

Hubbard-Stratonovic Decomposition

A Hubbard-Stratonovic decomposition, performed afterwards, has exactly the same structure as for the non-rotated case (4.13) Thus, the partition function has the form

$$\begin{aligned} Z &= \int \mathcal{D}^2\Omega(k,\tau) \int \mathcal{D}\tilde{\Psi}^* \mathcal{D}\tilde{\Psi} \int \mathcal{D}^2\Delta_{c,s}(k,\tau) \\ &\qquad \exp\left[-\frac{1}{\hbar} \left(S_0 + \int_0^{\hbar\beta} \sum_{k=1}^{N} \left\{ \frac{1}{U} \left(\Delta^2_c + \Delta^2_s \right) - \mathrm{i}\Delta_c \tilde{n}_k - \Delta_s \tilde{s}_k \right\} \right) \right], \quad (4.23) \end{aligned}$$

which includes an integration over all directions of the quantization axis The angles can again depend on the site and Matsubara time, as indicated by the arguments

Saddle-point Approximation

The next step could be a saddle-point approximation [44] The notion of such an approximation is that only such parts of the integral over the auxiliary fields contribute for which the action has a minimum. Then an integral can be simplified in the following way

$$\begin{aligned}\int_{-\infty}^{\infty} \mathrm{e}^{-f(\tau)}\mathrm{d}\tau &= \int_{-\infty}^{\infty} \exp\left[-\left\{f(x_0)+(\tau-\tau_0)f'(x_0)+\frac{1}{2}(\tau-\tau_0)^2 f''(\tau_0)+\ .\ \right\}\right] \\ &\approx \mathrm{e}^{-f(x_0)}\cdot\sqrt{\frac{2\pi}{f''(x_0)}}, \end{aligned} \tag{4 24}$$

provided that $f'(\tau_0)=0$ and $f''(x_0)>0$, that is that x_0 is a (local) minimum of the function f.

Nevertheless, it is not the aim to perform a complete saddle point approximation Instead, a linear transformation onto the saddle point will be done For the charge auxiliary field Δ_c the following integral has to be considered

$$I_c := \int \mathrm{d}\Delta_c \exp\left[-\frac{1}{\hbar}\left(\frac{1}{U}\Delta_c^2 - \imath\Delta_c\tilde{n}_k\right)\right] = \int \mathrm{d}\Delta_c \exp[-f_c(\Delta_c)]$$

The function f has the derivatives

$$f_c(\Delta_c)=\frac{1}{U\hbar}\Delta_c^2-\frac{\imath}{\hbar}\Delta_c\tilde{n}_k, \quad f_c'(\Delta_c)=\frac{2}{U\hbar}\Delta_c-\frac{\imath}{\hbar}\tilde{n}_k, \quad f_c''(\Delta_c)=\frac{2}{U\hbar}.$$

Assuming that a situation close to half-filling is considered, the occupation number can be approximated by $\tilde{n}_k \approx 1$ Then the minimum is at $\Delta_{c\,0}=\frac{\imath U}{2}$ In terms of a new integration variable $\delta_c = \Delta_c - \Delta_{c,0}$, which describes the fluctuations around the saddle point, the integral can be given in the form

$$\begin{aligned} I_c &= \int \mathrm{d}\delta_c \exp\left[-\left\{f_c\left(\frac{\mathrm{i}U}{2}\right)+\delta_c f_c'\left(\frac{\imath U}{2}\right)+\frac{1}{2}\delta_c^2 f_c''\left(\frac{\imath U}{2}\right)\right\}\right] \\ &= \int \mathrm{d}\delta_c \exp\left[-\frac{1}{\hbar}\left(-\frac{U}{4}+\frac{U}{2}\tilde{n}_k+\mathrm{i}\delta_c(1-\tilde{n}_k)+\frac{1}{U}\delta_c^2\right)\right] \end{aligned} \tag{4 25}$$

Analogous, one obtains for the spin auxiliary field Δ_s with the assumption $\tilde{s}_k \approx -1$ and the fluctuation variable $\delta_s = \Delta_s - \Delta_{s,0} = \Delta_s - \left(-\frac{U}{2}\right)$

$$\begin{aligned} I_s &:= \int \mathrm{d}\Delta_s \exp\left[-\frac{1}{\hbar}\left(\frac{1}{U}\Delta_s^2 - \Delta_s \tilde{s}_k\right)\right] = \int \mathrm{d}\Delta_s \exp[-f_s(\Delta_s)] \\ &= \int \mathrm{d}\delta_s \exp\left[-\left\{f_s\left(-\frac{U}{2}\right) + \delta_s f_s'\left(-\frac{U}{2}\right) + \frac{1}{2}\delta_s^2 f_s''\left(-\frac{U}{2}\right)\right\}\right] \\ &= \int \mathrm{d}\delta_s \exp\left[-\frac{1}{\hbar}\left(\frac{U}{4} + \frac{U}{2}\tilde{s}_k - \delta_s(1+\tilde{s}_k) + \frac{1}{U}\delta_s^2\right)\right] \end{aligned} \tag{4.26}$$

After this movement to the saddle point the expression for the action looks like this

$$\begin{aligned} S &= \int_0^{\hbar\beta} \mathrm{d}\tau \sum_{k=1}^{N} \left\{\tilde{\xi}_k^* \left(\hbar\partial_\tau - \mu + \frac{U}{2}(\mathbb{1}_2 + \sigma_z)\right)\tilde{\xi}_k\right\} \\ &+ \int_0^{\hbar\beta} \mathrm{d}\tau \sum_{k=1}^{N} \left\{\tilde{\xi}_k^* \hat{R}_k^+ (\partial_\tau \hat{R}_k)\tilde{\xi}_k\right\} \\ &+ \int_0^{\hbar\beta} \mathrm{d}\tau \sum_{k=1}^{N} \left\{-t\left(\tilde{\xi}_k^* \hat{R}_k^+ \hat{R}_{k+1}\tilde{\xi}_{k+1} \mathrm{e}^{\frac{2\pi \mathrm{i}}{N}\frac{\Phi}{\Phi_0}} + \tilde{\xi}_{k+1}^* \hat{R}_{k+1}^+ \hat{R}_k \tilde{\xi}_k \mathrm{e}^{-\frac{2\pi \mathrm{i}}{N}\frac{\Phi}{\Phi_0}}\right)\right\} \\ &+ \int_0^{\hbar\beta} \mathrm{d}\tau \sum_{k=1}^{N} \left\{-\mathrm{i}\delta_c(\tilde{n}_k - 1) - \delta_s(\tilde{s}_k + 1) + \frac{1}{U}\left(\delta_c^2 + \delta_s^2\right)\right\} \end{aligned} \tag{4.27}$$

It determines the partition function

$$Z = \int \mathcal{D}^2\Omega(k,\tau) \int \mathcal{D}\tilde{\Psi}^* \mathcal{D}\tilde{\Psi} \int \mathcal{D}^2\delta_{c,s}(k,\tau) \exp[-S/\hbar], \tag{4.28}$$

where the functional differential is now

$$\mathcal{D}^2\delta_{c,s}(k,\tau) = \prod_{k=1}^{N} \lim_{N_\tau \to \infty} \prod_{j=1}^{N_\tau} \left(\frac{\mathrm{d}\delta_c(k, \tau_j = \frac{\hbar\beta}{N_\tau} j)\mathrm{d}\delta_s(k,\tau_j)}{N_\tau} \quad \frac{\beta}{\pi U}\right) \tag{4.29}$$

Apart from the fact that only fluctuations of δ_c, δ_s around the saddle point up to second order are taken into consideration, this result is still exact It has to be emphasized that in order to evaluate the partition function there are still four integrations to be done That is quite a difficult task

4.4.2 Simplifications, Half Filling

In order to get a feeling for the situation we will try now to make things as simple as possible This includes the following five points.

1 A rotation Ω of the spin-quantization axis with only one degree of freedom is considered The most convenient way to do this is to set ζ identical zero Hence,

$$\hat{R}_k(\theta, \zeta \equiv 0) = \hat{R}_k(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

2 At some points it is helpful to determine how θ depends on the site k. As explained in section 4 3 the difference of the angles of adjacent sites should be small Furthermore, a handy connection between the site and the angle, which does not favour any of the sites, is wanted. The simplest way to implement these conditions is a rotation around the circumference of the ring by equal steps $\theta_k = \frac{2\pi}{N} k \cdot w$, where w ("angle phase winding number") is a small positive integer

3 Fluctuations around the saddle point are not taken into consideration, $\delta_c = \delta_s = 0$ This is a hard constraint. The saddle points were derived under certain assumptions, from which one was $\tilde{n}_k \approx 1$ To neglect fluctuations is only justified if these assumptions are fulfilled In other words, the following calculations are only true for half filling ($M = N$) or for a situation which is very close to it

4 There is no dependence on the temperatur (imaginary time) Dependencies can also be neglected in the high-temperature limit, because $\beta \to 0$ as $T \to \infty$

5. Furthermore, the chemical potential μ is set to be zero, which can be done by an appropriate energy shift

What then remains of the action is essentially an altered Hamiltonian of the system Thus, it is denoted with the same symbol

$$\begin{aligned}\mathcal{H} &= \frac{U}{2}\sum_{k=1}^{N}\tilde{\xi}_k^*\left(\mathbb{1}_2+\sigma_z\right)\tilde{\xi}_k - t\sum_{k=1}^{N}\left\{\tilde{\xi}_k^*\hat{R}_k^+\hat{R}_{k+1}\tilde{\xi}_{k+1}\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}+\tilde{\xi}_{k+1}^*\hat{R}_{k+1}^+\hat{R}_k\tilde{\xi}_k\mathrm{e}^{-\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}\right\}\\ &\approx U\sum_{k=1}^{N}\tilde{\xi}_k^*\begin{pmatrix}1&0\\0&0\end{pmatrix}\tilde{\xi}_k - t\sum_{k=1}^{N}\left\{\tilde{\xi}_k^*\begin{pmatrix}1&-\vartheta\\ \vartheta&1\end{pmatrix}\tilde{\xi}_{k+1}e^{\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}+\mathrm{h\,c}\right\}\end{aligned} \tag{4 30}$$

In the second line the fact was used that the combination of the two rotations effectively is a rotation over the difference of the angles,

$$\vartheta=\frac{1}{2}\left(\theta_{k+1}-\theta_k\right)=\frac{1}{2}\frac{2\pi}{N}w=\frac{\pi w}{N}.$$

The approximation is such that $\cos\vartheta\approx 1$ and $\sin\vartheta\approx\vartheta$ for large N

If no integration is performed it is also not necessary to use Grassmann numbers Instead, we introduce rotated creation and annihilation operators via

$$\tilde{c}_k\equiv\begin{pmatrix}\tilde{c}_{k,\uparrow}\\ \tilde{c}_{k,\downarrow}\end{pmatrix}=\hat{R}_k^+(\theta,\zeta)\begin{pmatrix}c_{k,\uparrow}\\ c_{k,\downarrow}\end{pmatrix}\quad\Longleftrightarrow\quad\tilde{c}_k^\dagger\equiv\left(\tilde{c}_{k,\uparrow}^\dagger\,\tilde{c}_{k,\downarrow}^\dagger\right)=\left(c_{k,\uparrow}^\dagger\,c_{k,\downarrow}^\dagger\right)R_k(\theta,\zeta), \tag{4 31}$$

and the Hamiltonian becomes

$$\begin{aligned}\mathcal{H}=U\sum_k\tilde{c}_{k,\uparrow}^\dagger\tilde{c}_{k,\uparrow}-t\sum_k\left\{\tilde{c}_{k,\uparrow}^\dagger\tilde{c}_{k+1,\uparrow}+\tilde{c}_{k,\downarrow}^\dagger\tilde{c}_{k+1,\downarrow}+\vartheta\left(\tilde{c}_{k,\downarrow}^\dagger\tilde{c}_{k+1,\uparrow}-\tilde{c}_{k,\uparrow}^\dagger\tilde{c}_{k+1,\downarrow}\right)\right\}\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}\\ -t\sum_k\left\{\tilde{c}_{k+1,\uparrow}^\dagger\tilde{c}_{k,\uparrow}+\tilde{c}_{k+1,\downarrow}^\dagger\tilde{c}_{k,\downarrow}+\vartheta\left(\tilde{c}_{k+1,\uparrow}^\dagger\tilde{c}_{k,\downarrow}-\tilde{c}_{k+1,\downarrow}^\dagger\tilde{c}_{k,\uparrow}\right)\right\}\mathrm{e}^{-\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}\end{aligned} \tag{4 32}$$

A problem of calculations with such a Hamiltonian is that the commutation relations between rotated operators and normal operators, as used in the states, are not necessarily straight-forward anymore The easiest way to avoid such difficulties is to return to the normal fermionic operators in the Hamiltonian

A procedure like this means in essence that the rotation is maintained only during the Hubbard Stratonovic decomposition. Only here it is necessary to ensure rotation invariance. If one returns afterwards to normal operators, then the kinetic energy part will be restored in its old shape However, this is not the case for the interaction part

From (4 31) it follows for the several components of the rotated operators

$$\begin{aligned} \tilde{c}_{k,\uparrow} &= \cos\tfrac{\theta_k}{2} c_{k,\uparrow} + \sin\tfrac{\theta_k}{2} c_{k,\downarrow} & \tilde{c}^\dagger_{k,\uparrow} &= \cos\tfrac{\theta_k}{2} c^\dagger_{k,\uparrow} + \sin\tfrac{\theta_k}{2} c^\dagger_{k,\downarrow} \\ \tilde{c}_{k,\downarrow} &= -\sin\tfrac{\theta_k}{2} c_{k,\uparrow} + \cos\tfrac{\theta_k}{2} c_{k,\downarrow} & \tilde{c}^\dagger_{k,\downarrow} &= -\sin\tfrac{\theta_k}{2} c^\dagger_{k,\uparrow} + \cos\tfrac{\theta_k}{2} c^\dagger_{k,\downarrow} \end{aligned} \tag{4 33}$$

provided that the rotation is over one angle only. Hence,

$$\begin{aligned} \tilde{c}^\dagger_{k,\uparrow}\tilde{c}_{k,\uparrow} &= \left(\cos\frac{\theta_k}{2} c^\dagger_{k,\uparrow} + \sin\frac{\theta_k}{2} c^\dagger_{k,\downarrow}\right)\left(\cos\frac{\theta_k}{2} c_{k,\uparrow} + \sin\frac{\theta_k}{2} c_{k,\downarrow}\right) \\ &= \cos^2\frac{\theta_k}{2} c^\dagger_{k,\uparrow} c_{k,\uparrow} + \sin^2\frac{\theta_k}{2} c^\dagger_{k,\downarrow} c_{k,\downarrow} + \sin\frac{\theta_k}{2}\cos\frac{\theta_k}{2}\left(c^\dagger_{k,\uparrow} c_{k,\downarrow} + c^\dagger_{k,\downarrow} c_{k,\uparrow}\right) \\ &= \frac{1}{2}\Big\{(1+\cos\theta_k)\, c^\dagger_{k,\uparrow} c_{k,\uparrow} + (1-\cos\theta_k)\, c^\dagger_{k,\downarrow} c_{k,\downarrow} \\ &\qquad + \sin\theta_k\left(c^\dagger_{k,\uparrow} c_{k,\downarrow} + c^\dagger_{k,\downarrow} c_{k,\uparrow}\right)\Big\}, \end{aligned}$$

which leads to the Hamiltonian

$$\begin{aligned} \mathcal{H} &= \frac{U}{2}\sum_{k=1}^{N}\Big\{\left(c^\dagger_{k,\uparrow} c_{k,\uparrow} + c^\dagger_{k,\downarrow} c_{k,\downarrow}\right) + \cos\theta_k\left(c^\dagger_{k,\uparrow} c_{k,\uparrow} - c^\dagger_{k,\downarrow} c_{k,\downarrow}\right) \\ &\qquad + \sin\theta_k\left(c^\dagger_{k,\uparrow} c_{k,\downarrow} + c^\dagger_{k,\downarrow} c_{k,\uparrow}\right)\Big\} \qquad (4\ 34) \\ &- t\sum_{k=1}^{N}\left\{\left(c^\dagger_{k,\uparrow} c_{k+1,\uparrow} + c^\dagger_{k,\downarrow} c_{k+1,\downarrow}\right) e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}} + \left(c^\dagger_{k+1,\uparrow} c_{k,\uparrow} + c^\dagger_{k+1,\downarrow} c_{k,\downarrow}\right) e^{-\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\right\}. \end{aligned}$$

The following steps will be analogous to those in the previous chapter We shall find the expectation value, take derivatives with respect to one of the parameters and try to solve the Hartree-Fock equations If this is possible, the total energy and afterwards the persistent current can be calculated

The expectation value shall first of all be evaluated with the same states as already used in section 3 4,

$$|\psi\rangle_{S_\uparrow S_\downarrow} = \underbrace{\prod_{n\in S_\uparrow}\left(\sum_{i_n=1}^{N}\beta^n_{i_n} c^\dagger_{i_n,\uparrow}\right)}_{\sim|0\rangle=|\psi\rangle_{S_\uparrow}} \underbrace{\prod_{m\in S_\downarrow}\left(\sum_{i_m=1}^{N}\beta^m_{i_m} c^\dagger_{i_m,\downarrow}\right)}_{\sim|0\rangle=|\psi\rangle_{S_\downarrow}} |0\rangle \tag{4 35}$$

Then the calculations for the hopping part are absolutely the same as already done there The terms of the interaction part shall be examined next

$${}_{S_\uparrow}\langle\psi|c^\dagger_{k,\uparrow} c_{k,\uparrow}|\psi\rangle_{S_\uparrow} = \sum_{A=1}^{M_\uparrow}\sum_{j_1}\cdots\sum_{j_{M_\uparrow}}\sum_{\wp\in\mathcal{P}(M_\uparrow)}(-1)^{\mathrm{sgn}\wp}\beta^{n_1 *}_{j_1}\cdots\beta^{n_{M_\uparrow} *}_{j_{M_\uparrow}}\beta^{n_{\wp(1)}}_{j_1}\cdots\beta^{n_{\wp(M_\uparrow)}}_{j_{M_\uparrow}}\delta_{j_A,k}$$

and accordingly for the opposite spin direction Derivative with an $n_C \in S_\uparrow$·

$$\begin{aligned}\frac{\partial}{\partial\beta_\tau^{nC*}}\left({}_{S_\uparrow}\langle\psi|c_{k,\uparrow}^\dagger c_{k,\uparrow}|\psi\rangle_{S_\uparrow}\right) &= \underbrace{\beta_k^{nC}\delta_{k,\tau}}_{\varphi=\mathrm{id},A=C} + \underbrace{\sum_{\substack{A=1\\A\neq C}}^{M_\uparrow}|\beta_k^{nA}|^2\beta_\tau^{nC}}_{\varphi=\mathrm{id},A\neq C} \\ &\quad \underbrace{-\sum_{\substack{A=1\\A\neq C}}^{M_\uparrow}\beta_k^{nA*}\beta_k^{nC*}\beta_x^{nA}}_{\varphi(A)=C,\varphi(C)=A} \\ \frac{\partial}{\partial\beta_\tau^{nC*}}\left({}_{S_\uparrow,S_\downarrow}\langle\psi|c_{k,\downarrow}^\dagger c_{k,\downarrow}|\psi\rangle_{S_\uparrow,S_\downarrow}\right) &= {}_{S_\downarrow}\langle\psi|c_{k,\downarrow}^\dagger c_{k\downarrow}|\psi\rangle_{S_\downarrow}\cdot\frac{\partial}{\partial\beta_x^{nC*}}\left({}_{S_\uparrow}\langle\psi|\psi\rangle_{S_\uparrow}\right) \\ &= \sum_{B=1}^{M_\downarrow}|\beta_k^{mB}|^2\cdot\beta_\tau^{nC}\end{aligned}$$

What remains are expressions of the form

$${}_{S_\uparrow,S_\downarrow}\langle\psi|c_{k,\uparrow}^\dagger c_{k,\downarrow}|\psi\rangle_{S_\uparrow,S_\downarrow}$$

If the operators are understood to operate on the ket-state $|\psi\rangle_{S_\uparrow,S_\downarrow}$, then the ket-state consists afterwards of one down-spin particle less and one up-spin particle more than the bra-state Since the number of up-spin a down-spin is conserved, respectively, the product of these two states has to be zero All such expressions simply vanish

Therefore, the following set of Hartree-Fock equations are obtained ($n_C \in S_\uparrow$):

$$\begin{aligned}&-\sum_{\substack{n\in S_\uparrow\\n\neq n_C}}\sum_{k=1}^{N}\beta_k^{n*}\left\{t\left(\beta_{k+1}^{n}e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}+\beta_{k-1}^{n}e^{-\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\right)-\frac{U}{2}\cos\theta_k\beta_k^n\right\}\beta_i^{nC} \\ &+\sum_{\substack{n\in S_\uparrow\\n\neq n_C}}\sum_{k=1}^{N}\beta_k^{n*}\left\{t\left(\beta_{k+1}^{nC}e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}+\beta_{k-1}^{nC}e^{-\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\right)-\frac{U}{2}\cos\theta_k\beta_k^{nC}\right\}\beta_x^{n} \\ &-\sum_{m\in S_\downarrow}\sum_{k=1}^{N}\beta_k^{m*}\left\{t\left(\beta_{k+1}^{m}e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}+\beta_{k-1}^{m}e^{-\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\right)-\frac{U}{2}\cos\theta_k\beta_k^m\right\}\beta_x^{nC} \\ &-t\left(\beta_{\tau+1}^{nC}e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}+\beta_{\tau-1}^{nC}e^{-\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\right)+\frac{U}{2}\left(M_\uparrow+M_\downarrow+\cos\theta_\iota\right)\beta_i^{nC} \\ &=\lambda\beta_\tau^{nC}\end{aligned} \tag{4.36}$$

This set of equations is in general not solved by Bloch wave functions anymore However, for the special case that no rotation is applied, $\theta_k \doteq 0\,\forall k$, the interaction

part in these equations simplifies to

$$\frac{U}{2}\left(M_\uparrow + M_\downarrow + 1 + M_\uparrow - 1 - M_\downarrow\right)\beta_x^{nc} = UM_\uparrow\beta_x^{nc}$$

and the solution becomes apparently a Bloch-type solution It is worth noting that in this case the equations do not reduce to those derived in section 3.4. The interaction energy derived in these previous calculations was $U\frac{M_\uparrow M_\downarrow}{N}$ What we obtain here is completely different. Even in the saddle-point approximation the Hubbard-Stratonovic decomposition apparently does not lead to Hartree-Fock results The reason might be an inappropriate choice of the saddle point

There are further inconveniences related to these equations The method of rotating the fermionic operators backwards after the Hubbard- Stratonovic decomposition led to the result, that the kinetic energy part again completely decouples from the interaction part. Neither the coupling constant U nor the spin structure $\{\theta_k\}_{k=1}^N$ appears in the hopping part, and the interaction part has nothing to do with the flux Φ

It should be possible to solve the equations above also for the general case, because they stem from a linear operator. However, for the mentioned reasons this particular approach shall not be investigated further Instead, another possibility of looking at things will be tried now

4.4.3 Rotated States

First Idea

The states which are used for expectation values are also constructed with the help of creation and annihilation operators Therefore, it is possible to rotate the operators at this position and to leave the Hamiltonian unchanged That means that

$$|\tilde{\psi}\rangle_{S_\uparrow,S_\downarrow} = \prod_{n\in S_\uparrow}\left(\sum_{i_n=1}^{N}\beta_{i_n}^{n}\tilde{c}_{i_n,\uparrow}^{\dagger}\right)\prod_{m\in S_\downarrow}\left(\sum_{i_m=1}^{N}\beta_{i_m}^{m}\tilde{c}_{i_m\downarrow}^{\dagger}\right)|0\rangle \qquad (4\ 37)$$

Such a state can afterwards be transformed again to an expression with non-rotated operators only To see how this works the case of two up-spin particles is considered first. Again the transformation (4 33) is used.

$$
\begin{aligned}
|\tilde{\psi}\rangle_{\{n_1,n_2\},\emptyset} &= \sum_{i_1,i_2} \beta_{i_1}^{n_1}\beta_{i_2}^{n_2}\tilde{c}_{i_2,\uparrow}\tilde{c}_{i_1,\uparrow}^{\dagger}|0\rangle \\
&= \sum_{i_1,i_2} \beta_{i_1}^{n_1}\beta_{i_2}^{n_2}\Big\{\cos\theta_{i_2}\cos\theta_{i_1}c_{i_2,\uparrow}^{\dagger}c_{i_1,\uparrow}^{\dagger} + \sin\theta_{i_2}\sin\theta_{i_1}c_{i_2,\downarrow}^{\dagger}c_{i_1,\downarrow}^{\dagger} \\
&\qquad + \sin\theta_{i_2}\cos\theta_{i_1}c_{i_2,\downarrow}^{\dagger}c_{i_1,\uparrow}^{\dagger} + \cos\theta_{i_2}\sin\theta_{i_1}c_{i_2,\uparrow}^{\dagger}c_{i_1,\downarrow}^{\dagger}\Big\}|0\rangle \\
\langle\tilde{\psi}|\tilde{\psi}\rangle_{\{n_1,n_2\},\emptyset} &= \sum_{i_1,i_2}\left|\beta_{i_1}^{n_1}\right|^2\left|\beta_{i_2}^{n_2}\right|^2\left(\cos^2\theta_{i_1}+\sin^2\theta_{i_1}\right)\left(\cos^2\theta_{i_2}+\sin^2\theta_{i_2}\right) \\
&- \sum_{i_1,i_2}\beta_{i_1}^{n_1}\beta_{i_2}^{n_1*}\beta_{i_2}^{n_2}\beta_{i_1}^{n_2*}\left(\cos^2\theta_{i_1}+\sin^2\theta_{i_1}\right)\left(\cos^2\theta_{i_2}+\sin^2\theta_{i_2}\right) \\
&= \sum_{i_1,i_2}\left\{\left|\beta_{i_1}^{n_1}\right|^2\left|\beta_{i_2}^{n_2}\right|^2 - \beta_{i_1}^{n_1}\beta_{i_2}^{n_1*}\beta_{i_2}^{n_2}\beta_{i_1}^{n_2*}\right\} \qquad (4\,38)
\end{aligned}
$$

The last result is the same as for the unrotated states This statement reminds us of a fact already explained in connection with formula (4 21) The operators $\tilde{c}_{i,\uparrow}^{\dagger}$ and $\tilde{c}_{i,\uparrow}$ obey the same anti-commutation relations as $c_{i,\uparrow}^{\dagger}$ and $c_{i,\uparrow}$ Therefore, one can also calculate with rotated operators in the familiar way.

As another implication one might argue that normalization constraints like ${}_{\{n_1\},\emptyset}\langle\tilde{\psi}|\tilde{\psi}\rangle_{\{n_1\},\emptyset} = 1$ and ${}_{\{n_1,n_2\},\emptyset}\langle\tilde{\psi}|\tilde{\psi}\rangle_{\{n_1,n_2\},\emptyset} = 1$ indicate that the β-factors in the states are, similar to the Bloch-case, orthonormal wave functions

$$\sum_i |\beta_i^{n_1}|^2 = 1 \quad \text{and} \quad \sum_i \beta_i^{n_1}\beta_i^{n_2*} = 0$$

Second Idea

In principle, there are two ways imaginable to obtain the expectation value of the hopping part

1 One could try to express also the Hamiltonian in rotated operators, assuming that an electron hops from one rotated site to the next rotated site However, to transform states and Hamiltonians at the same time does not change the physics and all calculations can be done as if there were no rotation That is what has essentially been done before

Even if additional operators in the form of the 2nd and 4th term of the Hamiltonian

$$\hat{H}_{\text{hop}} = -t\sum_{k=1}^{N}\Big\{\underbrace{\tilde{c}_{k,\uparrow}^{\dagger}\tilde{c}_{k+1,\uparrow}}_{1} + \underbrace{\tilde{c}_{k,\uparrow}^{\dagger}\tilde{c}_{k+1,\downarrow}}_{2} + \underbrace{\tilde{c}_{k,\downarrow}^{\dagger}\tilde{c}_{k+1,\uparrow}}_{3} + \underbrace{\tilde{c}_{k,\downarrow}^{\dagger}\tilde{c}_{k+1,\downarrow}}_{4} + \text{h c.}\Big\}$$

are introduced with the argument that because of the rotation there is no justification for spin preservation, nothing new appears When taking the average ${}_{S_\uparrow,S_\downarrow}\langle\tilde{\psi}|\hat{H}_{\text{hop}}|\tilde{\psi}\rangle_{S_\uparrow,S_\downarrow}$ these terms vanish.

2. It is more reasonable to start with unrotated hopping terms, only concentrating on the fact that the electron changes its site, but not characterizing the structure of different sites That brings us back to the situation on page 90 with the transformed Hamiltonian

$$\hat{H}_{\text{hop}} = -t\sum_{k=1}^{N}\left\{\tilde{c}_k^\dagger\begin{pmatrix}\cos\vartheta & -\sin\vartheta\\ \sin\vartheta & \cos\vartheta\end{pmatrix}\tilde{c}_{k+1}e^{\frac{2\pi\mathrm{i}}{\Lambda}\frac{\Phi}{\Phi_0}} + \text{h c.}\right\}, \tag{4 39}$$

where ϑ is the difference in the θ-angle of two adjacent sites, assumed to be fix In the average the mixed terms disappear again and the dependence on the spin-space reference frame expresses itself in a global factor

$${}_{S_\uparrow,S_\downarrow}\langle\tilde{\psi}|\hat{H}_{\text{hop}}|\tilde{\psi}\rangle_{S_\uparrow,S_\downarrow} = -t\cos\vartheta\sum_{k=1}^{N}\langle\tilde{\psi}|\left(\tilde{c}_{k,\uparrow}^\dagger\tilde{c}_{k+1,\uparrow}+\tilde{c}_{k,\downarrow}^\dagger\tilde{c}_{k+1,\downarrow}\right)e^{\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}+\text{h c.}|\tilde{\psi}\rangle$$

Both ways show the problem that mixed terms like $\tilde{c}_{k,\uparrow}^\dagger\tilde{c}_{k+1,\downarrow}$ always have to disappear The reason is the fixed number of up-spin and down-spin particles respectively However, such a behaviour is not really understandable If for instance two adjacent sites have a mutual angle of 90° between the spin-quantization axes it is not clear why the hopping $\tilde{c}_{k,\uparrow}^\dagger\tilde{c}_{k+1,\uparrow}$ is possible but not $\tilde{c}_{k,\uparrow}^\dagger\tilde{c}_{k+1,\downarrow}$.

In general, for sites with arbitrary rotations spin-flip processes should be allowed In other words, it does not make sense any-more to distinguish between a group of up-spin particles $S_\uparrow$ and a group of down-spin particles $S_\downarrow$ Only the total number of particles should be an integral of the system

This idea does not change the fact that a certain state is characterized by a set of quantum numbers $\{n_i\}_{i=1}^M$ which determine the coefficients in the field operator representation. The only difference is that the spin direction is not regulated any more Such conditions are satisfied by

$$|\tilde{\psi}\rangle_{n_1} = C_1\sum_{i=1}^{N}\gamma_i^{n_1}\left\{\tilde{c}_{i,\uparrow}^\dagger|0\rangle+\tilde{c}_{i,\downarrow}^\dagger|0\rangle\right\}$$

for the case of one particle. Here C_1 is a normalization constant which has because of

$$ {}_{n_1}\langle\tilde{\psi}|\tilde{\psi}\rangle_{n_1} = C_1^2 \sum_{i,j} \gamma_j^{n_1 *}\gamma_i^{n_1} \langle 0| \left(\tilde{c}_{j,\uparrow} + \tilde{c}_{j,\downarrow}\right)\left(\tilde{c}^\dagger_{i,\uparrow} + \tilde{c}^\dagger_{i,\downarrow}\right)|0\rangle = C_1^2 \sum_{i,j} \gamma_j^{n_1 *}\gamma_i^{n_1} 2\delta_{i\,j} $$

the value $C_1 = 1/\sqrt{2}$, when for convenience the γ-parameters are chosen in such a way that $\sum_{i=1}^{N} |\gamma_i|^2 = 1$.

Consequently, an arbitrary M-particle state has the following form

$$ |\tilde{\psi}\rangle_{n_1,\ \ldots,n_M} = C_M \sum_{i_1,\ \ldots,i_M} \sum_{\sigma_1,\ \ldots,\sigma_M}^{\sigma_i \in \{\uparrow,\downarrow\}} \gamma_{i_1}^{n_1} \cdot \quad \ldots \quad \gamma_{i_M}^{n_M} \tilde{c}^\dagger_{i_M,\sigma_M} \quad \ldots \quad \tilde{c}^\dagger_{i_1,\sigma_1}|0\rangle \quad (4\,40) $$

$$ {}_{n_1,\ \ldots,n_M}\langle\tilde{\psi}| = C_M^* \sum_{j_1,\ \ldots,j_M} \sum_{\eta_1,\ \ldots,\eta_M}^{\eta_i \in \{\uparrow,\downarrow\}} \gamma_{j_1}^{n_1 *} \cdot \ \ldots \cdot \gamma_{j_M}^{n_M *} \langle 0|\tilde{c}_{j_1,\eta_1} \cdot \ \ldots \cdot \tilde{c}_{j_M,\eta_M} \quad (4\,41) $$

That means that the wave functions, determined by the quantum numbers, are not changed, but for each particle both possibilities (up- and down-spin) are allowed Such a construction makes it possible to deal with spin flips

The normalization constant is easily evaluated if the overlap of two states is expressed in terms of fully contractions[3]:

$$ {}_{n_1,\ \ldots,n_M}\langle\tilde{\psi}|\tilde{\psi}\rangle_{n_1,\ \ldots,n_M} = |C_M|^2 \sum_{\substack{i_1 \\ j_1,}} \sum_{\substack{i_M \\ j_M}} \sum_{\substack{\sigma_1, \\ \eta_1,}} \sum_{\substack{\sigma_M \\ \eta_M}} \gamma_{j_1}^{n_1 *} \cdot \ \ldots \quad \gamma_{j_M}^{n_M *}\gamma_{i_1}^{n_1} \cdot \ \ldots \cdot \gamma_{i_M}^{n_M} * $$

$$ \ldots * \langle 0|\tilde{c}_{j_1,\eta_1} \cdot \quad \ldots \quad \tilde{c}_{j_M,\eta_M}\tilde{c}^\dagger_{i_M,\sigma_M} \quad \ldots \quad \tilde{c}^\dagger_{i_1,\sigma_1}|0\rangle $$

1st possibility:

2nd possibility

However, such "crossings" as in the second possibility lead to vanishing sums $\sum_k \gamma_k^{n_i *}\gamma_k^{n_j}$ with $n_i \neq n_j$. Therefore, only the first possibility, the identical permutation, remains, leading to

$$ {}_{n_1,\ \ldots,n_M}\langle\tilde{\psi}|\tilde{\psi}\rangle_{n_1,\ \ldots,n_M} = |C_M|^2 \sum_{\sigma_1,\ \ldots,\sigma_M} 1 \quad \Longrightarrow \quad C_M = 2^{-M/2}. $$

Now the task is, to determine the expectation values of the hopping part in the second proposed form (4 39).

[3]This method is explained in appendix F

$$
\begin{aligned}
&\frac{\partial}{\partial\gamma_x^{n_C}{}^*}{}_{n_1,\ \ ,n_M}\langle\tilde\psi|\tilde c^\dagger_{k,\uparrow}\tilde c_{k+1,\uparrow}|\tilde\psi\rangle_{n_1,\ldots,n_M}\\
&= 2^{-M}\sum_{\substack{i_1\\ j_1}}^{j_C=x}\sum_{\substack{i_M\\ j_M}}\sum_{\substack{\sigma_1\\ \eta_1}}\sum_{\substack{\sigma_M\\ \eta_M}}\gamma_{j_1}^{n_1*}\ \ldots\widehat{\gamma_{j_C}^{n_C*}}\cdot\gamma_{j_M}^{n_M*}\gamma_{i_1}^{n_1}\cdot\ldots\ \ \gamma_{i_M}^{n_M}{}^*\\
&\qquad *\langle 0|\tilde c_{j_1,\eta_1}\cdot\ \cdot\tilde c_{j_M,\eta_M}\tilde c^\dagger_{k,\uparrow}\tilde c_{k+1,\uparrow}\tilde c^\dagger_{i_M,\sigma_M}\ \cdot\ \tilde c^\dagger_{i_1,\sigma_1}|0\rangle\\
&= \frac{2^{M-2}}{2^M}\sum_{\substack{A=1\\ A\neq C}}^{M}\sum_{\substack{i_A,j_A\\ i_C\,j_C}}\sum_{\substack{\sigma_A,\eta_A\\ \sigma_C,\eta_C}}\gamma_{j_A}^{n_A*}\gamma_{i_A}^{n_A}\gamma_{i_C}^{n_C}\delta_{j_C,x}*\\
&\qquad \ldots *\langle 0|\ \tilde c_{j_A,\eta_A}\ \ \tilde c_{j_C,\eta_C}\ \ \tilde c^\dagger_{k,\uparrow}\tilde c_{k+1,\uparrow}\ \ \tilde c^\dagger_{i_C,\sigma_C}\ \ \tilde c^\dagger_{i_A,\sigma_A}\ \cdot|0\rangle\\
&\qquad\qquad +\ \text{(pairing)}\\
&\qquad\qquad -\ \text{(pairing)}\\
&\qquad\qquad -\ \text{(pairing)}\\
&\quad +\frac{2^{M-1}}{2^M}\sum_{i_C,j_C}\sum_{\sigma_C,\eta_C}\gamma_{i_C}^{n_C}\langle 0|\cdot\ \ldots\ \ \tilde c_{j_C,\eta_C}\ \ldots\tilde c^\dagger_{k,\uparrow}\tilde c_{k+1,\uparrow}\ \ \tilde c^\dagger_{i_C,\sigma_C}\ \ |0\rangle\\
&= \frac{1}{4}\ 2\sum_{\substack{A=1\\ A\neq C}}^{M}\left\{\gamma_k^{n_A*}\gamma_{k+1}^{n_A}\gamma_x^{n_C}-\gamma_k^{n_A*}\gamma_x^{n_A}\gamma_{k+1}^{n_C}-\underbrace{\sum_{j_A}\gamma_{j_A}^{n_A*}\gamma_{j_A}^{n_C}}_{=0}\gamma_{k+1}^{n_A}{}^*\delta_{k,x}\right\}+\frac{1}{2}\gamma_{k+1}^{n_C}\delta_{k,x}
\end{aligned}
$$

After exactly the same calculations in the other three cases one obtains

$$
\begin{aligned}
\frac{\partial}{\partial\gamma_y^{n_C}{}^*}\langle\tilde\psi|\sum_{k=1}^{N}\tilde c^\dagger_{k,\uparrow}\tilde c_{k+1,\uparrow}|\tilde\psi\rangle &= \frac{1}{2}\sum_{\substack{A=1\\ A\neq C}}^{M}\sum_{k=1}^{N}\gamma_k^{n_A*}\left\{\gamma_{k+1}^{n_A}\gamma_x^{n_C}-\gamma_x^{n_A}\gamma_{k+1}^{n_C}\right\}+\frac{1}{2}\gamma_{x+1}^{n_C}\\
\frac{\partial}{\partial\gamma_z^{n_C}{}^*}\langle\tilde\psi|\sum_{k=1}^{N}\tilde c^\dagger_{k,\uparrow}\tilde c_{k+1,\uparrow}|\tilde\psi\rangle &= \frac{1}{2}\sum_{\substack{A=1\\ A\neq C}}^{M}\sum_{k=1}^{N}\gamma_k^{n_A*}\left\{\gamma_{k+1}^{n_A}\gamma_z^{n_C}-\gamma_z^{n_A}\gamma_{k+1}^{n_C}\right\}+\frac{1}{2}\gamma_{z+1}^{n_C}\\
\frac{\partial}{\partial\gamma_x^{n_C}{}^*}\langle\tilde\psi|\sum_{k=1}^{N}\tilde c^\dagger_{k,\uparrow}\tilde c_{k+1,\uparrow}|\tilde\psi\rangle &= \frac{1}{2}\sum_{\substack{A=1\\ A\neq C}}^{M}\sum_{k=1}^{N}\gamma_k^{n_A*}\left\{\gamma_{k+1}^{n_A}\gamma_z^{n_C}-\gamma_z^{n_A}\gamma_{k+1}^{n_C}\right\}+\frac{1}{2}\gamma_{x+1}^{n_C}\\
\frac{\partial}{\partial\gamma_z^{n_C}{}^*}\langle\tilde\psi|\sum_{k=1}^{N}\tilde c^\dagger_{k,\uparrow}\tilde c_{k+1,\uparrow}|\tilde\psi\rangle &= \frac{1}{2}\sum_{\substack{A=1\\ A\neq C}}^{M}\sum_{k=1}^{N}\gamma_k^{n_A*}\left\{\gamma_{k+1}^{n_A}\gamma_z^{n_C}-\gamma_z^{n_A}\gamma_{k+1}^{n_C}\right\}+\frac{1}{2}\gamma_{z+1}^{n_C}
\end{aligned}
$$

The fact that the result is in all four cases the same shows that the chosen states are not sensitive to spin directions. The surprising consequence is that eventually spin-flip processes disappear again. This is because of the minus sign in the rotation matrix of the Hamiltonian

$$
\hat H_{\text{hop}}=-t\sum_{k=1}^{N}\left\{\tilde c_k^\dagger\begin{pmatrix}\cos\vartheta & -\sin\vartheta\\ \sin\vartheta & \cos\vartheta\end{pmatrix}\tilde c_{k+1}e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}+\text{h c}\right\},
$$

leading to the effect that the two mixed-spin terms cancel each other.

The interaction also needs to be calculated again

$$\hat{V} = U \sum_{k=1}^{N} \tilde{c}_k^\dagger \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tilde{c}_k = U \sum_{k=1}^{N} \tilde{c}_{k,\uparrow}^\dagger \tilde{c}_{k,\uparrow}$$

$$\begin{aligned} \frac{\partial}{\partial \gamma_x^{n_C *}} \langle \tilde{\psi} | \sum_{k=1}^{N} \tilde{c}_{k,\uparrow}^\dagger \tilde{c}_{k,\uparrow} | \tilde{\psi} \rangle_{n_1, \ldots, n_M} &= \frac{1}{2} \sum_{\substack{A=1 \\ A \neq C}}^{M} \sum_{k=1}^{N} \gamma_k^{n_A *} \{ \gamma_k^{n_A} \gamma_\tau^{n_C} - \gamma_\tau^{n_A} \gamma_k^{n_C} \} + \frac{1}{2} \gamma_x^{n_C} \\ &= \frac{1}{2} \sum_{\substack{A=1 \\ A \neq C}}^{M} \{ 1 \cdot \gamma_x^{n_C} - 0 \cdot \gamma_k^{n_C} \} + \frac{1}{2} \gamma_x^{n_C} = \frac{M}{2} \gamma_x^{n_C} \end{aligned}$$

All together the γ-problem has the following structure

$$\begin{aligned} &- t \cos\vartheta \sum_{\substack{A=1 \\ A \neq C}}^{M} \sum_{k=1}^{N} \gamma_k^{n_A *} \left(\gamma_{k+1}^{n_A} \mathrm{e}^{\frac{2\pi \mathrm{i}}{N} \frac{\Phi}{\Phi_0}} + \gamma_{k-1}^{n_A} \mathrm{e}^{-\frac{2\pi \mathrm{i}}{N} \frac{\Phi}{\Phi_0}} \right) \gamma_\tau^{n_C} \\ &+ t \cos\vartheta \sum_{\substack{A=1 \\ A \neq C}}^{M} \sum_{k=1}^{N} \gamma_k^{n_A *} \left(\gamma_{k+1}^{n_C} \mathrm{e}^{\frac{2\pi \mathrm{i}}{N} \frac{\Phi}{\Phi_0}} + \gamma_{k-1}^{n_C} \mathrm{e}^{-\frac{2\pi \mathrm{i}}{N} \frac{\Phi}{\Phi_0}} \right) \gamma_\tau^{n_A} \\ &- t \cos\vartheta \left(\gamma_{x+1}^{n_C} \mathrm{e}^{\frac{2\pi \mathrm{i}}{N} \frac{\Phi}{\Phi_0}} + \gamma_{x-1}^{n_C} \mathrm{e}^{-\frac{2\pi \mathrm{i}}{N} \frac{\Phi}{\Phi_0}} \right) + U \frac{M}{2} \gamma_x^{n_C} \\ &= \lambda \gamma_x^{n_C} \end{aligned} \tag{4 42}$$

Unfortunately, the situation is not much better than in the Hartree-Fock equations (4 36) The interaction and the hopping part are again completely decoupled The influence of the rotation only changed from the former to the latter However, if all simplifications proposed in subsection 4 4 2 are used, then $\cos\vartheta = \cos\frac{\pi}{N} \approx 1$ for large N, and no rotation at all remains

The γ-problem has again an exact solution Bloch wave functions satisfy all equations, as can easily be seen Thus, the energy of the system is within this model described by

$$E = \frac{1}{2} MU - 2t \cos\vartheta \sum_{A=1}^{M} \cos\left(\frac{2\pi}{N} \left(n_A + \frac{\Phi}{\Phi_0} \right) \right) \tag{4 43}$$

This expression needs to be minimized with the help of the free parameters It is always possible to choose the set of quantum numbers $\{n_A\}_{A=1}^{M}$ such that the cosine is positive Therefore, the ground state is characterized by $\vartheta = 0$, which

means that all spin quantization axes point in the same direction No matter what the value of the flux is. it does not lead to interesting spin structures within this model

4.5 Decomposition First

A different approach is to start with the Hubbard-Stratonovic decomposition and to apply the rotations afterwards. The notion of rotation in this sense is not in the first place the preservation of rotation invariance during the process of Hubbard-Stratonovic decomposition This was the main aim of the last section By introducing a spin-space reference frame before the decomposition and integrating over all possible angles afterwards, we wanted to restore the rotation invariance which gets lost during Hubbard- Stratonovic transformation

By altering the order of transformations, the emphasis is slightly changed The Hubbard-Stratonovic decomposition remains a tool to simplify the interaction part. The spin-space reference frame displays degrees of freedom of the system, which implies possibilities to describe the system much more detailed It is for example possible to use the angles θ and ζ to construct spin waves on the ring Those spin waves are assumed to be a good description of (excited) states

In more general terms the spin-space reference frame allows to have an SU(2) gauge invariance in the limit of strong interaction. Something similar is for instance done in superconductivity by introducing order parameters as coherent wave functions for a macroscopic body In this system the gauge invariance enabled Josephson to predict correctly how two superconductors behave when they are brought together For our system, a gauge invariance for each site is also connected with the hope to describe it qualitatively more correctly and to discover effects which keep hidden otherwise

4.5.1 Derivation of the Hamiltonian

The interaction part of the Hubbard model is spin-rotation invariant Thus, for many of its transformations it is not really relevant whether it is performed with normal or with rotated Grassmann numbers The same steps as already in the

previous section can be used

Hubbard-Stratonovic Decomposition

The result (4 13) from the explanation of this decomposition is carried forward

$$e^{-S/\hbar} = \int \mathcal{D}^2\Delta_{c,s}(k,\tau)\exp\left[-\frac{1}{\hbar}\left(S_0+\int_0^{\hbar\beta}d\tau\sum_{k=1}^{N}\left\{\frac{1}{U}\left(\Delta_c^2+\Delta_s^2\right)-\right.\right.\right.$$
$$\left.\left.\left.-\,i\Delta_c n_k-\Delta_s s_k\right\}\right)\right],$$

where

$$S_0 = \int_0^{\hbar\beta}d\tau\sum_{k=1}^{N}\sum_{\sigma=\uparrow,\downarrow}\left\{\xi^*_{k,\sigma}\left(\hbar\partial_\tau-\mu\right)\xi_{k,\sigma}-t\left(\xi^*_{k,\sigma}\xi_{k+1,\sigma}e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}+\ldots\right.\right.$$
$$\left.\left.\ldots+\xi^*_{k+1,\sigma}\xi_{k,\sigma}e^{-\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\right)\right\}$$

and

$$Z = \int \mathcal{D}\Psi^*\mathcal{D}\Psi\, e^{-S/\hbar}$$

Saddle-point Approximation

The movement to the saddle point works in analogy to (4 27)

$$e^{-S/\hbar} = \int \mathcal{D}^2\delta_{c,s}(k\ \tau)\exp\left[-\frac{1}{\hbar}\left(S_0+\int_0^{\hbar\beta}\sum_{k=1}^{N}\left\{\frac{U}{2}\xi^*_k\left(\mathbb{1}_2+\sigma_z\right)\xi_k-\right.\right.\right.$$
$$\left.\left.\left.\ldots-i\delta_c\left(n_k-1\right)-\delta_s\left(s_k+1\right)+\frac{1}{U}\left(\delta_c^2+\delta_s^2\right)\right\}\right)\right]$$

Simplifications

With the same simplifications 1 - 5 as in the previous chapter the Hamiltonian becomes

$$\mathcal{H} = \frac{U}{2}\sum_{k=1}^{N}c^\dagger_k\left(\mathbb{1}_2+\sigma_z\right)c_k-t\sum_{k=1}^{N}\left\{c^\dagger_{k,\sigma}c_{k+1,\sigma}e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}+c^\dagger_{k+1,\sigma}c^\dagger_{k,\sigma}e^{-\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}\right\},$$

where Grassmann numbers are again replaced by annihilation and creation operators

Rotation

To introduce a rotation at this point leads for the first time to modifications compared to the calculations in the previous section

$$H = \frac{U}{2}\sum_{k=1}^{N}\tilde{c}^\dagger_k\hat{R}^+_k\left(\mathbb{1}_2+\sigma_z\right)\hat{R}_k\tilde{c}_k-t\sum_{k=1}^{N}\left\{\tilde{c}^\dagger_k\hat{R}^+_k\hat{R}_{k+1}\tilde{c}_{k+1}e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}+\text{h c.}\right\}$$

$$
\begin{aligned}
&= U\sum_{k=1}^{N}\tilde{c}_k^{\dagger}\begin{pmatrix}\cos^2\frac{\theta_k}{2} & -\sin\frac{\theta_k}{2}\cos\frac{\theta_k}{2}\\ -\sin\frac{\theta_k}{2}\cos\frac{\theta_k}{2} & \sin^2\frac{\theta_k}{2}\end{pmatrix}\tilde{c}_k \\
&\qquad -t\sum_{k=1}^{N}\left\{\tilde{c}_k^{\dagger}\begin{pmatrix}\cos\vartheta & -\sin\vartheta\\ \sin\vartheta & \cos\vartheta\end{pmatrix}\tilde{c}_{k+1}e^{\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}}+\mathrm{h\,c}\right\} \\
&= \frac{U}{2}\sum_{k=1}^{N}\left\{\left(\tilde{c}_{k,\uparrow}^{\dagger}\tilde{c}_{k,\uparrow}+\tilde{c}_{k,\downarrow}^{\dagger}\tilde{c}_{k,\downarrow}\right)+\cos\theta_k\left(\tilde{c}_{k,\uparrow}^{\dagger}\tilde{c}_{k,\uparrow}-\tilde{c}_{k,\downarrow}^{\dagger}\tilde{c}_{k,\downarrow}\right)-\dots\right. \\
&\qquad \left.-\sin\theta_k\left(\tilde{c}_{k,\uparrow}^{\dagger}\tilde{c}_{k,\downarrow}+\tilde{c}_{k,\downarrow}^{\dagger}\tilde{c}_{k,\uparrow}\right)\right\} \\
&- t\sum_{k=1}^{N}\left\{\cos\vartheta\left(\tilde{c}_{k,\uparrow}^{\dagger}\tilde{c}_{k+1,\uparrow}+\tilde{c}_{k,\downarrow}^{\dagger}\tilde{c}_{k+1,\downarrow}+\mathrm{h\,c.}\right)+\sin\vartheta\left(\tilde{c}_{k,\downarrow}^{\dagger}\tilde{c}_{k+1,\uparrow}-\tilde{c}_{k,\uparrow}^{\dagger}\tilde{c}_{k+1\downarrow}+\mathrm{h\,c.}\right)\right\}
\end{aligned}
\tag{4.44}
$$

This structure of the Hamiltonian is actually a mixture of the two ways discussed in the subsections 4.4.2 and 4.4.3. In the former subsection we evaluated the Hamiltonian with unrotated states. The backward rotation of the Hamiltonian had for the hopping part the consequence that $\tilde{c}_{k,\uparrow}^{\dagger}\tilde{c}_{k,\uparrow}$ was transformed to an expression with non-rotated operators. That is exactly the same what we are doing in this section, apart from the fact that the transformation goes now in the other direction, from unrotated to rotated operators. Thus, the appearing angles are essentially negative. The hopping part above is the same as the hopping part in the latter of the mentioned subsections, were calculations were performed with rotated states.

4.5.2 Search for Solutions

Because of the above mentioned similarities to the previous section, one only needs to combine the results obtained there in order to obtain the Hartree-Fock equations. It is reasonable to use not only the idea of rotated states but to take also the possibility of spin-flip into consideration. After having done this, the four possible combinations of operators in the interaction part have again all the same expectation value. This missing spin sensitivity leads for instance to the disappearance of the term proportional to $\cos\theta_k$ [1]. If all necessary terms are collected one obtains

[1] By using the equality $\frac{\partial}{\partial\gamma_x^n c}\langle\tilde{\psi}|\tilde{c}_{k,\uparrow}^{\dagger}\tilde{c}_{k\downarrow}|\tilde{\psi}\rangle = \left(\frac{\partial}{\partial\gamma_x^n c}\langle\tilde{\psi}|\tilde{c}_{k\downarrow}^{\dagger}\tilde{c}_{k,\uparrow}|\tilde{\psi}\rangle\right)^*$ and performing the derivate on the right hand side, it is possible to check this result in another way. Such an equality also implies that the expectation values must be real.

$$
\begin{aligned}
&- \sum_{\substack{A=1\\A\neq C}}^{M}\sum_{k=1}^{N} \gamma_k^{n_A *}\left\{t\cos\vartheta\left(\gamma_{k+1}^{n_A}\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}+\gamma_{k-1}^{n_A}\mathrm{e}^{-\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}\right)+\frac{U}{2}\sin\theta_k\gamma_k^{n_A}\right\}\gamma_x^{n_C}\\
&+ \sum_{\substack{A=1\\A\neq C}}^{M}\sum_{k=1}^{N} \gamma_k^{n_A *}\left\{t\cos\vartheta\left(\gamma_{k+1}^{n_C}\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}+\gamma_{k-1}^{n_C}\mathrm{e}^{-\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}\right)+\frac{U}{2}\sin\theta_k\gamma_k^{n_C}\right\}\gamma_x^{n_A}\\
&\qquad -t\cos\vartheta\left(\gamma_{x+1}^{n_C}\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}+\gamma_{\tau-1}^{n_C}\mathrm{e}^{-\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}\right)+\frac{U}{2}\left(M-\sin\theta_\tau\right)\gamma_x^{n_C}\\
&= \lambda\gamma_x^{n_C} \qquad (4\,45)
\end{aligned}
$$

One can try to use Bloch wave functions to solve this set of equations Provided that the angle-site dependence is used which was proposed as simplification 2 on page 89 one obtains the following results for the potential energy part.

$$
\begin{aligned}
-\frac{U}{2}\sum_{\substack{A=1\\A\neq C}}^{M}\sum_{k=1}^{N}\gamma_k^{n_A *}\sin\theta_k\,\gamma_k^{n_A} &= -\frac{U}{2N}\sum_{\substack{A=1\\A\neq C}}^{M}\sum_{k=1}^{N}\sin\left(\frac{2\pi}{N}k\cdot w\right)=0\\
\frac{U}{2}\sum_{\substack{A=1\\A\neq C}}^{M}\sum_{k=1}^{N}\gamma_k^{n_A *}\sin\theta_k\,\gamma_k^{n_C}\frac{\gamma_x^{n_A}}{\gamma_x^{n_C}} &= \frac{U}{2N}\sum_{\substack{A=1\\A\neq C}}^{M}\frac{1}{2\mathrm{i}}\left(\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}k\,w}-\mathrm{e}^{-\frac{2\pi\mathrm{i}}{N}k\,w}\right)\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}(x-k)(n_A-n_C)}\\
&= \frac{U}{2}\sum_{\substack{A=1\\A\neq C}}^{M}\frac{1}{2\mathrm{i}}\left(\delta_{w,n_A-n_C}-\delta_{w,n_C-n_A}\right)\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}x(n_A-n_C)}\\
\text{if } \delta_{w\,n_A-n_C}=1=\delta_{w,n_C-n_A}, &= \frac{U}{2}\frac{1}{2\mathrm{i}}\left(\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}x\,w}-\mathrm{e}^{-\frac{2\pi\mathrm{i}}{N}x\,w}\right)=\frac{U}{2}\sin\theta_x \qquad (4\,46)
\end{aligned}
$$

Since solutions are only obtained if the final expression does not depend on the parameters x and n_C, we have found the following result

If every quantum number n_A is occupied by one particle (half filling) then the condition in (4 46) is always fulfilled The appearing sin-function cancels with the similar expression in the last but one line of (4 45) leading to the desired independence of x and n_C. Hence, Bloch wave functions satisfy in this case the equations, no matter what the value of w is For exactly half filling the kinetic energy vanishes and, hence, there exists only the one energy $\frac{1}{2}UM$

One might think of another situation $w = 2$ and every second quantum number is occupied. However, this is too far away from half filling to be described with our simplifications Nevertheless, if w is a large number and only every wth position in momentum space is empty, then the equations are also fulfilled This indicates that such spin structures with Bloch wave functions might exist.

4.6 Zeemann effect

One important phenomenon has not yet been taken into consideration. It was mentioned in section 2.4 that a current around the circumference of the ring gives rise to a magnetic moment, which interacts with the external magnetic field. This effect has been considered by including the flux in the hopping part of the Hamiltonian. However, there is also a magnetic moment of individual electrons which gives rise to a total spin of the system. The interaction of an electron spin with a magnetic field is called Zeemann effect.

In many other papers this effect is not taken into consideration. One reason is the assumption of a Aharonov-Bohm situation, where the particles move in field-free space. Another reason is the SU(2) invariance of the Hubbard model. It has the consequence that the modulus squared and an arbitrary component of the total spin operator commute with the Hamiltonian [43]. Hence, one can find a common set of eigenstates, and the Zeemann term has only the effect of an energy shift. However, if the SU(2) symmetry gets lost the Zeemann effect needs to be considered. Therefore, the following comments are necessary.

In our situation the magnetic field is supposed to be strictly perpendicular to the plane of the ring, that means the magnetic field vector B points in the z-direction. The magnetic moment of a single electron is called Bohr's magneton and is denoted by μ_B. Combined with the Landé factor g the exchange energy becomes

$$\hat{H}_{\text{Zeem}} = -g\mu_B B_z \sum_{k=1}^{N} \hat{s}_k, \tag{4.47}$$

since $\sum_k \hat{s}_k$ measures the z-component of the total spin of the system.

In this paper the flux dependence is of particular interest. Therefore, whenever the Zeemann term is included into consideration it is useful to express it in a form where the flux is more explicit. The flux is determined by the product of the magnetic field and the area A enclosed by the ring. With the help of its circumference $L = aN$ one can write

$$\Phi = B_z \ A = B_z \ \frac{L^2}{4\pi} = B_z \cdot \frac{a^2 N^2}{4\pi}$$

Together with all the other quantities one obtains:

$$g\ \mu_B \cdot B_z = g\ \frac{e\hbar}{2m_e c} \cdot \frac{4\pi\Phi}{a^2 N^2} \cdot \frac{hc}{e\Phi_0} = \frac{gh^2}{m_e a^2 N^2} \frac{\Phi}{\Phi_0} =: \frac{\Delta_Z}{N^2} \frac{\Phi}{\Phi_0}, \tag{4 48}$$

where $\Delta_Z = \frac{gh^2}{m_e a^2}$ is just an energy constant If the distance between two sites, a, is supposed to be approximately 3 Å then Δ_Z is of the order of magnitude $1 \times 10^{-18} J \approx 10 eV$ Especially for systems with a low number of sites the Zeemann energy is therefore not negligible

Consequently, the Zeemann term (4 47) would have the following structure:

$$\hat{H}_{\text{Zeem}} = -\frac{\Delta_Z}{N^2} \frac{\Phi}{\Phi_0} \sum_{k=1}^{N} \left\{ c^\dagger_{k,\uparrow} c_{k,\uparrow} - c^\dagger_{k,\downarrow} c_{k,\downarrow} \right\}$$

The problem with this notation is that one has to be careful with rotations The expression above is correct if and only if the spin quantization axis is parallel to the magnetic field. If this is changed then only the projection of the spin on the z-axis contributes Therefore, if calculations are performed with a rotated Hamiltonian then the Zeemann term has the following form

$$\hat{H}_{\text{Zeem}} = -\frac{\Delta_Z}{N^2} \frac{\Phi}{\Phi_0} \sum_{k=1}^{N} \cos\theta_k \left\{ \tilde{c}^\dagger_{k,\uparrow} \tilde{c}_{k,\uparrow} - \tilde{c}^\dagger_{k,\downarrow} \tilde{c}_{k,\downarrow} \right\} \tag{4.49}$$

In more general terms, the Zeemann term brakes the rotational symmetry of the system Since the external magnetic field has a fixed direction, the fact that the spin is coupled with the field leads to a preferred spin direction

Unfortunately, such terms vanish within our description of the situation The reason is again the chosen structure of the states It implies that the expectation value of $\tilde{c}^\dagger_{k,\uparrow} \tilde{c}_{k,\uparrow}$ equals the expectation value of $\tilde{c}^\dagger_{k,\downarrow} \tilde{c}_{k,\downarrow}$ The missing spin sensitivity is shown here most drastically To choose the same prefactor $\gamma_k^{n_4}$ for up-spin and down-spin particles negates a preference in a certain spin direction.

Remark: A conclusion of the strategy of this chapter might also be to handle the Zeemann term as follows The Hamiltonian is the one given in (4 49) if it is evaluated with unrotated states When using rotated stated, the Hamiltonian should first of all be expressed in normal operators leaving rotational effects to the states. However, the cosine factor has to remain since the same angle between the two forms of operators exists in both cases Such an *ansatz* leads in the trial

to obtain only one kind of operators to

$$
\begin{aligned}
&\hat{H}_{\text{Zeem}} \\
&= -\frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\sum_{k=1}^{N}\cos\theta_k\left\{c^\dagger_{k,\uparrow}c_{k,\uparrow}-c^\dagger_{k,\downarrow}c_{k,\downarrow}\right\} \\
&= -\frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\sum_{k=1}^{N}\cos\theta_k\,\tilde{c}^\dagger_k\hat{R}^\dagger_k\sigma_z\hat{R}_k\tilde{c}_k \\
&= -\frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\sum_{k=1}^{N}\cos\theta_k\,\tilde{c}^\dagger_k\begin{pmatrix}\cos^2\frac{\theta_k}{2}-\sin^2\frac{\theta_k}{2} & -2\sin\frac{\theta_k}{2}\cos\frac{\theta_k}{2}\\ -2\sin\frac{\theta_k}{2}\cos\frac{\theta_k}{2} & \sin^2\frac{\theta_k}{2}-\cos^2\frac{\theta_k}{2}\end{pmatrix}\tilde{c}_k \\
&= -\frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\sum_{k=1}^{N}\cos\theta_k\left\{\cos\theta_k\left(\tilde{c}^\dagger_{k,\uparrow}\tilde{c}_{k,\uparrow}-\tilde{c}^\dagger_{k,\downarrow}\tilde{c}_{k,\downarrow}\right)-\sin\theta_k\left(\tilde{c}^\dagger_{k,\uparrow}\tilde{c}_{k,\downarrow}+\tilde{c}^\dagger_{k,\downarrow}\tilde{c}_{k,\uparrow}\right)\right\} \\
&= -\frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\sum_{k=1}^{N}\left\{\cos^2\theta_k\left(\tilde{c}^\dagger_{k,\uparrow}\tilde{c}_{k,\uparrow}-\tilde{c}^\dagger_{k,\downarrow}\tilde{c}_{k,\downarrow}\right)-\frac{1}{2}\sin(2\theta_k)\left(\tilde{c}^\dagger_{k,\uparrow}\tilde{c}_{k,\downarrow}+\tilde{c}^\dagger_{k,\downarrow}\tilde{c}_{k,\uparrow}\right)\right\}
\end{aligned}
$$

Then after calculating the expectation value only a term proportional to $\sin(2\theta_k)$ survives, forcing the spin in the limit of a strong magnetic field B_z to point in the direction of $\theta_k = \frac{3}{4}\pi$. Obviously, this does not describe the physics correctly □

Chapter 5

Trials of Improvement

The considerations in the previous chapter allow to gain a feeling for the notion of rotation. Even so some changes have already been applied, there are still major difficulties connected to the present model. In addition to the missing spin sensitivity three others are mentioned in the sections 5.1 and 5.3. Possibilities how to improve the situation, also by using fewer simplifications, are suggested. As a consequence new systems of equations have to be solved. This is tried for systems of a limited size in the sections 5.2 and 5.4.

5.1 Away from Half Filling

If one looks at the results in the previous chapter it strikes that U always appears in the numerator. However, U is the coupling constant in the Hamiltonian

$$\mathcal{H} = -t \sum_{k=1}^{N} \left\{ c_{k,\uparrow}^{\dagger} c_{k+1,\uparrow} \mathrm{e}^{\frac{2\pi \mathrm{i}}{N} \frac{\Phi}{\Phi_0}} + c_{k,\downarrow}^{\dagger} c_{k+1,\downarrow} \mathrm{e}^{-\frac{2\pi \mathrm{i}}{N} \frac{\Phi}{\Phi_0}} + \mathrm{h.c.} \right\} + U \sum_{k=1}^{N} \hat{n}_{k,\uparrow} \hat{n}_{k,\downarrow}$$

and determines the interaction between fermions with different spins on the same site. For large U the Hamiltonian is obviously minimized if all particles are strongly localized and no site is double occupied. Even in the limit $U \to \infty$ this kind of behaviour leads to a finite energy, provided that the band is less than half filled. In contrast to this statement, the obtained result on the previous pages diverges as U increases. There is no possibility to get all coefficients in front of U to vanish.

It would be much more reasonable to have U in the denominator. This is what actually happens when the Hubbard-Stratonovic decomposition is applied as can be seen in section 4.2 Only the move to the saddle point as proposed by Schulz [44] and performed on page 87 *f.* changed this fact. It resulted in the diverging term $\frac{1}{2}MU$ The reason why the transformation to the saddle point does not always lead to exact energy values lies in the limited validity of this transformation. It was not possible to perform it without a couple of assumptions One of them was $\hat{n}_k \approx 1$ which refers to half-filling

Therefore, it seems to be a good idea to perform the calculations without the movement to the saddle point For this purpose the various steps are briefly repeated By allowing now rotations with two degrees of freedom we shall also forget about the simplifications in this direction

The starting point is the form of the action after the Hubbard-Stratonovic decomposition as has been given now already several times

$$\mathrm{e}^{-S/\hbar} = \int \mathcal{D}^2\Delta_{c,s}(k,\tau)\exp\left[-\frac{1}{\hbar}\left(S_0 + \int_0^{\hbar\beta}\sum_{k=1}^{N}\left\{\frac{1}{U}\left(\Delta_c^2+\Delta_s^2\right) - \mathrm{i}\Delta_c n_k - \Delta_s s_k\right\}\right)\right].$$

Assuming that there is no dependence of the physical quantities on imaginary time and handling the chemical potential as a constant which can set to be zero, one obtains the following expression for the Hamiltonian

$$\begin{aligned}\mathcal{H} &= -t\sum_{k=1}^{N}\left(c_k^\dagger c_{k+1}\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}} + c_{k+1}^\dagger c_k \mathrm{e}^{-\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}\right) \\ &+ \frac{N}{U}\left(\Delta_c^2+\Delta_s^2\right) - \mathrm{i}\Delta_c\sum_{k=1}^{N}c_k^\dagger \mathbb{1}_2\, c_k - \Delta_s\sum_{k=1}^{N}c_k^\dagger\sigma_z c_k - \frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\sum_{k=1}^{N}c_k^\dagger\sigma_z c_k\end{aligned} \tag{5 1}$$

now without any movement to the saddle point, but with the Zeemann term It should be pointed out again that in such expressions creation (annihilation) operators without a spin index denote the spinors

$$c_k^\dagger = \left(c_{k,\uparrow}^\dagger\; c_{k,\downarrow}^\dagger\right) \quad \text{and} \quad c_k = \begin{pmatrix} c_{k,\uparrow} \\ c_{k,\downarrow}\end{pmatrix}$$

For the three-dimensional rotation every term shall be handled separately. First, the hopping part:

$$
\begin{aligned}
c_k^\dagger c_{k+1} &= \tilde{c}_k^\dagger \hat{R}^+(\theta_k,\zeta_k)\hat{R}(\theta_{k+1},\zeta_{k+1})\,\tilde{c}_{k+1} \\
&= \tilde{c}_k^\dagger \begin{pmatrix} \cos\frac{\theta_k}{2} & e^{-i\zeta_k}\sin\frac{\theta_k}{2} \\ -e^{i\zeta_k}\sin\frac{\theta_k}{2} & \cos\frac{\theta_k}{2} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta_{k+1}}{2} & -e^{-i\zeta_{k+1}}\sin\frac{\theta_{k+1}}{2} \\ e^{i\zeta_{k+1}}\sin\frac{\theta_{k+1}}{2} & \cos\frac{\theta_{k+1}}{2} \end{pmatrix} \tilde{c}_{k+1} \\
&= \tilde{c}_k^\dagger \bar{R}_k(\theta_k,\zeta_k,\theta_{k+1},\zeta_{k+1})\,\tilde{c}_{k+1} \quad \text{with} \\
&\qquad \begin{aligned}
\bar{R}_{k,\uparrow\uparrow} &= \cos\tfrac{\theta_k}{2}\cos\tfrac{\theta_{k+1}}{2} + e^{i(-\zeta_k+\zeta_{k+1})}\sin\tfrac{\theta_k}{2}\sin\tfrac{\theta_{k+1}}{2} \\
\bar{R}_{k,\uparrow\downarrow} &= e^{-i\zeta_k}\sin\tfrac{\theta_k}{2}\cos\tfrac{\theta_{k+1}}{2} - e^{-i\zeta_{k+1}}\cos\tfrac{\theta_k}{2}\sin\tfrac{\theta_{k+1}}{2} \\
\bar{R}_{k,\downarrow\uparrow} &= -e^{i\zeta_k}\sin\tfrac{\theta_k}{2}\cos\tfrac{\theta_{k+1}}{2} + e^{i\zeta_{k+1}}\cos\tfrac{\theta_k}{2}\sin\tfrac{\theta_{k+1}}{2} \\
\bar{R}_{k,\downarrow\downarrow} &= \cos\tfrac{\theta_k}{2}\cos\tfrac{\theta_{k+1}}{2} + e^{i(\zeta_k-\zeta_{k+1})}\sin\tfrac{\theta_k}{2}\sin\tfrac{\theta_{k+1}}{2}
\end{aligned} \qquad (5.2) \\
&= \bar{R}_{k,\uparrow\uparrow}\tilde{c}_{k,\uparrow}^\dagger\tilde{c}_{k+1,\uparrow} + \bar{R}_{k,\uparrow\downarrow}\tilde{c}_{k,\uparrow}^\dagger\tilde{c}_{k+1,\downarrow} + \bar{R}_{k,\downarrow\uparrow}\tilde{c}_{k,\downarrow}^\dagger\tilde{c}_{k+1,\uparrow} + \bar{R}_{k,\downarrow\downarrow}\tilde{c}_{k,\downarrow}^\dagger\tilde{c}_{k+1,\downarrow}
\end{aligned}
$$

In general, the matrix $\bar{R}_k(\theta_k,\zeta_k;\theta_{k+1},\zeta_{k+1})$ cannot be simplified The previously used argument of an addition of two rotations (one forward, one backward) does not hold in the three-dimensional case The reason is that already the first rotation implies a change of the coordinate system, so that the angles of the second rotation are defined with respect to different axes Only in special cases one can return to the old picture If for instance the longitude angle is the same for every site, $\zeta \equiv \zeta_k = \zeta_{k+1}$, then

$$
\bar{R}_k(\theta_k,\zeta,\theta_{k+1},\zeta) = \begin{pmatrix} \cos\vartheta & -e^{-i\zeta}\sin\vartheta \\ e^{i\zeta}\sin\vartheta & \cos\vartheta \end{pmatrix},
$$

where ϑ denotes again the difference $\frac{1}{2}(\theta_{k+1}-\theta_k)$ and can also depend on the site.[1]

Nevertheless, the matrix elements of $\bar{R}_k$ depend on each other in a simple, characteristic way:

$$
\bar{R}^*_{k,\uparrow\uparrow} = \bar{R}_{k,\downarrow\downarrow} \quad \text{and} \quad \bar{R}^*_{k,\uparrow\downarrow} = -\bar{R}_{k,\downarrow\uparrow}, \qquad (5.3)
$$

where the stars denote "complex conjugate" values This is even more helpful for calculations than the fact that $\bar{R}_k$ as a product of unitary matrices also has to be

[1] If $\hat{R}$ is defined as an adjunct matrix $\bar{R}^+$ then $\vartheta = \frac{1}{2}(\theta_k - \theta_{k+1})$ and the signs in the matrix change

unitary, with the consequence that

$$\begin{aligned} |\bar{R}_{k,\uparrow\uparrow}|^2 + |\bar{R}_{k,\downarrow\uparrow}|^2 &= 1 = |\bar{R}_{k,\downarrow\downarrow}|^2 + |\bar{R}_{k,\uparrow\downarrow}|^2 \\ \bar{R}^*_{k,\uparrow\uparrow}\bar{R}_{k,\uparrow\downarrow} + \bar{R}^*_{k,\downarrow\uparrow}\bar{R}_{k,\downarrow\downarrow} &= 0 = \bar{R}^*_{k,\uparrow\downarrow}\bar{R}_{k,\uparrow\uparrow} + \bar{R}^*_{k,\downarrow\downarrow}\bar{R}_{k,\downarrow\uparrow}. \end{aligned} \tag{5 4}$$

Only the first of these four equations does not follow from (5 3)

For the interaction and Zeemann part the rotation has the following effect:

$$c_k^\dagger \mathbb{1}_2 c_k = \tilde{c}_k^\dagger \hat{R}^+(\theta_k,\zeta_k)\mathbb{1}_2\hat{R}(\theta_k,\zeta_k)\tilde{c}_k = \tilde{c}_k^\dagger \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tilde{c}_k$$

$$c_k^\dagger \sigma_z c_k = \tilde{c}_k^\dagger \hat{R}^+(\theta_k,\zeta_k)\sigma_z\hat{R}(\theta_k,\zeta_k)\tilde{c}_k = \tilde{c}_k^\dagger \begin{pmatrix} \cos\theta_k & -\mathrm{e}^{-\mathrm{i}\zeta_k}\sin\theta_k \\ -\mathrm{e}^{\mathrm{i}\zeta_k}\sin\theta_k & -\cos\theta_k \end{pmatrix} \tilde{c}_k$$

Together the Hamiltonian (5.1) becomes

$$\begin{aligned} \mathcal{H} = & - t\sum_{k=1}^{N}\sum_{\sigma,\sigma'}\left\{\bar{R}_{k,\sigma\sigma'}\tilde{c}^\dagger_{k,\sigma}\tilde{c}_{k+1,\sigma'}\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}} + \bar{R}^*_{k,\sigma\sigma'}\tilde{c}^\dagger_{k+1,\sigma}\tilde{c}_{k,\sigma'}\mathrm{e}^{-\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}}\right\} \\ & + \frac{N}{U}\left(\Delta_c^2+\Delta_s^2\right) - \mathrm{i}\Delta_c\sum_{k=1}^{N}\tilde{c}_k^\dagger\tilde{c}_k - \frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\sum_{k=1}^{N}\cos\theta_k\tilde{c}_k^\dagger\sigma_z\tilde{c}_k \\ & - \Delta_s\sum_{k=1}^{N}\cos\theta_k\,\tilde{c}_k^\dagger\sigma_z\tilde{c}_k + \Delta_s\sum_{k=1}^{N}\sin\theta_k\left\{\tilde{c}^\dagger_{k,\uparrow}\tilde{c}_{k,\downarrow}\mathrm{e}^{-\mathrm{i}\zeta_k} + \mathrm{h\ c}\right\} \end{aligned} \tag{5.5}$$

with the matrix elements $\bar{R}_{k,\sigma\sigma'}$ defined in (5 2)

A variational calculation with the rotated states

$$|\tilde{\psi}\rangle_{n_1,\ \ ,n_M} = 2^{-M/2}\sum_{\iota_1,\ \ \iota_M}\ \sum_{\sigma_1,\ \ ,\sigma_M}^{\sigma_\iota\in\{\uparrow,\downarrow\}} \gamma^{n_1}_{\iota_1}\cdot\ \ \cdot\gamma^{n_M}_{\iota_M}\tilde{c}^\dagger_{\iota_M,\sigma_M}\ \ \cdot\ \ \tilde{c}^\dagger_{\iota_1,\sigma_1}|0\rangle$$

works along the same lines as before One obtains the Hartree-Fock equations

$$\begin{aligned} & - t\sum_{k=1}^{N}\sum_{\sigma\,\sigma'}\left\{\bar{R}_{k,\sigma\sigma'}\left[\frac{1}{2}\sum_{\substack{A=1\\A\neq C}}^{M}\gamma_k^{n_A*}\left(\gamma^{n_A}_{k+1}\gamma^{n_C}_{\tau} - \gamma^{n_A}_{\tau}\gamma^{n_C}_{k+1}\right) + \frac{1}{2}\gamma^{n_C}_{k+1}\delta_{\tau,k}\right]\mathrm{e}^{\frac{2\pi\mathrm{i}}{N}\frac{\Phi}{\Phi_0}} + \text{“h c”}\right\} \\ & + \frac{N}{U}\left(\Delta_c^2+\Delta_s^2\right)\gamma^{n_C}_{\tau} - \mathrm{i}\Delta_c\sum_{k=1}^{N}2\left[\frac{1}{2}\sum_{\substack{A=1\\A\neq C}}^{M}\gamma_k^{n_A*}\left(\gamma^{n_A}_{k}\gamma^{n_C}_{\tau} - \gamma^{n_A}_{\tau}\gamma^{n_C}_{k}\right) + \frac{1}{2}\gamma^{n_C}_{k}\delta_{\tau,k}\right] \\ & - \frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\sum_{k=1}^{N}\cos\theta_k\ \ 0\ -\ \Delta_s\sum_{k=1}^{N}\cos\theta_k\cdot 0 \\ & + \Delta_s\sum_{k=1}^{N}\sin\theta_k\left[\frac{1}{2}\sum_{\substack{A=1\\A\neq C}}^{M}\gamma_k^{n_A*}\left(\gamma^{n_A}_{k}\gamma^{n_C}_{x} - \gamma^{n_A}_{\tau}\gamma^{n_C}_{k}\right) + \frac{1}{2}\gamma^{n_C}_{k}\delta_{x,k}\right]\left(\mathrm{e}^{-\mathrm{i}\zeta_k} + \mathrm{e}^{\mathrm{i}\zeta_k}\right) = \lambda\gamma^{n_C}_{x} \end{aligned}$$

This expression shall be modified next For the hopping the characteristic dependence (5 3) of the matrix elements of $\bar{R}$ can be used to prove the following statements for any $z \in \mathbb{C}$

$$\begin{aligned} \left\{\left(\bar{R}_{k,\uparrow\uparrow} + \bar{R}_{k,\downarrow\downarrow}\right) z + \text{h c}\right\} &= \left(\bar{R}_{k,\uparrow\uparrow} + \bar{R}_{k,\downarrow\downarrow}\right)\{z + \text{h c.}\} \\ \left\{\left(\bar{R}_{k\,\uparrow\downarrow} + \bar{R}_{k,\downarrow\uparrow}\right) z + \text{h c}\right\} &= \left(\bar{R}_{k,\uparrow\downarrow} + \bar{R}_{k,\downarrow\uparrow}\right)\{z - \text{h c.}\} \end{aligned} \tag{5 6}$$

Furthermore,

$$\begin{aligned} \left\{z e^{\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}} + \text{h.c.}\right\} &= \{z + \text{h c}\}\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) + \imath\{z - \text{h c}\}\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \\ \left\{z e^{\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}} - \text{h c.}\right\} &= \{z - \text{h c}\}\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) + \imath\{z + \text{h c}\}\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \end{aligned} \tag{5 7}$$

Hence, in the hopping part of the Hartree-Fock equation the sum over σ and σ' becomes essentially

$$\begin{aligned} &\left\{\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\left(\bar{R}_{k,\uparrow\uparrow} + \bar{R}_{k,\downarrow\downarrow}\right) + \imath\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\left(\bar{R}_{k,\uparrow\downarrow} + \bar{R}_{k,\downarrow\uparrow}\right)\right\} * \Big[\,.. \quad + \text{h c}\Big] \\ &\left\{\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\left(\bar{R}_{k,\uparrow\downarrow} + \bar{R}_{k,\downarrow\uparrow}\right) + \imath\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\left(\bar{R}_{k,\uparrow\uparrow} + \bar{R}_{k,\downarrow\downarrow}\right)\right\} * \Big[\quad - \text{h c.}\Big] \end{aligned} \tag{5 8}$$

After a careful handling of the various trigonometric functions one finally ends up with the following set of equations.

$$
\begin{aligned}
\lambda\gamma_x^{nC} = \\
&- t\sum_{k=1}^{N}\sum_{\substack{A=1\\A\neq C}}^{M}\left\{\gamma_k^{nA*}\left(\gamma_{k+1}^{nA}\gamma_x^{nC}-\gamma_x^{nA}\gamma_{k+1}^{nC}\right)+\gamma_k^{nA*}\left(\gamma_{k-1}^{nA}\gamma_x^{nC}-\gamma_x^{nA}\gamma_{k-1}^{nC}\right)\right\}* \\
&\quad . .*\left\{\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\frac{\theta_k}{2}\cos\frac{\theta_{k+1}}{2}+\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\frac{\theta_k}{2}\sin\frac{\theta_{k+1}}{2}\cos(\zeta_k-\zeta_{k+1})\right. \\
&\quad\left.-\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\frac{\theta_k}{2}\sin\frac{\theta_{k+1}}{2}\sin\zeta_{k+1}+\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\frac{\theta_k}{2}\cos\frac{\theta_{k+1}}{2}\sin\zeta_k\right\} \\
&- t\sum_{k=1}^{N}\sum_{\substack{A=1\\A\neq C}}^{M}\mathrm{i}\left\{\gamma_k^{nA*}\left(\gamma_{k+1}^{nA}\gamma_x^{nC}-\gamma_x^{nA}\gamma_{k+1}^{nC}\right)-\gamma_k^{nA*}\left(\gamma_{k-1}^{nA}\gamma_x^{nC}-\gamma_x^{nA}\gamma_{k-1}^{nC}\right)\right\}*.. \\
&\quad *\left\{\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\frac{\theta_k}{2}\cos\frac{\theta_{k+1}}{2}+\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\frac{\theta_k}{2}\sin\frac{\theta_{k+1}}{2}\cos(\zeta_k-\zeta_{k+1})\right. \\
&\quad\left.+\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\frac{\theta_k}{2}\sin\frac{\theta_{k+1}}{2}\sin\zeta_{k+1}-\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\frac{\theta_k}{2}\cos\frac{\theta_{k+1}}{2}\sin\zeta_k\right\} \\
&- t\left(\gamma_{\tau+1}^{nC}+\gamma_{\tau-1}^{nC}\right)* \quad . \\
&\quad \ldots *\left\{\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\frac{\theta_x}{2}\cos\frac{\theta_{x+1}}{2}+\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\frac{\theta_x}{2}\sin\frac{\theta_{x+1}}{2}\cos(\zeta_x-\zeta_{x+1})\right. \\
&\quad\left.-\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\frac{\theta_x}{2}\sin\frac{\theta_{x+1}}{2}\sin\zeta_{x+1}+\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\frac{\theta_x}{2}\cos\frac{\theta_{x+1}}{2}\sin\zeta_x\right\} \\
&- t\,\mathrm{i}\left(\gamma_{\tau+1}^{nC}-\gamma_{\tau-1}^{nC}\right)*\ldots \\
&\quad . .*\left\{\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\frac{\theta_x}{2}\cos\frac{\theta_{x+1}}{2}+\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\frac{\theta_x}{2}\sin\frac{\theta_{x+1}}{2}\cos(\zeta_x-\zeta_{x+1})\right. \\
&\quad\left.+\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\frac{\theta_x}{2}\sin\frac{\theta_{x+1}}{2}\sin\zeta_{x+1}-\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\frac{\theta_x}{2}\cos\frac{\theta_{x+1}}{2}\sin\zeta_x\right\} \\
&+ \Delta_s\sum_{k=1}^{N}\sum_{\substack{A=1\\A\neq C}}^{M}\sin\theta_k\gamma_k^{nA*}\left(\gamma_k^{nA}\gamma_\tau^{nC}-\gamma_x^{nA}\gamma_k^{nC}\right)\cos\zeta_k \;+\; \Delta_s\sin\theta_\tau\gamma_\tau^{nC}\cos\zeta_\tau \\
&+ \frac{N}{U}\left(\Delta_c^2+\Delta_s^2\right)\gamma_x^{nC} \;-\; \mathrm{i}\Delta_c M\gamma_x^{nC} \qquad (5\,9)
\end{aligned}
$$

It might be necessary to add a couple of remarks on these equations As an expectation value of a hermitian operator one expects the energy to be a real value. Hence, it strikes that the imaginary unit i appears twice in the equation. However, this is not much of a problem, since the brackets behind it consist of a complex number and its complex conjugate (at least after a devision by γ_x^{nC}) A little bit more suspicious is the fact that the first of the interaction terms does not necessarily give a real number. This can for instance be seen in the case of Bloch waves below. Here the reason is that on the right hand side of the Hartree-Fock equations an expectation value is not really calculated An important fact is that the sum over τ is missing Only if the expressions become independent of x, if

proper solutions are found, this constraint vanishes

It shall be examined next whether Bloch wave functions and these Hartree-Fock equations go together. If the former are inserted into the latter one obtains expressions like

$$\gamma_k^{n_A*}\left(\gamma_{k+1}^{n_A}-\gamma_{k+1}^{n_C}\frac{\gamma_x^{n_A}}{\gamma_x^{n_C}}\right)+\text{h c} = \frac{2}{N}\left\{\cos\left(\frac{2\pi}{N}n_A\right)-\cos\left(\frac{2\pi}{N}n_C+\frac{2\pi}{N}(n_C-n_A)(k-x)\right)\right\}$$

$$\gamma_k^{n_A*}\left(\gamma_k^{n_A}-\gamma_k^{n_C}\frac{\gamma_x^{n_A}}{\gamma_x^{n_C}}\right) = \frac{2}{N}\left\{1-\cos\left(\frac{2\pi}{N}(n_C-n_A)(k-x)\right)-\dots\right.$$

$$\left.\dots-\text{i}\sin\left(\frac{2\pi}{N}(n_C-n_A)(k-x)\right)\right\}$$

which combine to the energy $E =$

$$-2t\sum_{\substack{A=1\\A\neq C}}^{M}\frac{1}{N}\sum_k\left[\cos\left(\frac{2\pi}{N}\left(n_A+\frac{\Phi}{\Phi_0}\right)\right)-\cos\left(\frac{2\pi}{N}\left(n_C+\frac{\Phi}{\Phi_0}+(n_C-n_A)(k-x)\right)\right)\right]*$$

$$.\quad *\left\{\cos\frac{\theta_k}{2}\cos\frac{\theta_{k+1}}{2}+\sin\frac{\theta_k}{2}\sin\frac{\theta_{k+1}}{2}\cos(\zeta_k-\zeta_{k+1})\right\}$$

$$-2t\cos\left(\frac{2\pi}{N}n_C\right)\left\{\cos\frac{\theta_x}{2}\cos\frac{\theta_{x+1}}{2}+\sin\frac{\theta_x}{2}\sin\frac{\theta_{x+1}}{2}\cos(\zeta_x-\zeta_{x+1})\right\}$$

$$+2t\sum_{\substack{A=1\\A\neq C}}^{M}\frac{1}{N}\sum_k\left[\sin\left(\frac{2\pi}{N}\left(n_A+\frac{\Phi}{\Phi_0}\right)\right)-\sin\left(\frac{2\pi}{N}\left(n_C+\frac{\Phi}{\Phi_0}+(n_C-n_A)(k-x)\right)\right)\right]*$$

$$..*\left\{\cos\frac{\theta_k}{2}\sin\frac{\theta_{k+1}}{2}\sin\zeta_{k+1}-\sin\frac{\theta_k}{2}\cos\frac{\theta_{k+1}}{2}\sin\zeta_k\right\}$$

$$+2t\sin\left(\frac{2\pi}{N}n_C\right)\left\{\cos\frac{\theta_x}{2}\sin\frac{\theta_{x+1}}{2}\sin\zeta_{x+1}-\sin\frac{\theta_x}{2}\cos\frac{\theta_{x+1}}{2}\sin\zeta_x\right\}$$

$$-\Delta_c\sum_{\substack{A=1\\A\neq C}}^{M}\sum_k\sin\theta_k\left\{\cos\left(\frac{2\pi}{N}(n_C-n_A)(k-x)\right)+\text{i}\sin\left(\frac{2\pi}{N}(n_C-n_A)(k-x)\right)\right\}\cos\zeta_k$$

$$+\Delta_c\frac{M-1}{N}\sum_k\sin\theta_k\cos\zeta_k+\Delta_s\sin\theta_x\cos\zeta_x$$

$$-\text{i}\Delta_c M+\frac{N}{U}\left(\Delta_c^2+\Delta_s^2\right) \qquad (3\,10)$$

For the case of an arbitrary rotation this expression can hardly be simplified further The fact that x and n_C appear several times indicates that Bloch wave functions are apparently not proper solution. One possibility of continuation could be to use them as an approximation and to minimize with respect to the mean fields Δ_c and Δ_s accordingly Another possibility, and this one has been chosen, is to reduce the size of the system For these simpler configurations it should be possible to construct the wave functions by hand with the hope to be able to generalize their solutions to larger systems.

5.2 Limited System Size

5.2.1 One Particle / One Site ($M = 1, N = 1$)

Whenever we have a situation with only one particle, sums of the form $\sum_{\substack{A=1 \\ A \neq C}}^{M}$ in the expression for the energy (5.9) disappear because of the constraint $A \neq C$. Furthermore, for the special case of $N = 1$ it is $\gamma_{k+1} = \gamma_{k-1} = \gamma_k = \gamma$ if we try to use again periodic boundary conditions[2]. The same is true for the angles θ_k and ζ_k. Thus, the only remaining term of the hopping part is

$$\begin{aligned} & -t\left(\gamma_{x+1}^{nc} + \gamma_{x-1}^{nc}\right) * \dots \\ & \quad * \left\{ \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \cos\frac{\theta_x}{2} \cos\frac{\theta_{x+1}}{2} + \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \sin\frac{\theta_x}{2} \sin\frac{\theta_{x+1}}{2} \cos(\zeta_x - \zeta_{x+1}) - \right. \\ & \quad \left. - \sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \cos\frac{\theta_x}{2} \sin\frac{\theta_{x+1}}{2} \sin\zeta_{x+1} + \sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \sin\frac{\theta_x}{2} \cos\frac{\theta_{x+1}}{2} \sin\zeta_x \right\} \\ = \; & -2t\gamma \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \end{aligned}$$

For the interaction part the symbols

$$\begin{aligned} a_k &= \Delta_s \sin\theta_k \cos\zeta_k \\ \text{and} \qquad E_F^{(M,N)} &= \frac{N}{U}\left(\Delta_c^2 + \Delta_s^2\right) - i\Delta_c M \end{aligned} \tag{5.11}$$

shall be introduced to simplify writing

Therefore, the complicated energy equation reduces in this case to

$$E\gamma = -2t\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\gamma + a_1\gamma + E_F^{(1,1)}\gamma \tag{5.12}$$

with the solutions

$$\boxed{\begin{aligned} E &= -2t\cos\left(2\pi\frac{\Phi}{\Phi_0}\right) + \Delta_s \sin\theta_1 \cos\zeta_1 - i\Delta_c + \frac{1}{U}\left(\Delta_c^2 + \Delta_s^2\right) \\ \gamma &= e^{i\chi} \end{aligned}} \tag{5.13}$$

where χ can be an arbitrary phase

[2]The upper index for the quantum number is omitted because only one number appears

A saddle point approximation in the charge mean fields is achieved for $\Delta_{c,0} = \frac{iU}{2}$ For the spin mean field it depends on the angles The absolute minimum corresponds to $\theta_1 = \frac{\pi}{2}, \zeta_1 = 0$ and $\Delta_{s,0} = -\frac{U}{2}$. This choice, which is by the way identical to former consideration on page 87 (half-filling), has the effect that the two contributions cancel each other Only the term proportional to t remains for the energy This is the correct result because for one particle there should not be any interaction

5.2.2 One Particle / Two Sites ($M = 1, N = 2$)

Even here it is $\gamma_{x+1} = \gamma_{x-1}$ for $x = 1, 2$ because of the periodic boundary conditions A closer look at the hopping terms

$$
\begin{aligned}
x = 1 \quad & -2t\gamma_2 \left\{ \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \cos\frac{\theta_1}{2}\cos\frac{\theta_2}{2} + \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\cos(\zeta_1 - \zeta_2) - \right. \\
& \left. - \sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \cos\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\sin\zeta_2 + \sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \sin\frac{\theta_1}{2}\cos\frac{\theta_2}{2}\sin\zeta_1 \right\} \\
x = 2 \cdot \quad & -2t\gamma_1 \left\{ \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \cos\frac{\theta_2}{2}\cos\frac{\theta_1}{2} + \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \sin\frac{\theta_2}{2}\sin\frac{\theta_1}{2}\cos(\zeta_2 - \zeta_1) - \right. \\
& \left. - \sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \cos\frac{\theta_2}{2}\sin\frac{\theta_1}{2}\sin\zeta_1 + \sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) \sin\frac{\theta_2}{2}\cos\frac{\theta_1}{2}\sin\zeta_2 \right\}
\end{aligned}
$$

shows that variables w_1 and w_2 can be introduced such that the terms can be written in the form

$$
\begin{aligned}
x = 1 \quad & -2t\gamma_2 (w_1 + w_2) \\
x = 2 \quad . \quad & -2t\gamma_1 (w_1 - w_2)
\end{aligned}
\tag{5 14}
$$

which is based on the fact that in (5 8)

$$\bar{R}_{1,\uparrow\uparrow} = \bar{R}_{2,\downarrow\downarrow}, \quad \bar{R}_{1,\downarrow\downarrow} = \bar{R}_{2,\uparrow\uparrow}, \quad \bar{R}_{1,\uparrow\downarrow} = -\bar{R}_{2,\downarrow\uparrow}, \quad \bar{R}_{1,\downarrow\uparrow} = -\bar{R}_{2,\uparrow\downarrow}$$

Then for this particular case the following system of equations in γ has to be solved

$$
\begin{aligned}
\left(E - a_1 - E_F^{(1,2)}\right)\gamma_1 \; + \; & 2t\,(w_1 + w_2)\,\gamma_2 \; = \; 0 \\
2t\,(w_1 - w_2)\,\gamma_1 \; + \; & \left(E - a_2 - E_F^{(2,1)}\right)\gamma_2 \; = \; 0
\end{aligned}
\tag{5 15}
$$

Apart from the trivial solution $\gamma_1 = \gamma_2 = 0$, which contradicts normalization conditions, the only possibility to obtain further solutions is that

$$
0 \; = \; \det \begin{pmatrix} E - a_1 - E_F^{(1,2)} & 2t\,(w_1 + w_2) \\ 2t\,(w_1 - w_2) & E - a_2 - E_F^{(1,2)} \end{pmatrix}
$$

$$
\begin{aligned}
\Longleftrightarrow \quad 0 &= E^2 - E(2E_F^{(1,2)} + a_1 + a_2) + (E_F^{(1,2)} + a_1)(E_F^{(1,2)} + a_2) - 4t^2\left(w_1^2 - w_2^2\right) \\
\Longrightarrow E_{\mathrm{I,II}} &= \frac{1}{2}\Big(2E_F^{(1,2)} + a_1 + a_2 \pm \sqrt{(2E_F^{(1,2)} + a_1 + a_2)^2 - \ .} \\
&\qquad\qquad \overline{\ldots - 4(E_F^{(1,2)} + a_1)(E_F^{(1,2)} + a_2) + 16t^2\left(w_1^2 - w_2^2\right)}\Big) \\
&= \frac{1}{2}\left(2E_F^{(1,2)} + a_1 + a_2 \pm \sqrt{(a_2 - a_1)^2 + 16t^2\left(w_1^2 - w_2^2\right)}\right)
\end{aligned}
$$

If one puts this result into the first or the second of the equations (5 15) one can obtain a relation between γ_1 and γ_2 which together with the normalization condition determines the wave function

$$
\begin{aligned}
\Longrightarrow \quad \gamma_1 &= \frac{4t\,(w_1 + w_2)\,\gamma_2}{(a_1 - a_2) \mp \sqrt{(a_1 - a_2)^2 + 16t^2\left(w_1^2 - w_2^2\right)}} = r_{\mathrm{I,II}}\,\gamma_2 \\
\Longleftrightarrow \quad \gamma_1 &= \frac{(a_1 - a_2) \pm \sqrt{(a_1 - a_2)^2 + 16t^2\left(w_1^2 - w_2^2\right)}}{4t\,(w_2 - w_1)}\,\gamma_2 = r_{\mathrm{I,II}}\,\gamma_2
\end{aligned}
\tag{5 16}
$$

Together with $1 = \gamma_1\gamma_1^* + \gamma_2\gamma_2^* = \left(1 + r_{\mathrm{I,II}}^2\right)\gamma_2\gamma_2^*$ this leads to the following solution:

$$
\boxed{
\begin{gathered}
E_{\mathrm{I,II}} = \frac{1}{2}\left(a_1 + a_2 \pm \sqrt{(a_1 - a_2)^2 + 16t^2\left(w_1^2 - w_2^2\right)}\right) - \mathrm{i}\Delta_c + \frac{2}{U}\left(\Delta_c^2 + \Delta_s^2\right) \\
\gamma_1^{\mathrm{I,II}} = \frac{r_{\mathrm{I,II}}}{\sqrt{1 + r_{\mathrm{I,II}}^2}}\,\mathrm{e}^{\mathrm{i}\chi^{\mathrm{I,II}}}, \quad \gamma_2^{\mathrm{I,II}} = \frac{1}{\sqrt{1 + r_{\mathrm{I,II}}^2}}\,\mathrm{e}^{\mathrm{i}\chi^{\mathrm{I\,II}}}
\end{gathered}
}
\tag{5 17}
$$

Again the wave functions include an arbitrary phase χ It is not very helpful to give an extended version (without auxiliary variables) for the energy because the expression would be too complicated. Nevertheless, one can mention some interesting points which are connected to the structure of the solution for the wave functions

1. The ratio of γ_1 and γ_2 is apparently of particular interest for the wave function. Since it does not include the variable $E_F^{(1,2)}$, the wave functions apparently does not depend on the mean field associated with the charge degree of freedom. This is reasonable, because the total number of particles

and hence the the total charge is assumed to be fixed within the model under consideration

2 What is less understandable is the fact that the qualitative difference between the two possible solutions I and II is also independent of the mean field associated with the spin degree of freedom. In the product

$$r_{\mathrm{I}} \cdot r_{\mathrm{II}} = -\frac{w_1 + w_2}{w_1 - w_2} = \frac{\gamma_1^{\mathrm{I}}}{\gamma_2^{\mathrm{I}}} \frac{\gamma_1^{\mathrm{II}}}{\gamma_2^{\mathrm{II}}}$$

only quantities related to the hopping part appear.

3 There exist some special situations for the solutions of the wave function

two equal solutions	$\gamma^{\mathrm{I}} \equiv \gamma^{\mathrm{II}}$	$\Longleftrightarrow$	$0 \overset{!}{=} (a_2 - a_1)^2 + 16t^2 (w_1^2 - w_2^2)$
mirrored solutions:	$\frac{\gamma_1^{\mathrm{I}}}{\gamma_2^{\mathrm{I}}} = \frac{\gamma_2^{\mathrm{II}}}{\gamma_1^{\mathrm{II}}}$	$\Longleftrightarrow$	$0 \overset{!}{=} w_1$
equal distribution:	$\lvert\gamma_1\rvert^2 = \lvert\gamma_2\rvert^2$	$\Longleftrightarrow$	$(a_1 - a_2) \overset{!}{=} \pm 4t\, w_2$
localized solutions:	$\gamma_1 = 0$	$\Longrightarrow$	$w_1 = -w_2 \wedge E = a_2 + E_F^{(1,2)}$
	$\gamma_2 = 0$	$\Longrightarrow$	$w_1 = w_2 \wedge E = a_1 + E_F^{(1,2)}$

In the last situation the interaction energy is that of the 1 particle / 1 site problem This is not the case for the kinetic energy, because even if not occupied the hopping "feels" the existence of adjacent sites Only if both sites were identical, $\Omega_1 = \Omega_2$, then also the kinetic energy would have the value of the previous case.

4 If the magnetic flux is close to half a flux quantum, the expression under the square root

$$\sqrt{(a_1 - a_2)^2 + 16t^2 (w_1^2 - w_2^2)}$$

can become negative, since in this region w_2 might be greater than w_1 Not only does this lead to complex energy values, it might also have the effect of diverging expressions for the components of the wave function The most likely conclusion is that certain[3] configurations are simply forbidden

[3]This term "certain" is difficult to specify, because already for two sites the equations are too complex Nevertheless, one can say that for $\zeta_1 = \zeta_2 \approx 0$ no difficulties appear

Based on these statements one could try to investigate the dependence of the system on the external flux. There are two possible approaches One is to fix a certain spin configuration and to study how the wave function alters if the magnetic field is changed The flux dependence is mainly determined by the two variables

$$\begin{aligned} w_1 &= \cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\left\{\cos\frac{\theta_1}{2}\cos\frac{\theta_2}{2}+\sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\cos(\zeta_1-\zeta_2)\right\} \quad \text{and} \\ w_2 &= \sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\left\{\sin\frac{\theta_1}{2}\cos\frac{\theta_2}{2}\sin\zeta_1-\cos\frac{\theta_1}{2}\sin\frac{\theta_2}{2}\sin\zeta_2\right\}. \end{aligned} \tag{5 18}$$

Therefore, one can observe that the probability of the particle to be on site 1 or on site 2 changes periodically Depending on the parameters, it can happen that the particle can for some values of Φ only be found on one site With increasing flux it then moves to the other site until the flux is again large enough for a preference of the first site. A continuous increase of the flux, therefore, leads to an oscillation in the particle distribution

A more accurate approach does not *a priori* fix a certain set of angles On the contrary, it is supposed that the spin structure is determined by the external magnetic field Whenever a non-zero flux appears, θ_k and ζ_k are chosen in such a way that the total energy becomes a minimum Therefore, the angles might be a function of Φ A trial to obtain a minimization with the help of derivatives leads to long, cumbersome equations Thus, a qualitative discussion of the energy is necessary

If one starts such a discussion with the case $\zeta_1 = \zeta_2 = 0$ and $\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) = 0$ then the minimal energy is determined by

$$E_{\parallel} = \frac{1}{2}\left(a_1 + a_2 - |a_1 - a_2|\right) + E_{\Gamma}^{(1,2)}; \qquad a_k = \Delta_s \sin\theta_k$$

For both of the possibilities $a_1 < a_2$ and $a_1 > a_2$ only one angle remains Hence, it is without loss of generality sufficient to perform a minimization of a_1 with respect to θ_1, because then $a_1 < a_2$ is automatically fulfilled. The result of this minimization is $\theta_1 = \frac{3\pi}{2}$ The next two steps are to drop first of all the constraint $\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) = 0$ and two allow later non-zero values $\zeta_1 = \zeta_2 = \zeta$ Looking at the energy

$$E_{\text{II}} = \frac{1}{2}\Delta_s(\sin\theta_1+\sin\theta_2)\cos\zeta - \frac{1}{2}\sqrt{\Delta_s^2(\sin\theta_1-\sin\theta_2)^2\cos^2\zeta + 16t^2\cos^2\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos^2\left(\frac{\theta_1}{2}-\frac{\theta_2}{2}\right) - \ldots \overline{\ldots - 16t^2\sin^2\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin^2\left(\frac{\theta_1}{2}-\frac{\theta_2}{2}\right)\sin^2\zeta}} + E_F^{(1,2)},$$

one can see that the flux minimizes the energy even further and most of all if $\theta_1 = \theta_2$. On the other hand, the ζ angle leads to an increase in the energy because $|\cos\zeta| \leq 1$ and because of the minus sign in front of $\sin^2\zeta$. This is less apparent but also true for $\zeta_1 \neq \zeta_2$.

Hence, to choose θ_k and ζ_k in such a way that the total energy becomes a minimum means to have

$$\theta_1 = \theta_2 = \frac{3\pi}{2};\quad \zeta_1 = \zeta_2 = 0 \qquad \Longleftrightarrow \qquad \theta_1 = \theta_2 = \frac{\pi}{2};\quad \zeta_1 = \zeta_2 = \pi.$$

This result leads flux-independently to the energy

$$E = -\Delta_s - 2t\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right) - \mathrm{i}\Delta_c + \frac{2}{U}\left(\Delta_c^2+\Delta_s^2\right). \tag{5.19}$$

Furthermore, the saddle point for the mean fields is $\Delta_{c,0} = \frac{\mathrm{i}U}{4}$ and $\Delta_{s,0} = \frac{U}{4}$. It leads, similarly to the previous case, to the non-interaction energy $E = -2t\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)$.

5.2.3 Two Particles / Two Sites ($M = 2, N = 2$)

The previous two cases were not very interesting because the existence of only one particle does not allow any interaction. This is different for the situation which is now under consideration. Therefore, it is also not possible to combine the solutions for one particle to a solution for two particles. By calling

$$\gamma_x^{nC} =: \gamma_x \quad \text{and} \quad \gamma_x^{n\downarrow} = \beta_x$$

one obtains from (5.9) the following general equation

$$\begin{aligned} E\gamma_x = &- t\left[2\beta_1^*(\beta_2\gamma_x - \beta_x\gamma_2)(w_1+w_2) + 2\beta_2^*(\beta_1\gamma_x - \beta_x\gamma_1)(w_1-w_2)\right] \\ &- t(\gamma_{x+1}+\gamma_{x-1})(w_1 \pm w_2) \\ &+ a_1\beta_1^*(\beta_1\gamma_x - \beta_x\gamma_1) + a_2\beta_2^*(\beta_2\gamma_x - \beta_x\gamma_2) + a_x\gamma_x + E_F^{(2,2)}\gamma_x \end{aligned}$$

which leads to the set of equations

$$\begin{aligned} x=1: \quad 0 &= \gamma_1\left[-2t\beta_1^*\beta_2(w_1+w_2)+\beta_2^*\beta_2 a_2+a_1+E_F^{(2,2)}-E\right] \\ &+ \gamma_2\left[+2t\beta_1^*\beta_1(w_1+w_2)-2t(w_1+w_2)-\beta_2^*\beta_1 a_2\right] \\ x=2: \quad 0 &= \gamma_1\left[+2t\beta_2^*\beta_2(w_1-w_2)-2t(w_1-w_2)-\beta_1^*\beta_2 a_1\right] \\ &+ \gamma_2\left[-2t\beta_2^*\beta_1(w_1-w_2)+\beta_1^*\beta_1 a_1+a_2+E_F^{(2,2)}-E\right] \end{aligned} \tag{5 20}$$

Provided that the two wave functions γ, β are distinct, the existence of a non-trivial solution is equivalent to the condition

$$\begin{aligned} 0 &= \left[-2t\beta_1^*\beta_2(w_1+w_2)+\beta_2^*\beta_2 a_2+a_1+E_F^{(2,2)}-E\right]*\ldots \\ &\quad *\left[-2t\beta_2^*\beta_1(w_1-w_2)+\beta_1^*\beta_1 a_1+a_2+E_F^{(2,2)}-E\right] \\ &- \left[+2t\beta_2^*\beta_2(w_1+w_2)+\beta_2^*\beta_1 a_2\right]*\left[+2t\beta_1^*\beta_1(w_1-w_2)+\beta_1^*\beta_2 a_1\right], \end{aligned}$$

for which also the normalization condition $|\beta_1|^2+|\beta_2|^2=1$ is used twice. If one multiplies these brackets it turns out that many terms cancel each other leaving the following equation for discussion

$$\begin{aligned} 0 = &- 2t\beta_1^*\beta_2(w_1+w_2)(a_1+a_2+E_F^{(2,2)}-E) \\ &- 2t\beta_2^*\beta_1(w_1-w_2)(a_1+a_2+E_F^{(2,2)}-E) \\ &+ |\beta_1|^2 a_1(a_1+E_F^{(2,2)}-E) \;+\; |\beta_2|^2 a_2(a_2+E_F^{(2,2)}-E) \\ &+ (a_1+E_F^{(2,2)}-E)(a_2+E_F^{(2,2)}-E) \end{aligned} \tag{5 21}$$

Just looking at the imaginary part of equation (5 21), one has to deal with

$$\begin{aligned} 0 = &- 2t\,\mathrm{Im}\,(\beta_1^*\beta_2)\,(w_1+w_2)(a_1+a_2+E_F^{(2,2)}-E) \\ &- 2t\,\mathrm{Im}\,(\beta_2^*\beta_1)\,(w_1-w_2)(a_1+a_2+E_F^{(2,2)}-E) \\ \Longleftrightarrow \quad 0 = &\quad 2t\,\mathrm{Im}\,(\beta_1^*\beta_2)\,w_2\,(a_1+a_2+E_F^{(2,2)}-E) \end{aligned} \tag{5 22}$$

The equality is satisfied if one of the factors is zero. That leaves the possibilities that there is no phase difference between β_1 and β_2, that a special spin configuration is realized or that the energy has a certain value. The statement about the energy is of particular interest, and used for (5 21):

$$0 = |\beta_1|^2 a_1(-a_2)+|\beta_2|^2 a_2(-a_2)+(-a_1)(-a_2)$$

one can see that $E_{\rm I} = a_1 + a_2 + E_F^{(2,2)}$ is also a solution for the whole equation.

This result makes it much easier to find also the second energy solution of the quadratic equation (5 21), written in the form

$$\begin{aligned} 0 &= (E - E_F^{(2,2)})^2 + (E - E_F^{(2,2)})\Big[2t\beta_1^*\beta_2(w_1 + w_2) + 2t\beta_2^*\beta_1(w_1 - w_2) - . \\ &\qquad \ldots - |\beta_1|^2 a_1 - |\beta_2|^2 a_2 - (a_1 + a_2)\Big] + \Big\{\ldots\Big\} \end{aligned}$$

$\Longrightarrow$

$$\Big[\ .\Big] = -(E_{\rm I} - E_F^{(2,2)}) - (E_{\rm II} - E_\Gamma^{(2,2)}) = E_F^{(2,2)} - (a_1 + a_2) - E_{\rm II}$$

Hence, the two solutions for the energy are

$$\boxed{\begin{aligned} E_{\rm I} &= a_1 + a_2 + E_F^{(2,2)} \\ E_{\rm II} &= 2t\beta_1^*\beta_2(w_1 + w_2) + 2t\beta_2^*\beta_1(w_1 - w_2) - |\beta_1|^2 a_1 - |\beta_2|^2 a_2 + E_\Gamma^{(2,2)} \end{aligned}} \qquad (5\ 23)$$

The next step is to determine the wave functions belonging to these energies If the obtained energies are plugged into the equations (5 2 3) one ends up with two (per construction dependent) equations For $E = E_{\rm I}$ it is not difficult to see that they are fulfilled for

$$\beta_1 = \beta_2 = \frac{1}{\sqrt{2}}\,e^{i\chi_1} \quad \text{and} \quad \gamma_1 = -\gamma_2 = \frac{1}{\sqrt{2}}\,e^{i\chi_2} \qquad (5.24)$$

or vice versa

For $E = E_{\rm II}$ the situation is much more difficult. Looking back at the discussion of equation (5 22) one can conclude that in this case there is no phase difference between β_1 and β_2, provided that not a special spin configuration is realized such that $w_2 = 0$ Without loss of generality one can therefore assume that the components of β (and γ) are real. Then the equations (5 2 3) can be written as

$$\begin{aligned} \gamma_1\left[2t\beta_1(w_1 - w_2) + \beta_2 a_1\right] &= \gamma_2\left[2t\beta_2(w_1 + w_2) + \beta_1 a_2\right] \quad \text{and accordingly} \\ \beta_1\left[2t\gamma_1(w_1 - w_2) + \gamma_2 a_1\right] &= \beta_2\left[2t\gamma_2(w_1 + w_2) + \gamma_1 a_2\right], \end{aligned} \qquad (5\ 25)$$

where it has been used that non of the components is zero Together with the normalization conditions one now has four independent equations which can be

combined in various ways. Eventually, all these possibilities lead to the same quadratic equations, which are:

$$0 = z^2\left[16t^2w_1^2 + (a_1 - a_2)^2\right] - z\left[16t^2w_1(w_1 + w_2) + (a_1 - a_2)^2\right] + 4t^2(w_1 + w_2)^2$$
$$0 = \tilde{z}^2\left[16t^2w_1^2 + (a_1 - a_2)^2\right] - \tilde{z}\left[16t^2w_1(w_1 - w_2) + (a_1 - a_2)^2\right] + 4t^2(w_1 - w_2)^2$$

Here, z represents β_1^2 or γ_1^2, and $\tilde{z}$ stands for β_2^2 or γ_2^2.

The solutions of these equations are

$$z_\pm = \frac{1}{2}\left\{1 + \frac{16t^2w_1w_2}{p} \pm \sqrt{1 + \frac{(16t^2w_1^2)\cdot(16t^2w_2^2)}{p^2} - \frac{(16t^2w_1^2) + (16t^2w_2^2)}{p}}\right\}$$
$$\tilde{z}_\pm = \frac{1}{2}\left\{1 - \frac{16t^2w_1w_2}{p} \pm \sqrt{1 + \frac{(16t^2w_1^2)\ (16t^2w_2^2)}{p^2} - \frac{(16t^2w_1^2) + (16t^2w_2^2)}{p}}\right\}$$
$$\left(p = 16t^2w_1^2 + (a_1 - a_2)^2\right) \qquad (5\ 26)$$

They have the wanted property $z_+ + \tilde{z}_- = 1 = z_- + \tilde{z}_+$ Which allows the combinations

$$\left[\beta_1 = \sqrt{z_+} \wedge \beta_2 = \sqrt{\tilde{z}_-}\right] \quad \text{or} \quad \left[\beta_1 = \sqrt{z_-} \wedge \beta_2 = \sqrt{\tilde{z}_+}\right] \qquad (5.27)$$

and similarly for γ However, during the process of transforming (5 25) to the quadratic form the whole equation has to be squared once Since this is not an equivalent transformation, not all of the suggest solutions really have to fulfill (5 25) A thorough investigation into this question has been done, but is not worth repeating because of even bigger problems mentioned in the next section.

5.3 More Appropriate States

5.3.1 The Problem of Orthogonality

Looking back at the problem of 1 particle / 2 sites, we had in (5 17) two different solutions γ^{I} and γ^{II} for the wave function These two wave functions are not necessarily orthogonal On the contrary,

$$\gamma_1^{\mathrm{I}}\gamma_1^{\mathrm{II}} + \gamma_2^{\mathrm{I}}\gamma_2^{\mathrm{II}} = \frac{1 + r_{\mathrm{I}}\ r_{\mathrm{II}}}{\sqrt{1 + r_{\mathrm{I}}^2}\sqrt{1 + r_{\mathrm{II}}^2}} = \frac{1}{\sqrt{1 + r_{\mathrm{I}}^2}\sqrt{1 + r_{\mathrm{II}}^2}}\ \frac{2w_2}{w_2 - w_1} \qquad (5\ 28)$$

and orthogonality is only satisfied if $w_2 = 0$ In this special case, which is for instance fulfilled if $\zeta_1 = \zeta_2 = 0$, the solutions are identical with those of the 2 particles / 2 sites problem because

$$r_{\mathrm{I,II}}^{\lambda} = \frac{16t^2w_1^2}{\left(\sqrt{16t^2w_1^2 + (a_1 - a_2)^2} \mp (a_1 - a_2)\right)^2} = \frac{\sqrt{16t^2w_1^2 + (a_1 - a_2)^2} \pm (a_1 - a_2)}{\sqrt{16t^2w_1^2 + (a_1 - a_2)^2} \mp (a_1 - a_2)} = \frac{z_{\pm}}{\tilde{z}_{\mp}}.$$

For all other angle configurations our Hartree-Fock calculations for the 1 particle problem do not lead to two orthogonal solutions Hence, attempts to obtain a solution for the 2 particle problem which consist of a combination of two orthogonal wave functions are also very likely to fail

Therefore, we have to reconsider the strategy for the choice of the states In the preceding calculations the more general two-body state

$$|\psi\rangle_{n_1,n_2} = \frac{1}{2}\sum_{i_1,i_2}\sum_{\sigma_1,\sigma_2}\gamma_{i_1,i_2}^{n_1,n_2}c_{i_1,\sigma_1}^{\dagger}c_{i_2,\sigma_2}^{\dagger}|0\rangle$$

has, in a kind of separation *ansatz*, been split in the form

$$|\psi\rangle_{n_1,n_2} = \frac{1}{2}\sum_{i_1,i_2}\sum_{\sigma_1,\sigma_2}\gamma_{i_1}^{n_1}\gamma_{i_2}^{n_2}c_{i_1,\sigma_1}^{\dagger}c_{i_2,\sigma_2}^{\dagger}|0\rangle$$

If this step together with the normalization condition $\sum_i |\gamma_i^n|^2 = 1$ and the orthogonality constraint $\sum_i \gamma_i^{n_1}\gamma_i^{n_2} = 0$ for $n_1 \neq n_2$ is performed, one has two independently behaving particles in mind However, this is not a useful concept in the case that there is an interaction between particles. Due to the interaction there might appear new energy levels which are not simple combinations of the energies of single particles The wave function needs to be treated as a many-body problem

The solutions for the 2 particles / 2 sites problem on page 121 cannot be used because they are in general not orthogonal and, thus, contradict an assumption which is apparently wrong. It is necessary to forget about the orthogonality constraint and to perform the calculations again That means that the evaluation of the Hamiltonian (5 5) has to be altered, and consequently, a more general expression for the Hartree-Fock equation (5 9) has to be found.

For the expectation value of a typical operator without using orthogonality a compact notation shall be used It arises naturally when such operator chains

are fully contracted and makes use of an auxiliary quantum number n_0 for which the wave function is $\gamma_i^{n_0} = \delta_{i,k}$. Then

$$
\begin{aligned}
&{}_{n_1,\ \ ,n_M}\langle\psi|\tilde{c}^{\dagger}_{k,\uparrow}\tilde{c}_{k+1,\downarrow}|\psi\rangle_{n_1,\ \ ,n_M} \\
&\quad = \frac{1}{2}\sum_{j_1,\ \ ,j_M}\sum_{\wp\in\mathcal{P}(M+1)}^{\wp(0)\neq 0}(-1)^{\mathrm{sgn}\wp+1}\gamma_{j_1}^{n_1*}\cdots\gamma_{j_M}^{n_{M}*}\gamma_{j_1}^{n_{\wp(1)}}\cdot\ \ \gamma_{j_M}^{n_{\wp(M)}}\gamma_{k+1}^{n_{\wp(0)}} \\
&\frac{\partial}{\partial\gamma_\tau^{n_C*}}\left({}_{n_1,\ \ ,n_M}\langle\psi|\sum_{k=1}^{N}\tilde{c}^{\dagger}_{k,\uparrow}\tilde{c}_{k+1,\downarrow}|\psi\rangle_{n_1,\ \ ,n_M}\right) \\
&\quad = \frac{1}{2}\sum_{k=1}^{N}\sum_{j_1,\ \ ,j_M}^{j_C=\tau}\sum_{\wp\in\mathcal{P}(M+1)}^{\wp(0)\neq 0}(-1)^{\mathrm{sgn}\wp+1}\gamma_{j_1}^{n_1*}\cdot\cdot\ \widehat{\gamma_{j_C}^{n_C}}^{*}\cdot\ \ \gamma_{j_M}^{n_M*}\gamma_{j_1}^{n_{\wp(1)}}\cdot\cdot\ \gamma_{j_M}^{n_{\wp(M)}}\gamma_{k+1}^{n_{\wp(0)}} \\
&\quad = \frac{1}{2}\sum_{4=1}^{M}\sum_{j_1,\ \ ,j_M}^{j_C=x}\sum_{\wp\in\mathcal{P}(M)}(-1)^{\mathrm{sgn}\wp}\gamma_{j_1}^{n_1*}\cdot\ \ \widehat{\gamma_{j_C}^{n_C}}^{*}\cdot\ \cdot\gamma_{j_M}^{n_M*}\gamma_{j_1}^{n_{\wp(1)}}\ \cdot\ \gamma_{j_4+1}^{n_{\wp(4)}}\cdot\ \ \gamma_{j_M}^{n_{\wp(M)}}
\end{aligned}
$$

and the sum over all permutations cannot be reduced further

Hence the γ-problem has a much more complicated structure than (5 9)[4].

$$
\begin{aligned}
&E\sum_{j_1,\ \ ,j_M}^{j_C=\tau}\sum_{\wp\in\mathcal{P}(M)}(-1)^{\mathrm{sgn}\wp}\gamma_{j_1}^{n_1*}\cdot\ \cdot\widehat{\gamma_{j_C}^{n_C}}^{*}\ \ \gamma_{j_M}^{n_M*}\gamma_{j_1}^{n_{\wp(1)}}\ \cdot\ \gamma_{j_M}^{n_{\wp(M)}} = \\
&-t\sum_{k=1}^{\Lambda}\sum_{j_1,\ \ ,j_M}^{j_C=\iota}\sum_{\wp\in\mathcal{P}(M+1)}^{\wp(0)\neq 0}(-1)^{\mathrm{sgn}\wp+1}\gamma_{j_1}^{n_1*}\ \ \cdot\widehat{\gamma_{j_C}^{n_C}}^{*}\cdot\ \ \gamma_{j_M}^{n_M*}\gamma_{j_1}^{n_{\wp(1)}}\cdot\ \ \gamma_{j_M}^{n_{\wp(M)}}\left(\gamma_{k+1}^{n_{\wp(0)}}+\gamma_{k-1}^{n_{\wp(0)}}\right) \\
&\quad *\left\{\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\frac{\theta_k}{2}\cos\frac{\theta_{k+1}}{2}+\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\frac{\theta_k}{2}\sin\frac{\theta_{k+1}}{2}\cos(\zeta_k-\zeta_{k+1})-\right. \\
&\quad\left.-\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\frac{\theta_k}{2}\sin\frac{\theta_{k+1}}{2}\sin\zeta_{k+1}+\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\frac{\theta_k}{2}\cos\frac{\theta_{k+1}}{2}\sin\zeta_k\right\} \\
&-it\sum_{k=1}^{N}\sum_{j_1,\ \ ,j_M}^{j_C=\tau}\sum_{\wp\in\mathcal{P}(M+1)}^{\wp(0)\neq 0}(-1)^{\mathrm{sgn}\wp+1}\gamma_{j_1}^{n_1*}\ \cdot\ \widehat{\gamma_{j_C}^{n_C}}^{*}\ \ \gamma_{j_M}^{n_M*}\gamma_{j_1}^{n_{\wp(1)}}\ \ \gamma_{j_M}^{n_{\wp(M)}}\left(\gamma_{k+1}^{n_{\wp(0)}}-\gamma_{k-1}^{n_{\wp(0)}}\right) \\
&\quad *\left\{\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\frac{\theta_k}{2}\cos\frac{\theta_{k+1}}{2}+\sin\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\frac{\theta_k}{2}\sin\frac{\theta_{k+1}}{2}\cos(\zeta_k-\zeta_{k+1})-\right. \\
&\quad\left.+\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\cos\frac{\theta_k}{2}\sin\frac{\theta_{k+1}}{2}\sin\zeta_{k+1}-\cos\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\sin\frac{\theta_k}{2}\cos\frac{\theta_{k+1}}{2}\sin\zeta_k\right\} \\
&+\Delta_s\sum_{k=1}^{N}\sum_{j_1,\ \ ,j_M}^{j_C=\tau}\sum_{\wp\in\mathcal{P}(M+1)}^{\wp(0)\neq 0}(-1)^{\mathrm{sgn}\wp}\gamma_{j_1}^{n_1*}\ \cdot\ \widehat{\gamma_{j_C}^{n_C}}^{*}\ \cdot\ \gamma_{j_M}^{n_M*}\gamma_{j_1}^{n_{\wp(1)}}\ \ \cdot\gamma_{j_M}^{n_{\wp(M)}}\gamma_{k}^{n_{\wp(0)}}\sin\theta_k\cos\zeta_k \\
&-i\Delta_c\sum_{k=1}^{N}\sum_{j_1,\ \ ,j_M}^{j_C=\iota}\sum_{\wp\in\mathcal{P}(M+1)}^{\wp(0)\neq 0}(-1)^{\mathrm{sgn}\wp+1}\gamma_{j_1}^{n_1*}\ \ \cdot\widehat{\gamma_{j_C}^{n_C}}^{*}\cdot\ \gamma_{j_M}^{n_M*}\gamma_{j_1}^{n_{\wp(1)}}\ \ \gamma_{j_M}^{n_{\wp(M)}}\gamma_{k}^{n_{\wp(0)}} \\
&+\frac{N}{U}\left(\Delta_c^2+\Delta_s^2\right)\sum_{j_1,\ \ ,j_M}^{j_C=\tau}\sum_{\wp\in\mathcal{P}(M)}(-1)^{\mathrm{sgn}\wp}\gamma_{j_1}^{n_1*}\ \ \widehat{\gamma_{j_C}^{n_C}}^{*}\ \ \gamma_{j_M}^{n_M*}\gamma_{j_1}^{n_{\wp(1)}}\ \ \gamma_{j_M}^{n_{\wp(M)}} \qquad (5\ 29)
\end{aligned}
$$

[4] If in the following sums $\wp(C) = 0$ then $\delta_{\iota_C,k}$ appears, which together with $\delta_{\iota_C\ x}$ leads via $\delta_{x\ k}$ to the effect that the sum over k vanishes and that all angles have the index x

For the special case of 2 particles these rather difficult equations can be reduced to the less cumbersome expression ($C = 2$).

$$
\begin{aligned}
& E \sum_{j_1=1}^{N} \gamma_{j_1}^{n_1 *} \left\{ \gamma_{j_1}^{n_1} \gamma_x^{n_C} - \gamma_{j_1}^{n_C} \gamma_x^{n_1} \right\} = \\
& - t \sum_{k=1}^{N} \sum_{j_1=1}^{N} \gamma_{j_1}^{n_1 *} \left\{ \gamma_{j_1}^{n_1} \gamma_x^{n_0} \left(\gamma_{k+1}^{n_C} + \gamma_{k-1}^{n_C} \right) - \gamma_{j_1}^{n_C} \gamma_x^{n_0} \left(\gamma_{k+1}^{n_1} + \gamma_{k-1}^{n_1} \right) - \cdot \cdot \right. \\
& \qquad \left. \cdot \cdot - \gamma_{j_1}^{n_0} \gamma_x^{n_1} \left(\gamma_{k+1}^{n_C} + \gamma_{k-1}^{n_C} \right) + \gamma_{j_1}^{n_0} \gamma_x^{n_C} \left(\gamma_{k+1}^{n_1} + \gamma_{k-1}^{n_1} \right) \right\} \left\{ \cos\left(\frac{2\pi}{N} \frac{\Phi}{\Phi_0} \right) \cdot \right\} \\
& - \imath t \sum_{k=1}^{N} \sum_{j_1=1}^{N} \gamma_{j_1}^{n_1 *} \left\{ \gamma_{j_1}^{n_1} \gamma_x^{n_0} \left(\gamma_{k+1}^{n_C} - \gamma_{k-1}^{n_C} \right) - \gamma_{j_1}^{n_C} \gamma_x^{n_0} \left(\gamma_{k+1}^{n_1} - \gamma_{k-1}^{n_1} \right) - \cdot \right. \\
& \qquad \left. \cdots - \gamma_{j_1}^{n_0} \gamma_x^{n_1} \left(\gamma_{k+1}^{n_C} - \gamma_{k-1}^{n_C} \right) + \gamma_{j_1}^{n_0} \gamma_x^{n_C} \left(\gamma_{k+1}^{n_1} - \gamma_{k-1}^{n_1} \right) \right\} \left\{ \sin\left(\frac{2\pi}{N} \frac{\Phi}{\Phi_0} \right) \cdots \right\} \\
& + \Delta_s \sum_{k=1}^{N} \sum_{j_1=1}^{N} \gamma_{j_1}^{n_1 *} \left\{ \gamma_{j_1}^{n_1} \gamma_x^{n_0} \gamma_k^{n_C} - \gamma_{j_1}^{n_C} \gamma_x^{n_0} \gamma_k^{n_1} - \gamma_{j_1}^{n_0} \gamma_x^{n_1} \gamma_k^{n_C} + \gamma_{j_1}^{n_0} \gamma_x^{n_C} \gamma_k^{n_1} \right\} \sin\theta_k \cos\zeta_k \\
& - \imath \Delta_c \sum_{k=1}^{N} \sum_{j_1=1}^{N} \gamma_{j_1}^{n_1 *} \left\{ \gamma_{j_1}^{n_1} \gamma_x^{n_0} \gamma_k^{n_C} - \gamma_{j_1}^{n_C} \gamma_x^{n_0} \gamma_k^{n_1} - \gamma_{j_1}^{n_0} \gamma_x^{n_1} \gamma_k^{n_C} + \gamma_{j_1}^{n_0} \gamma_x^{n_C} \gamma_k^{n_1} \right\} \\
& + \frac{N}{U} \left(\Delta_c^2 + \Delta_s^2 \right) \sum_{j_1=1}^{N} \gamma_{j_1}^{n_1 *} \left\{ \gamma_{j_1}^{n_1} \gamma_x^{n_C} - \gamma_{j_1}^{n_C} \gamma_x^{n_1} \right\}
\end{aligned}
\tag{5 30}
$$

For the sub-case of 2 sites one obtains by

- calling again $\gamma_x^{n_C} =: \gamma_x$ and $\gamma_x^{n_1} = \beta_\iota$,
- keeping in mind that $\gamma_{x+1}^{n} = \gamma_{x-1}^{n}$ and
- neglecting normalization conditions for the single particle[5]

the following set of equations

$$
\begin{aligned}
& E \left\{ \gamma_x \left(\beta_1^* \beta_1 + \beta_2^* \beta_2 \right) - \beta_x \left(\beta_1^* \gamma_1 + \beta_2^* \gamma_2 \right) \right\} = \\
& \quad - 2t \left\{ \beta_1^* \left(\beta_2 \gamma_x - \beta_x \gamma_2 \right) (w_1 + w_2) + \beta_2^* \left(\beta_1 \gamma_x - \beta_x \gamma_1 \right) (w_1 - w_2) \right\} \\
& \quad - 2t \left\{ \gamma_{x+1} \left(\beta_1^* \beta_1 + \beta_2^* \beta_2 \right) - \beta_{x+1} \left(\beta_1^* \gamma_1 + \beta_2^* \gamma_2 \right) \right\} \left(w_1 - (-1)^{\iota} w_2 \right) \\
& \quad + a_1 \beta_1^* \left(\beta_1 \gamma_x - \beta_x \gamma_1 \right) + a_2 \beta_2^* \left(\beta_2 \gamma_x - \beta_x \gamma_2 \right) \\
& \quad + a_x \left\{ \gamma_x \left(\beta_1^* \beta_1 + \beta_2^* \beta_2 \right) - \beta_x \left(\beta_1^* \gamma_1 + \beta_2^* \gamma_2 \right) \right\} \\
& \quad - 2\mathrm{i} \Delta_c \left\{ \gamma_x \left(\beta_1^* \beta_1 + \beta_2^* \beta_2 \right) - \beta_x \left(\beta_1^* \gamma_1 + \beta_2^* \gamma_2 \right) \right\} \\
& \quad + \frac{2}{U} \left(\Delta_c^2 + \Delta_s^2 \right) \left\{ \gamma_x \left(\beta_1^* \beta_1 + \beta_2^* \beta_2 \right) - \beta_x \left(\beta_1^* \gamma_1 + \beta_2^* \gamma_2 \right) \right\}
\end{aligned}
$$

[5] Even if they were used, the result would be the same

$x = 1$

$$\begin{aligned} 0 &= \gamma_1 \Big[-2t\beta_1^*\beta_2(w_1+w_2) + 2t\beta_1^*\beta_2(w_1+w_2) + a_2\beta_2^*\beta_2 + a_1\beta_2^*\beta_2 - \\ &\quad -2\imath\Delta_c\beta_2^*\beta_2 + \frac{2}{U}\left(\Delta_c^2+\Delta_s^2\right)\beta_2^*\beta_2 - E\beta_2^*\beta_2 \Big] \\ &+ \gamma_2 \Big[2t\beta_1^*\beta_2(w_1+w_2) - 2t\beta_1^*\beta_1(w_1+w_2) - a_2\beta_2^*\beta_1 - a_1\beta_2^*\beta_1 + \\ &\quad +2\imath\Delta_c\beta_2^*\beta_1 - \frac{2}{U}\left(\Delta_c^2+\Delta_s^2\right)\beta_2^*\beta_1 + E\beta_2^*\beta_1 \Big] \end{aligned}$$

$\imath = 2$:

$$\begin{aligned} 0 &= \gamma_1 \Big[2t\beta_2^*\beta_2(w_1-w_2) - 2t\beta_2^*\beta_2(w_1-w_2) - a_1\beta_1^*\beta_2 - a_2\beta_1^*\beta_2 + \\ &\quad +2\imath\Delta_c\beta_1^*\beta_2 - \frac{2}{U}\left(\Delta_c^2+\Delta_s^2\right)\beta_1^*\beta_2 + E\beta_1^*\beta_2 \Big] \\ &+ \gamma_2 \Big[-2t\beta_2^*\beta_1(w_1-w_2) + 2t\beta_2^*\beta_1(w_1-w_2) + a_1\beta_1^*\beta_1 + a_2\beta_1^*\beta_1 - \\ &\quad -2\imath\Delta_c\beta_1^*\beta_1 + \frac{2}{U}\left(\Delta_c^2+\Delta_s^2\right)\beta_1^*\beta_1 - E\beta_1^*\beta_1 \Big] \end{aligned}$$

Surprisingly, these two equations can be simplified a lot, leading to

$$\begin{aligned} 0 &= \left(a_1 + a_2 + E_F^{(2,2)} - E\right)\beta_2^*\left(\gamma_1\beta_2 - \gamma_2\beta_1\right) \\ 0 &= \left(a_1 + a_2 + E_F^{(2,2)} - E\right)\beta_1^*\left(\gamma_1\beta_2 - \gamma_2\beta_1\right) \end{aligned} \tag{5 31}$$

The result offers two possibilities One is that the energy of the system has the value

$$\boxed{E = \Delta_s\left(\sin\theta_1\cos\zeta_1 + \sin\theta_2\cos\zeta_2\right) - 2\imath\Delta_c + \frac{2}{U}\left(\Delta_c^2+\Delta_s^2\right).} \tag{5 32}$$

The saddle point approximation leads with $\theta_1 = \theta_2 = \frac{\pi}{2}$ and $\zeta_1 = \zeta_2 = 0$ to an energy $E = 0$ This is exactly the value which is obtained for noninteracting particles at the beginning of this paper in (2.37)

This solution is furthermore the same as the first of the solutions in the case when an orthogonality is used (Since the corresponding wave functions were orthogonal anyway, this is reasonable) However, in difference to the calculations there, it does not give any constraints what so ever for the choice of the wave function Apparently, the given energy value is highly degenerated

The second possibility, $\gamma \equiv \beta$, seems to imply that any energy value is allowed because the right hand sides of the equations above are zero independently

of the value for the energy. However, this possibility contradicts normalization conditions and is therefore not allowed.

5.3.2 Comparison with Bethe ansatz

In the paper of Kusmartsev *et al.* [14] the same system has been solved with the help of the Bethe *ansatz* Here for the wave function the expression

$$\psi(x_1,\ldots,x_N) = \sum_{p\in\mathcal{P}(M)} A(p)\exp\left[\mathrm{i}\sum_{j=1}^{M} k_{p(j)}x_j\right] \tag{5.33}$$

is used, which gives together with the Bethe equations the following set of equations:

$$Nk_j = 2\pi I_j + 2\pi\frac{\Phi}{\Phi_0} - 2\sum_{\beta=1}^{M_\uparrow}\arctan\left(4\frac{t\sin k_j-\lambda_\beta}{U}\right)$$

$$-2\sum_{j=1}^{M}\arctan\left(4\frac{t\sin k_j-\lambda_\beta}{U}\right) = 2\pi J_\beta + 2\sum_{\alpha=1}^{M_\uparrow}\arctan\left(2\frac{\lambda_\beta-\lambda_\alpha}{U}\right)$$

The quantum numbers I_j and J_β obey the equations

$$I_j \frac{M_\uparrow}{2} \pmod 1, \quad J_\beta = \frac{M-M_\uparrow+1}{2} \pmod 1$$

and have to be adjusted such that the energy is minimized

For one particle ($M=1$) it is.

$$\left.\begin{array}{lll} M_\uparrow = 0 \implies & Nk &= 2\pi\frac{\Phi}{\Phi_0} \\ M_\uparrow = 1 \implies & Nk &= 2\pi\frac{1}{2} + 2\pi\frac{\Phi}{\Phi_0} + 2\pi\frac{1}{2} = 2\pi\frac{\Phi}{\Phi_0} \end{array}\right\} \Longleftrightarrow k = \frac{2\pi}{N}\frac{\Phi}{\Phi_0}$$

Therefore, the solution is that of a free particle with flux This is clear because for a single particle there is no interaction

For two particles ($M=2, M_\uparrow=1$) and a sufficiently small flux ($\left|\frac{\Phi}{\Phi_0}\right| < \frac{1}{2}$) it is

$$Nk_j = 2\pi\frac{1}{2} + 2\pi\frac{\Phi}{\Phi_0} - 2\arctan\left(4\frac{t\sin k_j-\lambda}{U}\right); \quad -2\sum_{j=1}^{2}\arctan\left(4\frac{t\sin k_j-\lambda}{U}\right) = 0$$

$$\begin{aligned} N\frac{k_1+k_2}{2} &= 2\pi\frac{\Phi}{\Phi_0} \\ N\frac{k_1-k_2}{2} &= \arctan\left(4\frac{t\sin k_2-\lambda}{U}\right) - \arctan\left(4\frac{t\sin k_1-\lambda}{U}\right) \end{aligned}$$

$$= 2\arctan\left(\frac{4t\,(\sin k_2 - \sin k_1)}{2U}\right) = 2\arctan\left(\frac{4t\sin\left(\frac{k_1-k_2}{2}\right)\cos\left(\frac{k_1-k_2}{2}\right)}{U}\right)$$

$$= 2\arctan\left(\frac{\varepsilon}{\sin\left(\frac{k_1-k_2}{2}\right)}\right) \qquad \text{with} \quad \varepsilon = \frac{U}{4t\cos\left(\frac{2\pi\frac{\Phi}{\Phi_0}}{N}\right)}$$

If the number of sites is $N = 2$ then the situation is equivalent to that we have just studied. Kusmartsev *et al* found out that it is for this case possible to obtain an exact solution. Since

$$\tan\left(\frac{k_1-k_2}{2}\right)\,\sin\left(\frac{k_1-k_2}{2}\right) = \varepsilon \iff 1-\cos^2\left(\frac{k_1-k_2}{2}\right) = \varepsilon\cos\left(\frac{k_1-k_2}{2}\right),$$

one obtains the following expression for the wave vector

$$k_{1,2} = \pm\arccos\left(-\frac{\varepsilon}{2}+\sqrt{\frac{\varepsilon^2}{4}+1}\right)+\pi\frac{\Phi}{\Phi_0}$$

and for the ground state energy

$$E_{\text{ground}} = -2t\left(-\frac{\varepsilon}{2}+\sqrt{\frac{\varepsilon^2}{4}+1}\right)\cos\left(\pi\frac{\Phi}{\Phi_0}\right) \qquad \text{sin-terms cancel}$$

$$= -\frac{tU}{4t\cos\left(\pi\frac{\Phi}{\Phi_0}\right)}\left(-1+\sqrt{1+\frac{4(4t)^2\cos^2\left(\pi\frac{\Phi}{\Phi_0}\right)}{U^2}}\right)\cos\left(\pi\frac{\Phi}{\Phi_0}\right)$$

$$= \frac{1}{2}\left(\frac{U}{2}-\sqrt{\left(\frac{U}{2}\right)^2+16t^2\cos^2\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)}\right) \qquad (5\,34)$$

The expression for the energy obtained with the help of the Bethe *ansatz* has much more in common with our result for 1 particle / 2 sites than with the result for 2 particles For instance, for the choice

$$N = 2, \quad M = 2, \quad \zeta_1 = \zeta_2 = 0, \quad \theta_1 = \frac{\pi}{2}, \quad \theta_2 = 0, \quad \Delta_s = \frac{U}{2}, \quad \Delta_c = 0$$

the ground state energy (5 17) has the form

$$E = \frac{1}{2}\left(\frac{U}{2}-\sqrt{\left(\frac{U}{2}\right)^2+16t^2\cos^2\left(\frac{2\pi}{N}\frac{\Phi}{\Phi_0}\right)\frac{1}{2}}\right)+\frac{U}{2} \qquad (5\,35)$$

This indicates another problem of the states used so far The wave function for what was called so far "one particle' has the following structure

$$|\psi\rangle_{n_1} = \frac{1}{\sqrt{2}}\sum_{i_1}\sum_{\sigma_1=\uparrow,\downarrow}\gamma_{i_1}^{n_1}\tilde{c}^{\dagger}_{i_1,\sigma_1}|0\rangle = \frac{1}{\sqrt{2}}\sum_{i}\gamma_i^{n_1}\left\{\tilde{c}^{\dagger}_{i,\uparrow}|0\rangle+\tilde{c}^{\dagger}_{i,\downarrow}|0\rangle\right\}$$

The comparison with the Bethe *ansatz* calculations in essence shows that these kind of states include already a pair of particles, a mixture of a up-spin and a down-spin part. The problem could be that both parts have exactly the same weight γ_{x_1} for each site For this reason, derivatives are sensitive to both parts at the same time Therefore, the up-spin part influences, or one might even say interacts with, its own down-spin part.

The pair character becomes even clearer if one just looks at the normalization of a two-particle state

$$\begin{aligned}
\langle\psi|\psi\rangle &= \frac{1}{4}\sum_{\substack{i_1\,i_2\\ j_1\,j_2}}\sum_{\substack{\sigma_1,\sigma_2\\ \eta_1,\eta_2}} \gamma^*_{j_1}\beta^*_{j_2}\gamma_{i_1}\beta_{i_2}\langle 0|\tilde{c}_{j_2,\eta_2}\tilde{c}_{j_1,\eta_1}\tilde{c}^\dagger_{i_1,\sigma_1}\tilde{c}^\dagger_{i_2,\sigma_2}|0\rangle \\
&= \sum_{i_1,i_2}\left\{\gamma^*_{i_1}\beta^*_{i_2}\gamma_{i_1}\beta_{i_2} - \gamma^*_{i_2}\beta^*_{i_1}\gamma_{i_1}\beta_{i_2}\right\} \\
&= \begin{cases} 0 & \text{for } N=1 \\ \gamma^*_1\beta^*_2(\gamma_1\beta_2-\gamma_2\beta_1)+\gamma^*_2\beta^*_1(\gamma_2\beta_1-\gamma_1\beta_2) & \text{for } N=2 \end{cases}
\end{aligned}$$

A situation of 2 particles / 1 site is quantum mechanically allowed, but leads in our description to a vanishing wave function In the 2 sites situation the wave function vanishes if $\gamma \equiv \beta$ Again, this happens without the necessity according to the Pauli principle Furthermore, the 2 particles / 2 sites calculations in subsection 5 3 1 led to only one energy, which also indicates that actually a four-particle problem has been treated

We shall show next that all these troubles can be solved if we forget about the assumption that up- and down-spin particles can be handled with the same weight. Instead, both spin directions should have independent wave functions and a normalization should be applied only for their combination Not least thanks to the Zeemann effect such a step seems to be reasonable

This most general way of expressing the wave function has for a single particle the following form.

$$|\psi\rangle = \sum_{i=1}^{N}\psi_\uparrow(i)\tilde{c}^\dagger_{i,\uparrow}|0\rangle + \sum_{i=1}^{N}\psi_\downarrow(i)\tilde{c}^\dagger_{i,\downarrow}|0\rangle = \sum_{i=1}^{N}\sum_{\sigma=\uparrow,\downarrow}\psi_\sigma(i)\tilde{c}^\dagger_{i,\sigma}|0\rangle$$

It should be stressed again that $\psi_\uparrow$ and $\psi_\downarrow$ are now two (almost) independent functions This also includes the case that the particle has a fixed spin with no

possibility to change it, if for instance $\psi_\downarrow \equiv 0$ is chosen. However, the normalization condition

$$\langle\psi|\psi\rangle = \sum_{i,j}\sum_{\sigma,\eta}\psi^*_\eta(j)\psi_\sigma(i)\langle 0|\tilde{c}_{j,\eta}\tilde{c}^\dagger_{j,\sigma}|0\rangle = \sum_i\left\{|\psi_\uparrow(i)|^2+|\psi_\downarrow(i)|^2\right\} \stackrel{!}{=} 1$$

implies that the two functions still have something to do with one another

A straight forward generalization to M particles has the following form

$$|\psi\rangle_{n_1,\ \ldots,n_M} = C_M \sum_{i_1,\ \ldots,i_M}\sum_{\sigma_1,\ \ldots,\sigma_M}\psi^{n_1}_{\sigma_1}(i_1)\cdot\ \ldots\ \cdot\psi^{n_M}_{\sigma_M}(i_M)\tilde{c}^\dagger_{i_1,\sigma_1}\cdot\ \ldots\ \cdot\tilde{c}^\dagger_{i_M,\sigma_M}|0\rangle \quad (5\ 36)$$

These kind of states offer various possibilities. One positive consequence is that most of the mentioned problems do not arise any more For instance the above studied case of 2 particles becomes now

$$\begin{aligned}
1 \stackrel{!}{=}\ & {}_{n_1,n_2}\langle\psi|\psi\rangle_{n_1,n_2} \\
=\ & C_2^2\sum_{\substack{i_1\ i_2\\ j_1,j_2}}\sum_{\substack{\sigma_1,\sigma_2\\ \eta_1,\eta_2}}\left[\psi^{n_1}_{\eta_1}(j_1)\right]^*\left[\psi^{n_2}_{\eta_2}(j_2)\right]^*\psi^{n_1}_{\sigma_1}(i_1)\psi^{n_2}_{\sigma_2}(i_2)\langle 0|\tilde{c}_{j_2,\eta_2}\tilde{c}_{j_1,\eta_1}\tilde{c}^\dagger_{i_1,\sigma_1}\tilde{c}^\dagger_{i_2,\sigma_2}|0\rangle \\
=\ & C_2^2\sum_{i_1,i_2}\sum_{\sigma_1,\sigma_2}\left\{\left|\psi^{n_1}_{\sigma_1}(i_1)\right|^2\left|\psi^{n_2}_{\sigma_2}(i_2)\right|^2-\left[\psi^{n_1}_{\sigma_2}(i_2)\right]^*\left[\psi^{n_2}_{\sigma_1}(i_1)\right]^*\psi^{n_1}_{\sigma_1}(i_1)\psi^{n_2}_{\sigma_2}(i_2)\right\}
\end{aligned}$$

There are the positive contributions $\langle\uparrow\uparrow|\uparrow\uparrow\rangle$, $\langle\downarrow\downarrow|\downarrow\downarrow\rangle$, $\langle\uparrow\downarrow|\uparrow\downarrow\rangle$, $\langle\downarrow\uparrow|\downarrow\uparrow\rangle$ and the negative contributions $\langle\uparrow\uparrow|\downarrow\downarrow\rangle$, $\langle\downarrow\downarrow|\uparrow\uparrow\rangle$, $\langle\uparrow\downarrow|\downarrow\uparrow\rangle$, $\langle\downarrow\uparrow|\uparrow\downarrow\rangle$ to the overlap, and there is, in general, no need for them to cancel each other Even for only 1 site

$$\sum_{\sigma_1,\sigma_2}\left\{\left|\psi^{n_1}_{\sigma_1}\right|^2\left|\psi^{n_2}_{\sigma_2}\right|^2-\left[\psi^{n_1}_{\sigma_2}\right]^*\left[\psi^{n_2}_{\sigma_1}\right]^*\psi^{n_1}_{\sigma_1}\psi^{n_2}_{\sigma_2}\right\}$$

has a non-zero value for almost every configuration If the first particle has a certain ratio of the up-spin and the down-spin weights, $\psi^{n_1}_{\sigma_1}/\psi^{n_1}_{\sigma_2}$, an arbitrary ratio $\psi^{n_2}_{\sigma_1}/\psi^{n_2}_{\sigma_2}$ for the second particle is possible As mentioned before, this includes a combination of a pure up-spin and a pure down-spin particle However, it is enough if one particle "shows the up-spin character more" than the other one Only if the ratio is for both particles the same, the wave function vanishes again

A little bit problematic is the question of normalization The remarks of the previous subsection have led to the conclusion that wave functions of different

particles within the same state cannot necessarily be assumed to be orthogonal. Thus, the negative contribution to the 2-particle overlap above are not zero Nor do the various terms of the slater determinant in the many-particle case vanish

Unfortunately, this freedom of the system also effects the normalization of the single participating fermion If conditions like

$$\sum_{i_A} \left\{ |\psi_\uparrow^{n_A}(i_A)|^2 + |\psi_\downarrow^{n_A}(i_A)|^2 \right\} \stackrel{!}{=} 1$$

were maintained, the identical permutation in the slater determinant would already be equal to unity, which implies the orthogonality for the remaining terms which should be avoided

5.4 Again: Limited System Size

The derivation of the Hartree-Fock equations is again very similar to the derivation in section 5 1 Apart from the greater freedom of the wave function, the main difference is the fact that all derivatives are now taken with respect to a parameter $\left[\psi_\nu^{n_C}(x)\right]^*$ which also has a spin index ν However, this spin index can be treated very similar to the site index x and does not make calculations qualitatively more difficult

For the expectation value of a typical operator the same compact notation as already introduced in the previous subsection shall be used. The wave function with the quantum number n_0 is now a product of two Kronecker deltas, one for the site and one for the spin. If for instance the operator product $\tilde{c}_{k,\uparrow}^\dagger \tilde{c}_{k+1,\downarrow}$ is considered then $\psi_\sigma^{n_0}(i) = \delta_{i,k}\delta_{\sigma,\uparrow}$ Hence,

$$\begin{aligned} {}_{n_1,\ \ ,n_M}\langle\psi|\tilde{c}_{k,\uparrow}^\dagger \tilde{c}_{k+1,\downarrow}|\psi\rangle_{n_1,\ \ ,n_M} = \qquad\qquad (5\ 37) \\ C_M^2 \sum_{j_1,\ \ ,j_M} \sum_{\sigma_1,\ \ ,\sigma_M} \sum_{\wp(0)\neq 0 \atop \wp\in\mathcal{P}(M+1)} (-1)^{\mathrm{sgn}\wp+1} \left[\psi_{\sigma_1}^{n_1}(j_1)\right]^* \ldots \left[\psi_{\sigma_M}^{n_M}(j_M)\right]^* * \\ * \psi_{\sigma_1}^{n_{\wp(1)}}(j_1) \ldots \psi_{\sigma_M}^{n_{\wp(M)}}(j_M) \psi_\downarrow^{n_{\wp(0)}}(k+1) \end{aligned}$$

$$\frac{\partial}{\partial\left[\psi_\nu^{n_C}(x)\right]^*}\left({}_{n_1,\ \ ,n_M}\langle\psi|\tilde{c}^\dagger_{k,\uparrow}\tilde{c}_{k+1,\downarrow}|\psi\rangle_{n_1,\ ,n_M}\right) = \tag{5 38}$$

$$C_M^2 \sum_{j_1,\ \ ,j_M}^{j_C=x} \sum_{\sigma_1,\ \ ,\sigma_M}^{\sigma_C=\nu} \sum_{p\in\mathcal{P}(M+1)}^{p(0)\neq 0} (-1)^{\mathrm{sgn}p+1}\left[\psi_{\sigma_1}^{n_1}(j_1)\right]^* \cdot \left[\widehat{\psi_{\sigma_C}^{n_C}(j_C)}\right]^* \cdots \left[\psi_{\sigma_M}^{n_M}(j_M)\right]^* * \psi_{\sigma_1}^{n_{p(1)}}(j_1) \ \cdot\ \psi_{\sigma_M}^{n_{p(M)}}(j_M)\psi_\downarrow^{n_{p(0)}}(k+1)$$

are the kind of expressions which now appear in the Hartree-Fock equations The Hamiltonian is still the one given in (5 5). It shall be evaluated now for particular cases

5.4.1 One Particle / One Site ($M = 1, N = 1$)

For one particle one has to deal with the following derivatives:

$$\begin{aligned}
\frac{\partial}{\partial\left[\psi_\nu^{n_C}(x)\right]^*}\left({}_{n_C}\langle\psi|\psi\rangle_{n_C}\right) &= \psi_\nu^{n_C}(x)\\
\frac{\partial}{\partial\left[\psi_\nu^{n_C}(x)\right]^*}\left({}_{n_C}\langle\psi|\tilde{c}^\dagger_{k,\sigma}\tilde{c}_{k+1,\sigma'}|\psi\rangle_{n_C}\right) &= \delta_{x,k}\delta_{\nu,\sigma}\psi_{\sigma'}^{n_C}(k+1)\\
\frac{\partial}{\partial\left[\psi_\nu^{n_C}(x)\right]^*}\left({}_{n_C}\langle\psi|\sum_k \tilde{c}^\dagger_{k,\sigma}\tilde{c}_{k+1,\sigma'}|\psi\rangle_{n_C}\right) &= \delta_{\nu,\sigma}\,\psi_{\sigma'}^{n_C}(x+1)
\end{aligned}$$

which gives the following Hartree-Fock equations:[6]

$$\begin{aligned}
E\psi_\nu(x) = &- t\sum_{\sigma'}\left\{\bar{R}_{x,\nu\sigma'}\psi_{\sigma'}(x+1)\mathrm{e}^{\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}} + \bar{R}^*_{x-1,\nu\sigma'}\psi_{\sigma'}(x-1)\mathrm{e}^{-\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}}\right\}\\
&+ E_F^{(1,N)}\psi_\nu(x) - \left(\Delta_s + \frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\right)\cos\theta_x\left(\delta_{\nu,\uparrow}\psi_\uparrow(x) - \delta_{\nu,\downarrow}\psi_\downarrow(x)\right)\\
&+ \Delta_s\sin\theta_x\left\{\delta_{\nu,\uparrow}\psi_\downarrow(x)\mathrm{e}^{-\imath\zeta_x} + \delta_{\nu,\downarrow}\psi_\uparrow(x)\mathrm{e}^{\imath\zeta_x}\right\}
\end{aligned} \tag{5 39}$$

For only one site this simplifies to the two equations (for $\nu = \uparrow$ and $\nu = \downarrow$ respectively):

$$\begin{aligned}
0 &= \psi_\uparrow\left[-2t\cos\left(2\pi\mathrm{i}\frac{\Phi}{\Phi_0}\right) + E_F^{(1,1)} - \left(\Delta_s + \Delta_Z\frac{\Phi}{\Phi_0}\right)\cos\theta_1 - E\right] + \psi_\downarrow\left[\Delta_s\sin\theta_1\mathrm{e}^{-\imath\zeta_1}\right]\\
0 &= \psi_\uparrow\left[\Delta_s\sin\theta_1\mathrm{e}^{\imath\zeta_1}\right] + \psi_\downarrow\left[-2t\cos\left(2\pi\mathrm{i}\frac{\Phi}{\Phi_0}\right) + E_F^{(1,1)} + \left(\Delta_s + \Delta_Z\frac{\Phi}{\Phi_0}\right)\cos\theta_1 - E\right]
\end{aligned}$$

[6]The index for the quantum number is omitted

If this system of equations should have non-trivial solutions then a quadratic equation in the energy has to be fulfilled The two solutions are

$$\boxed{E_{1,2} = -2t\cos\left(2\pi i\frac{\Phi}{\Phi_0}\right) - i\Delta_c + \frac{1}{U}\left(\Delta_c^2 + \Delta_s^2\right) \pm \left(\Delta_s + \Delta_Z\frac{\Phi}{\Phi_0}\right)} \qquad (5\,40)$$

with the ground state energy

$$E = -2t\cos\left(2\pi i\frac{\Phi}{\Phi_0}\right) - \frac{gh^2}{m_e a^2}\frac{\Phi}{\Phi_0}. \qquad (5.41)$$

It will become clear soon that it is reasonable to rewrite the same system in a matrix form. For brevity the following two terms shall be defined

$$\Lambda_{s,Z}^{(N)} := \Delta_s + \frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}; \qquad \Lambda_{\text{hopp}}^{(N)} = -2t\cos\left(\frac{2\pi i}{N}\frac{\Phi}{\Phi_0}\right)$$

Hence,

$$\left(E - E_F^{(1,1)}\right)\begin{pmatrix}\psi_\uparrow(1)\\ \psi_\downarrow(1)\end{pmatrix} = H^{(1,1)}\begin{pmatrix}\psi_\uparrow(1)\\ \psi_\downarrow(1)\end{pmatrix} \qquad (5\,42)$$

with

$$H^{(1,1)} = \begin{pmatrix}\Lambda_{\text{hopp}}^{(1)}\bar{R}_{1,\uparrow\uparrow} & \Lambda_{\text{hopp}}^{(1)}\bar{R}_{1,\uparrow\downarrow}\\ \Lambda_{\text{hopp}}^{(1)}\bar{R}_{1,\downarrow\uparrow} & \Lambda_{\text{hopp}}^{(1)}\bar{R}_{1,\downarrow\downarrow}\end{pmatrix} + \begin{pmatrix}-\Lambda_{s,Z}^{(1)}\cos\theta_x & \Delta_s\sin\theta_1 e^{-i\zeta_1}\\ \Delta_s\sin\theta_x e^{-i\zeta_1} & \Lambda_{s,Z}^{(1)}\cos\theta_x\end{pmatrix} \qquad (5.43)$$

5.4.2 One Particle / Two Sites ($M = 1, N = 2$)

For 2 sites the equation (5 39) is still valid. Unfortunately, the arguments which led to w_1 and w_2 in section 5.2 2 are not applicable, since it is not summed anymore over all four matrix elements of $\bar{R}$. However, the properties of $\bar{R}$ for an arbitrary number of sites $\bar{R}^*_{k,\uparrow\uparrow} = \bar{R}_{k,\downarrow\downarrow}$ and $\bar{R}^*_{k,\uparrow\downarrow} = -\bar{R}_{k,\downarrow\uparrow}$ and particularly for two sites. $\bar{R}_{1,\uparrow\uparrow} = \bar{R}_{2,\downarrow\downarrow}, \bar{R}_{1,\downarrow\downarrow} = \bar{R}_{2,\uparrow\uparrow}, \bar{R}_{1,\uparrow\downarrow} = -\bar{R}_{2,\downarrow\uparrow}, \bar{R}_{1,\downarrow\uparrow} = -\bar{R}_{2,\uparrow\downarrow}$ still allow simplifications. The most convenient one is that for any spin combination

$$\bar{R}^*_{2,\sigma\sigma'} = \bar{R}_{1,\sigma\sigma'} \quad \text{and} \quad \bar{R}^*_{1\,\sigma\sigma'} = \bar{R}_{2\,\sigma\sigma'} \qquad (5\,44)$$

holds As a consequence the exponential functions in the flux can be expressed in form of a cosine

Another problem is that the wave function ψ possesses now $2 \times 2 = 4$ components Instead of solving an equation of fourth order directly, the equations shall

now be written as an eigenvalue problem. All equations are expressed with the help of the following matrix

$$H^{(1,2)} = \begin{pmatrix} -\Lambda^{(2)}_{s,Z}\cos\theta_1 & \Delta_s \sin\theta_1 e^{-i\zeta_1} & \Lambda_{\mathrm{hopp}^{(2)}}\bar{R}_{1,\uparrow\uparrow} & \Lambda^{(2)}_{\mathrm{hopp}}\bar{R}_{1,\uparrow\downarrow} \\ \Delta_s \sin\theta_1 e^{i\zeta_1} & \Lambda_{s,Z^{(2)}}\cos\theta_1 & \Lambda^{(2)}_{\mathrm{hopp}}\bar{R}_{1,\downarrow\uparrow} & \Lambda^{(2)}_{\mathrm{hopp}}\bar{R}_{1,\downarrow\downarrow} \\ \Lambda^{(2)}_{\mathrm{hopp}}\bar{R}_{2,\uparrow\uparrow} & \Lambda^{(2)}_{\mathrm{hopp}}\bar{R}_{2,\uparrow\downarrow} & -\Lambda_{s,Z}\cos\theta_2 & \Delta_s \sin\theta_2 e^{-i\zeta_2} \\ \Lambda^{(2)}_{\mathrm{hopp}}\bar{R}_{2,\downarrow\uparrow} & \Lambda^{(2)}_{\mathrm{hopp}}\bar{R}_{2,\downarrow\downarrow} & \Delta_s \sin\theta_2 e^{i\zeta_2} & \Lambda^{(2)}_{s,Z}\cos\theta_2 \end{pmatrix} \tag{5.45}$$

which determines the following matrix equation

$$\left(E - E_F^{(1,2)}\right)\begin{pmatrix} \psi_\uparrow(1) \\ \psi_\downarrow(1) \\ \psi_\uparrow(2) \\ \psi_\downarrow(2) \end{pmatrix} = H^{(1,2)}\begin{pmatrix} \psi_\uparrow(1) \\ \psi_\downarrow(1) \\ \psi_\uparrow(2) \\ \psi_\downarrow(2) \end{pmatrix} \tag{5.46}$$

5.4.3 Two Particles / One Site ($M = 2, N = 1$)

For two particles the derivatives (5.38) are at least twice as complicated as for one particle. The second particle, the one which does not have the quantum number n_C shall again be denoted by β, allowing to omit the index for the quantum numbers. Then the following kind of expressions have to be dealt with

$$\frac{\partial}{\partial\left[\psi_\nu(x)\right]^*}\left({}_{n_1,n_2}\langle\psi\,|\,\psi\rangle_{n_1,n_2}\right) = C_2^2\left\{\psi_\nu(x)\sum_j\sum_\eta\left|\beta_\eta(j)\right|^2 - \beta_\nu(x)\sum_j\sum_\eta\beta^*_\eta(j)\psi_\eta(j)\right\}$$

$$\frac{\partial}{\partial\left[\psi^{n_C}_\nu(x)\right]^*}\left({}_{n_1,n_2}\langle\psi\,|\tilde{c}^\dagger_{k,\sigma}\tilde{c}_{k+1,\sigma'}\,|\psi\rangle_{n_1,n_2}\right)$$

$$= C_2^2\sum_j\sum_\eta\beta^*_\eta(j)\Big\{\underbrace{\delta_{x,k}\delta_{\nu,\sigma}\beta_\eta(j)\psi_{\sigma'}(k+1)}_{\wp(120)=102} - \underbrace{\delta_{i,k}\delta_{\nu,\sigma}\psi_\eta(j)\beta_{\sigma'}(k+1)}_{\wp(120)=201} - \ldots$$

$$\ldots - \underbrace{\delta_{j,k}\delta_{\eta,\sigma}\beta_\nu(x)\psi_{\sigma'}(k+1)}_{\wp(120)=012} + \underbrace{\delta_{j,k}\delta_{\eta,\sigma}\psi_\nu(x)\beta_{\sigma'}(k+1)}_{\wp(120)=021}\Big\}$$

$$\frac{\partial}{\partial\left[\psi^{n_C}_\nu(x)\right]^*}\left({}_{n_1,n_2}\langle\psi\,|\sum_k\tilde{c}^\dagger_{k,\sigma}\tilde{c}_{k+1,\sigma'}\,|\psi\rangle_{n_1,n_2}\right)$$

$$= C_2^2\Big\{\delta_{\nu,\sigma}\psi_{\sigma'}(x+1)\sum_j\sum_\eta\left|\beta_\eta(j)\right|^2 - \delta_{\nu,\sigma}\beta_{\sigma'}(x+1)\sum_j\sum_\eta\beta^*_\eta(j)\psi_\eta(j) - \ldots$$

$$\ldots - \beta_\nu(x)\sum_k\beta^*_\sigma(k)\psi_{\sigma'}(k+1) + \psi_\nu(x)\sum_k\beta^*_\sigma(k)\beta_{\sigma'}(k+1)\Big\}$$

This leads to the following Hartree-Fock equations:

$$
\begin{aligned}
E\Big\{\psi_\nu(x)\sum_\jmath\sum_\eta|\beta_\eta 1(\jmath)|^2-\beta_\nu(x)\sum_\jmath\sum_\eta\beta^*_\eta(\jmath)\psi_\eta(\jmath)\Big\}=&\\
-\ t\sum_{\sigma'}\Big\{\bar R_{x,\nu\sigma'}\psi_{\sigma'}(x+1)\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2\mathrm{e}^{\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}}+\ldots&\\
+\bar R^*_{x-1,\nu\sigma'}\psi_{\sigma'}(x-1)\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2\mathrm{e}^{-\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}}\Big\}&\\
+\ t\sum_{\sigma'}\Big\{\bar R_{x,\nu\sigma'}\beta_{\sigma'}(x+1)\sum_\jmath\sum_\eta\beta^*_\eta(\jmath)\psi_\eta(\jmath)\mathrm{e}^{\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}}+\ldots&\\
\ldots+\bar R^*_{x-1,\nu\sigma'}\beta_{\sigma'}(x-1)\sum_\jmath\sum_\eta\beta^*_\eta(\jmath)\psi_\eta(\jmath)\mathrm{e}^{-\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}}\Big\}&\\
-\ t\psi_\nu(x)\sum_k\sum_{\sigma,\sigma'}\Big\{\bar R_{k,\sigma\sigma'}\beta^*_\sigma(k)\beta_{\sigma'}(k+1)\mathrm{e}^{\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}}+\bar R^*_{k-1,\sigma\sigma'}\beta^*_\sigma(k)\beta_{\sigma'}(k-1)\mathrm{e}^{-\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}}\Big\}&\\
+\ t\beta_\nu(x)\sum_k\sum_{\sigma,\sigma'}\Big\{\bar R_{k,\sigma\sigma'}\beta^*_\sigma(k)\psi_{\sigma'}(k+1)\mathrm{e}^{\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}}+\bar R^*_{k-1,\sigma\sigma'}\beta^*_\sigma(k)\psi_{\sigma'}(k-1)\mathrm{e}^{-\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}}\Big\}&\\
+\ \frac{N}{U}\left(\Delta_c^2+\Delta_s^2\right)\Big\{\psi_\nu(x)\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2-\beta_\nu(x)\sum_\jmath\sum_\eta\beta^*_\eta(\jmath)\psi_\eta(\jmath)\Big\}&\\
-\ 2\imath\Delta_c\Big\{\psi_\nu(x)\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2-\beta_\nu(x)\sum_\jmath\sum_\eta\beta^*_\eta(\jmath)\psi_\eta(\jmath)\Big\}&\\
-\ \left(\Delta_z+\frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\right)\Big\{(\delta_{\nu,\uparrow}-\delta_{\nu,\downarrow})\psi_\nu(x)\cos\theta_x\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2-\ .&\\
-(\delta_{\nu,\uparrow}-\delta_{\nu,\downarrow})\beta_\nu(x)\cos\theta_x\sum_\jmath\sum_\eta\beta^*_\eta(\jmath)\psi_\eta(\jmath)\Big\}&\\
-\ \left(\Delta_z+\frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\right)\Big\{\psi_\nu(x)\sum_k\cos\theta_k\left(\beta^*_\uparrow(k)\beta_\uparrow(k)-\beta^*_\downarrow(k)\beta_\downarrow(k)\right)-\ldots&\\
\ldots-\beta_\nu(x)\sum_k\cos\theta_k\left(\beta^*_\uparrow(k)\psi_\uparrow(k)-\beta^*_\downarrow(k)\psi_\downarrow(k)\right)\Big\}&\\
+\ \Delta_s\Big\{\left(\delta_{\nu,\uparrow}\psi_\downarrow(x)\mathrm{e}^{-\imath\zeta_x}+\delta_{\nu,\downarrow}\psi_\uparrow(x)\mathrm{e}^{\imath\zeta_x}\right)\sin\theta_x\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2-&\\
\ldots-\left(\delta_{\nu,\uparrow}\beta_\downarrow(\imath)\mathrm{e}^{-\imath\zeta_x}+\delta_{\nu,\downarrow}\beta_\uparrow(x)\mathrm{e}^{\imath\zeta_x}\right)\sin\theta_x\sum_\jmath\sum_\eta\beta^*_\eta(\jmath)\psi_\eta(\jmath)\Big\}&\\
+\ \Delta_s\Big\{\psi_\nu(\imath)\sum_k\sin\theta_k\left(\beta^*_\uparrow(k)\beta_\downarrow(k)\mathrm{e}^{-\imath\zeta_k}+\beta^*_\downarrow(k)\beta_\uparrow(k)\mathrm{e}^{\imath\zeta_k}\right)-\ .&\\
.-\beta_\nu(\imath)\sum_k\sin\theta_k\left(\beta^*_\uparrow(k)\psi_\downarrow(k)\mathrm{e}^{-\imath\zeta_k}+\beta^*_\downarrow(k)\psi_\uparrow(k)\mathrm{e}^{\imath\zeta_k}\right)\Big\}&
\end{aligned}
$$

(5 47)

For only one site these equations simplify again drastically. All terms which go with Δ_s disappear, and because $\bar{R}_{\uparrow\uparrow} = \bar{R}_{\downarrow\downarrow} = 1, \bar{R}_{\uparrow\downarrow} = \bar{R}_{\downarrow\uparrow} = 0$ it is

$$\begin{aligned}\left(E - E_F^{(2,1)}\right)\beta_\downarrow^*\left\{\psi_\uparrow\beta_\downarrow - \psi_\downarrow\beta_\uparrow\right\} &= -4t\cos\left(2\pi\frac{\Phi}{\Phi_0}\right)\beta_\downarrow^*\left\{\psi_\uparrow\beta_\downarrow - \psi_\downarrow\beta_\uparrow\right\} \\ \left(E - E_F^{(2,1)}\right)\beta_\uparrow^*\left\{\psi_\downarrow\beta_\uparrow - \psi_\uparrow\beta_\downarrow\right\} &= -4t\cos\left(2\pi\frac{\Phi}{\Phi_0}\right)\beta_\uparrow^*\left\{\psi_\downarrow\beta_\uparrow - \psi_\uparrow\beta_\downarrow\right\}\end{aligned}$$

The result for the energy is therefore

$$E = -4t\cos\left(2\pi\frac{\Phi}{\Phi_0}\right) - 2\imath\Delta_c + \frac{1}{U}\left(\Delta_c^2 + \Delta_s^2\right), \tag{5.48}$$

which is almost the sum of the two possible energy solutions (5.40) in the case that only one particle is sitting on the site. Only the term in front of the mean field does not have the factor 2, which indicates that the mean fields have higher values in the two-particle case.

The saddle point in this case is obtained by setting $\Delta_{c,0} = \imath U$ and $\Delta_{s,0} = 0$. It is related to the energy

$$E = -4t\cos\left(2\pi\frac{\Phi}{\Phi_0}\right) + U. \tag{5.49}$$

This expression describes the physical situation correctly. Both particles have the same quantum number $n = 0$ and are sitting on the same site. The former implies the term for the kinetic energy given, the latter leads to the effect that the potential energy is equivalent to the full Coulomb repulsion energy. That this has been obtained shows that we are on the right track.

5.4.4 Two Particles / Two Sites ($M = 2, N = 2$)

The situation of two particles on two sites is the one which is of particular interest for us because it allows an interaction as well a non-trivial distribution. The three cases before can be understood to be only a preparation for this task. One can use now the same Hartree-Fock equation as in the proceeding subsection and the same properties (5.44) of the matrix elements of $\bar{R}$ as in the subsection before. The four possible combinations of $\nu = \uparrow, \downarrow$ and $\alpha = 1, 2$ lead to the following four

equations:

$$
\begin{aligned}
&\left(E - E_F^{(2,2)}\right)\psi_\nu(x)\left[\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2 - \beta_\nu^*(k)\beta_\nu(k)\right] \\
&= \psi_\uparrow(1)\Lambda_{\text{hopp}}^{(2)}\left[-\beta_\uparrow^*(1)\bar{R}_{x,\nu\uparrow}\beta_\uparrow(x+1) - \beta_\uparrow^*(1)\bar{R}_{x,\nu\downarrow}\beta_\downarrow(x+1) - \right. \\
&\qquad \left. - \beta_\uparrow^*(2)\bar{R}_{2,\uparrow\uparrow}\beta_\nu(\imath) - \beta_\downarrow^*(2)\bar{R}_{2,\downarrow\uparrow}\beta_\nu(x) \quad + \delta_{x,2}\bar{R}_{\imath,\nu\uparrow}\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2\right] \\
&+ \psi_\downarrow(1)\Lambda_{\text{hopp}}^{(2)}\left[-\beta_\downarrow^*(1)\bar{R}_{x,\nu\uparrow}\beta_\uparrow(x+1) - \beta_\downarrow^*(1)\bar{R}_{x,\nu\downarrow}\beta_\downarrow(\imath+1) - \right. \\
&\qquad \left. - \beta_\uparrow^*(2)\bar{R}_{2,\uparrow\downarrow}\beta_\nu(x) - \beta_\downarrow^*(2)\bar{R}_{2,\downarrow\downarrow}\beta_\nu(x) \quad + \delta_{\imath,2}\bar{R}_{\imath,\nu\downarrow}\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2\right] \\
&+ \psi_\uparrow(2)\Lambda_{\text{hopp}}^{(2)}\left[-\beta_\uparrow^*(2)\bar{R}_{x,\nu\uparrow}\beta_\uparrow(x+1) - \beta_\uparrow^*(2)\bar{R}_{\imath,\nu\downarrow}\beta_\downarrow(\imath+1) - \right. \\
&\qquad \left. - \beta_\uparrow^*(1)\bar{R}_{2,\uparrow\uparrow}\beta_\nu(x) - \beta_\downarrow^*(1)\bar{R}_{2,\downarrow\uparrow}\beta_\nu(x) \quad + \delta_{x,1}\bar{R}_{x,\nu\uparrow}\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2\right] \\
&+ \psi_\downarrow(2)\Lambda_{\text{hopp}}^{(2)}\left[-\beta_\downarrow^*(2)\bar{R}_{x,\nu\uparrow}\beta_\uparrow(x+1) - \beta_\downarrow^*(2)\bar{R}_{x,\nu\downarrow}\beta_\downarrow(\imath+1) - \right. \\
&\qquad \left. - \beta_\uparrow^*(1)\bar{R}_{2,\uparrow\downarrow}\beta_\nu(x) - \beta_\downarrow^*(1)\bar{R}_{2,\downarrow\downarrow}\beta_\nu(x) \quad + \delta_{\imath,1}\bar{R}_{\imath,\nu\downarrow}\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2\right] \\
&+ \psi_\uparrow(1)\delta_{\nu,\uparrow}\left[\Lambda_{s,Z}^{(2)}\left(\cos\theta_1 + \cos\theta_x\right)\beta_\uparrow^*(1)\beta_\uparrow(\imath) - \right. \\
&\qquad - \Delta_s\sin\theta_x e^{-i\zeta_x}\beta_\uparrow^*(1)\beta_\downarrow(x) - \\
&\qquad \left. - \Delta_s\sin\theta_1 e^{i\zeta_1}\beta_\downarrow^*(1)\beta_\uparrow(\imath)\right] \\
&+ \psi_\uparrow(1)\delta_{\nu,\downarrow}\left[\Lambda_{s,Z}^{(2)}\left(\cos\theta_1 - \cos\theta_x\right)\beta_\uparrow^*(1)\beta_\downarrow(x) - \right. \\
&\qquad - \Delta_s\sin\theta_x e^{i\zeta_x}\beta_\uparrow^*(1)\beta_\uparrow(\imath) - \\
&\qquad \left. - \Delta_s\sin\theta_1 e^{i\zeta_1}\beta_\downarrow^*(1)\beta_\downarrow(x) \quad + \delta_{\imath,1}\Delta_s\sin\theta_x e^{i\zeta_x}\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2\right] \\
&+ \psi_\downarrow(1)\delta_{\nu,\uparrow}\left[\Lambda_{s,Z}^{(2)}\left(\cos\theta_x - \cos\theta_1\right)\beta_\downarrow^*(1)\beta_\uparrow(\imath) - \right. \\
&\qquad - \Delta_s\sin\theta_x e^{-i\zeta_x}\beta_\downarrow^*(1)\beta_\downarrow(\imath) - \\
&\qquad \left. - \Delta_s\sin\theta_1 e^{-i\zeta_1}\beta_\uparrow^*(1)\beta_\uparrow(x) \quad + \delta_{x,1}\Delta_s\sin\theta_x e^{-i\zeta_x}\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2\right] \\
&+ \psi_\downarrow(1)\delta_{\nu,\downarrow}\left[-\Lambda_{s,Z}^{(2)}\left(\cos\theta_x + \cos\theta_1\right)\beta_\downarrow^*(1)\beta_\downarrow(x) - \right. \\
&\qquad - \Delta_s\sin\theta_x e^{i\zeta_x}\beta_\downarrow^*(1)\beta_\uparrow(\imath) - \\
&\qquad \left. - \Delta_s\sin\theta_1 e^{-i\zeta_1}\beta_\uparrow^*(1)\beta_\downarrow(\imath)\right] \\
&+ \psi_\uparrow(2)\delta_{\nu,\uparrow}\left[\Lambda_{s,Z}^{(2)}\left(\cos\theta_\imath + \cos\theta_2\right)\beta_\uparrow^*(2)\beta_\uparrow(x) - \right. \\
&\qquad - \Delta_s\sin\theta_x e^{-i\zeta_x}\beta_\uparrow^*(2)\beta_\downarrow(x) - \\
&\qquad \left. - \Delta_s\sin\theta_2 e^{i\zeta_2}\beta_\downarrow^*(2)\beta_\uparrow(\imath)\right] \\
&+ \psi_\uparrow(2)\delta_{\nu,\downarrow}\left[\Lambda_{s,Z}^{(2)}\left(\cos\theta_2 - \cos\theta_x\right)\beta_\uparrow^*(2)\beta_\downarrow(\imath) - \right. \\
&\qquad - \Delta_s\sin\theta_x e^{i\zeta_x}\beta_\uparrow^*(2)\beta_\uparrow(x) - \\
&\qquad \left. - \Delta_s\sin\theta_2 e^{i\zeta_2}\beta_\downarrow^*(2)\beta_\downarrow(\imath) \quad + \delta_{x,2}\Delta_s\sin\theta_\imath e^{i\zeta_x}\sum_\jmath\sum_\eta\left|\beta_\eta(\jmath)\right|^2\right] \\
&+ \psi_\downarrow(2)\delta_{\nu,\uparrow}\left[\Lambda_{s,Z}^{(2)}\left(\cos\theta_\imath - \cos\theta_2\right)\beta_\downarrow^*(2)\beta_\uparrow(x) - \right.
\end{aligned}
$$

$$
\begin{aligned}
&\quad - \Delta_s \sin\theta_x \mathrm{e}^{-\mathrm{i}\zeta_x} \beta^*_\downarrow(2)\beta_\downarrow(x) - \ldots \\
&\ldots - \Delta_s \sin\theta_2 \mathrm{e}^{-\mathrm{i}\zeta_2} \beta^*_\uparrow(2)\beta_\uparrow(x) \qquad + \delta_{x,2}\Delta_s \sin\theta_x \mathrm{e}^{-\mathrm{i}\zeta_x} \sum_\jmath \sum_\eta \left|\beta_\eta(\jmath)\right|^2 \Big] \\
+ \quad \psi_\downarrow(2)\delta_{\nu,\downarrow} \Big[&-\Lambda^{(2)}_{s,Z} (\cos\theta_x + \cos\theta_2)\, \beta^*_\downarrow(2)\beta_\downarrow(x) - \ldots \\
&\ldots - \Delta_s \sin\theta_x \mathrm{e}^{\mathrm{i}\zeta_x} \beta^*_\downarrow(2)\beta_\uparrow(x) - \quad . \\
&\ldots - \Delta_s \sin\theta_2 \mathrm{e}^{-\mathrm{i}\zeta_2} \beta^*_\uparrow(2)\beta_\downarrow(x) \Big] \\
+ \quad \psi_\nu(x) \Big[&\Lambda^{(2)}_{\mathrm{hopp}} \sum_k \sum_{\sigma,\sigma'} \beta^*_\sigma(k) \bar{R}_{k,\sigma\sigma'} \beta_{\sigma'}(k+1) - \ldots \\
&\ldots - (\delta_{\nu,\uparrow} - \delta_{\nu,\downarrow}) \Lambda^{(2)}_{s,Z} \cos\theta_x \sum_\jmath \sum_\eta \left|\beta_\eta(\jmath)\right|^2 - . \\
&. \; - \Lambda^{(2)}_{s,Z} \sum_k \cos\theta_k \left(\beta^*_\uparrow(k)\beta_\uparrow(k) - \beta^*_\downarrow(k)\beta_\downarrow(k) \right) + \ldots \\
&. + \Delta_s \sum_k \sin\theta_k \left(\beta^*_\uparrow(k)\beta_\downarrow(k)\mathrm{e}^{-\mathrm{i}\zeta_k} + \beta^*_\downarrow(k)\beta_\uparrow(k)\mathrm{e}^{\mathrm{i}\zeta_k} \right) \Big]
\end{aligned}
\tag{5 50}
$$

If these equations are studied carefully one can find some structure in them. Especially, it is possible to rewrite the expression in a compact matrix form, similar to the cases before Trying various orders, we were able to find a specific structure We shall present it already in the more general case of N sites since in the two-sites system some features get lost

5.4.5 Two Particles / N Sites ($M = 2, N$ arbitrary)

Looking back at the Hartree-Fock equation on page 134, one can quickly see that the hopping part can be expressed in a more convenient form The first part, given in the form

$$
-t \sum_{\sigma'} \Big\{ \bar{R}_{x,\nu\sigma'} \psi_{\sigma'}(x+1) \sum_\jmath \sum_\eta \left|\beta_\eta(\jmath)\right|^2 \mathrm{e}^{\frac{2\pi\mathrm{i}}{\Lambda}\frac{\Phi}{\Phi_0}} + \\
+ \bar{R}^*_{x-1,\nu\sigma'} \psi_{\sigma'}(x-1) \sum_\jmath \sum_\eta \left|\beta_\eta(\jmath)\right|^2 \mathrm{e}^{-\frac{2\pi\mathrm{i}}{\Lambda}\frac{\Phi}{\Phi_0}} \Big\},
$$

does not mix contributions of the ψ-particle with those of the β-particle Keeping the definition of the elements of $\bar{R}$ in (5 2) or better in the form

$$
\bar{R}_{k,\sigma\sigma'} = \sum_\eta \hat{R}^+_{k,\sigma\eta} \hat{R}_{k+1\eta\sigma'} \quad \text{with} \quad \hat{R}_k = \begin{pmatrix} \cos\left(\frac{1}{2}\theta_k\right) & -\mathrm{e}^{-\mathrm{i}\zeta_k} \sin\left(\frac{1}{2}\theta_k\right) \\ \mathrm{e}^{\mathrm{i}\zeta_k} \sin\left(\frac{1}{2}\theta_k\right) & \cos\left(\frac{1}{2}\theta_k\right) \end{pmatrix}
$$

in mind, this part of the hopping can be expressed with the help of the matrix[7]

$$F_H = -t \begin{pmatrix} 0 & e^{\imath f}\hat{R}_1^+\hat{R}_2 & 0 & \cdots & 0 & e^{-\imath f}\hat{R}_1^+\hat{R}_N \\ e^{-\imath f}\hat{R}_2^+\hat{R}_1 & 0 & e^{\imath f}\hat{R}_2^+\hat{R}_3 & & & 0 \\ 0 & e^{-\imath f}\hat{R}_3^+\hat{R}_2 & 0 & & & \\ \cdot & & & \cdot & & \\ 0 & & & & 0 & e^{\imath f}\hat{R}_{N-1}^+\hat{R}_N \\ e^{\imath f}\hat{R}_N^+\hat{R}_1 & 0 & \cdots & 0 & e^{-\imath f}\hat{R}_N^+\hat{R}_{N-1} & 0 \end{pmatrix} \tag{5 51}$$

in the following form

$$\left(\sum_\jmath \sum_\eta (F_H)^{\nu x}_{\eta\jmath}\psi_\eta(\jmath)\right) * \left(\sum_\jmath \sum_\eta \left|\beta_\eta(\jmath)\right|^2\right), \tag{5 52}$$

where the superscripts at F_H denote the row and the subscripts denote the column of this matrix. It is worth noting that the structure of F_H is very similar to the matrix for the hopping part of unrotated tight-binding models as for instance on page 41 Nevertheless, the existence of the rotation matrices implies a qualitative difference. It might even be interesting to investigate its effect independently of the interaction part

The rest of the hopping part consists of many small matrices within a big matrix The contribution

$$-t\psi_\nu(x)\sum_k \sum_{\sigma,\sigma'} \left\{ \bar{R}_{k,\sigma\sigma'}\beta^*_\sigma(k)\beta_{\sigma'}(k+1)e^{\frac{2\pi\imath}{\Lambda}\frac{\Phi}{\Phi_0}} + \bar{R}^*_{k-1,\sigma\sigma'}\beta^*_\sigma(k)\beta_{\sigma'}(k-1)e^{-\frac{2\pi\imath}{\Lambda}\frac{\Phi}{\Phi_0}} \right\}$$

has the same F_H-matrix character For the other two terms

$$+ \quad t\sum_{\sigma'} \left\{ \bar{R}_{x,\nu\sigma'}\beta_{\sigma'}(x+1)\sum_\jmath \sum_\eta \beta^*_\eta(\jmath)\psi_\eta(\jmath)e^{\frac{2\pi\imath}{\Lambda}\frac{\Phi}{\Phi_0}} + \right.$$
$$\left. \cdot \; + \bar{R}^*_{x-1,\nu\sigma'}\beta_{\sigma'}(x-1)\sum_\jmath \sum_\eta \beta^*_\eta(\jmath)\psi_\eta(\jmath)e^{-\frac{2\pi\imath}{\Lambda}\frac{\Phi}{\Phi_0}} \right\}$$

$$+ \quad t\beta_\nu(x)\sum_k \sum_{\sigma,\sigma'} \left\{ \bar{R}_{k,\sigma\sigma'}\beta^*_\sigma(k)\psi_{\sigma'}(k+1)e^{\frac{2\pi\imath}{\Lambda}\frac{\Phi}{\Phi_0}} + \bar{R}^*_{k-1,\sigma\sigma'}\beta^*_\sigma(k)\psi_{\sigma'}(k-1)e^{-\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}} \right\}$$

the matrices, which are denoted with the symbol $P^{\nu x}_{\eta\jmath}$, have the following form.

[7] $f = \frac{2\pi}{N}\frac{\Phi}{\Phi_0}$

$f = \frac{2\pi}{N}\frac{\Phi}{\Phi_0}$

$$
P^{\uparrow x}_{\uparrow j} =
\begin{array}{c}
\begin{array}{cccccc}
\uparrow, x-1 & \downarrow, x-1 & \uparrow, x & \downarrow, x & \uparrow, x+1 & \downarrow, x+1
\end{array} \\
\begin{pmatrix}
 & & te^{if}\bar{R}_{j-1,\uparrow\uparrow} & & & \\
 & & te^{if}\bar{R}_{j-1,\downarrow\uparrow} & & & \\
te^{-if}\bar{R}_{x-1,\downarrow\downarrow} - te^{-if}\bar{R}_{x-1,\uparrow\downarrow} & & E & & te^{if}\bar{R}_{x,\uparrow\uparrow} & te^{if}\bar{R}_{x,\uparrow\downarrow} \\
 & & te^{-if}\bar{R}_{j,\downarrow\downarrow} & & & \\
 & & -te^{-if}\bar{R}_{j,\downarrow\uparrow} & & &
\end{pmatrix}
\end{array}
\begin{array}{l}
\uparrow, j-1 \\ \downarrow, j-1 \\ \uparrow, j \\ \downarrow, j \\ \uparrow, j+1 \\ \downarrow, j+1
\end{array}
$$

$$
P^{\downarrow\downarrow}_{\uparrow j} =
\begin{pmatrix}
 & & te^{if}\bar{R}_{j-1,\uparrow\uparrow} & & & \\
 & & te^{if}\bar{R}_{j-1,\downarrow\uparrow} & & & \\
-te^{-if}\bar{R}_{x-1,\downarrow\uparrow}\, te^{-if}\bar{R}_{x-1,\uparrow\uparrow} & & E & & te^{if}\bar{R}_{x,\downarrow\uparrow} & te^{if}\bar{R}_{x,\downarrow\downarrow} \\
 & & te^{-if}\bar{R}_{j,\downarrow\downarrow} & & & \\
 & & -te^{-if}\bar{R}_{j,\downarrow\uparrow} & & &
\end{pmatrix}
$$

$$
P^{\uparrow x}_{\downarrow j} =
\begin{pmatrix}
 & & te^{if}\bar{R}_{j-1,\uparrow\downarrow} & & & \\
 & & te^{if}\bar{R}_{j-1,\downarrow\downarrow} & & & \\
te^{-if}\bar{R}_{x-1\,\downarrow\downarrow} - te^{-if}\bar{R}_{x-1\,\uparrow\downarrow} & & & E & te^{if}\bar{R}_{x,\uparrow\uparrow} & te^{if}\bar{R}_{x,\uparrow\downarrow} \\
 & & -te^{-if}\bar{R}_{j,\uparrow\downarrow} & & & \\
 & & te^{-if}\bar{R}_{j\,\uparrow\uparrow} & & &
\end{pmatrix}
$$

$$
P^{\downarrow x}_{\downarrow j} =
\begin{pmatrix}
 & & & te^{if}\bar{R}_{j-1,\uparrow\downarrow} & & \\
 & & & te^{if}\bar{R}_{j-1,\downarrow\downarrow} & & \\
-te^{-if}\bar{R}_{x-1,\downarrow\uparrow}\, te^{-if}\bar{R}_{x-1,\uparrow\uparrow} & & & E & te^{if}\bar{R}_{x,\downarrow\uparrow} & te^{if}\bar{R}_{x,\downarrow\downarrow} \\
 & & & -te^{-if}\bar{R}_{j,\uparrow\downarrow} & & \\
 & & & te^{-if}\bar{R}_{j\,\uparrow\uparrow} & &
\end{pmatrix}
$$

(5 53)

Together with such matrices it is useful to introduce a vector notation for the wave functions. Their components shall be ordered in the following way

$$\begin{aligned}\psi &:= \left(\psi_\uparrow(1)\,\psi_\downarrow(1)\,\psi_\uparrow(2)\,\psi_\downarrow(2) \quad .\,\psi_\uparrow(N-1)\,\psi_\downarrow(N-1)\,\psi_\uparrow(N)\,\psi_\downarrow(N)\right)^T \\ \psi^* &= \left(\psi^*_\uparrow(1)\,\psi^*_\downarrow(1)\,\psi^*_\uparrow(2)\,\psi_\downarrow(2)^* \,. \quad \psi^*_\uparrow(N-1)\,\psi^*_\downarrow(N-1)\,\psi^*_\uparrow(N)\,\psi^*_\downarrow(N)\right)\end{aligned}$$

and β is defined accordingly The superscript T denotes the transposition; ψ is actually a column As one can see, the asterisk stands for complex conjugation as well as transposition.

Then the matrix character of the two last mentioned hopping terms is as follows:

$$P(\beta) = \begin{pmatrix} \beta^* P^{\uparrow 1}_{\uparrow 1}\beta & \beta^* P^{\uparrow 1}_{\downarrow 1}\beta & \beta^* P^{\uparrow 1}_{\uparrow 2}\beta & \beta^* P^{\uparrow 1}_{\downarrow 2}\beta & \cdots\cdots & \beta^* P^{\uparrow 1}_{\downarrow N}\beta \\ \beta^* P^{\downarrow 1}_{\uparrow 1}\beta & \beta^* P^{\downarrow 1}_{\downarrow 1}\beta & \beta^* P^{\downarrow 1}_{\uparrow 2}\beta & \beta^* P^{\downarrow 1}_{\downarrow 2}\beta & \cdots & \\ \beta^* P^{\uparrow 2}_{\uparrow 1}\beta & & \ddots & & & \\ & & & \cdot & & \\ \vdots & & & & \cdot\ \cdot & \beta^* P^{\uparrow N}_{\downarrow N}\beta \\ \beta^* P^{\downarrow N}_{\uparrow 1}\beta & \cdots\cdots\cdots & \cdots & \cdots\cdots & \beta^* P^{\downarrow N}_{\uparrow N}\beta & \beta^* P^{\downarrow N}_{\downarrow N}\beta \end{pmatrix} \tag{5 54}$$

Such a notation allows to express the whole system of Hartree-Fock equations in a compact form What has been investigated so far is the hopping part of the Hamiltonian which has the following structure

$$E\psi\,\langle\beta^*\cdot\beta\rangle \;=\; F_H\psi\,\langle\beta^*\cdot\beta\rangle \;+\; (\beta^* F_H \beta)\,\psi \;+\; P(\beta)\psi. \tag{5 55}$$

The fact that the matrix of the non-mixed contribution, F_H, appears again together with β is more than reasonable If one looks at the β-particle as being independent of the ψ-particle then $F_H\beta = E_\beta\beta$ is the eigenvalue equation for this particle Hence, $\beta^* F_H\beta = E_\beta(\beta^*\cdot\beta)$ That means that in the case that the β-particle and the ψ-particle can be handled independently one obtains the equation

$$E\psi\,\langle\beta^*\;\beta\rangle \;=\; F_H\psi\,\langle\beta^*\;\beta\rangle \;+\; E_\beta\,\langle\beta^*\cdot\beta\rangle\psi = (E_\psi\psi + E_\beta\psi)\,\langle\beta^*\;\beta\rangle$$

which means that the total energy E is just the sum $E_\psi + E_\beta$ of the energies of the two particles In this situation of independent particles it also does not matter what kind of normalizations are applied.

In this context the condition for independence is that the influence of the matrices $P^{\nu x}_{\eta\jmath}$ has to vanish The terms which are responsible for these matrices are given. The first of them contains with

$$\sum_{\jmath}\sum_{\eta}\beta^*_\eta(\jmath)\psi_\eta(\jmath) = \langle\beta^*\cdot\psi\rangle$$

the vector product of the wave vectors which are connected with the two separated particles. If orthogonality of the wave functions were assumed this product would give zero The same sum goes together with the energy E, which is the reason for the appearance of this term in the P matrix as well In the second mentioned term the sums

$$\sum_{k}\sum_{\sigma,\sigma'}\bar{R}_{k,\sigma\sigma'}\beta^*_\sigma(k)\psi_{\sigma'}(k+1)$$

are more difficult to handle. One can at least say that in the case of no rotations, when Bloch wave functions are solutions, this term also vanishes. The argument $(k+1)$ of ψ can for Bloch wave functions be avoided by splitting off a simple exponential function So, the non-orthogonality is apparently closely related to an exchange energy already within the hopping part

What remains are the terms for the interaction. The terms which are proportional to Δ_c and $\frac{N}{U}(\Delta_c^2+\Delta_s^2)$ can be taken into consideration by writing $E - E_F^{(2,N)}$ instead of E. The various terms which go with Δ_s can be split into those which mix the ψ-expression and β-expression and those which do not mix them

Terms including $\left|\beta_\eta(\jmath)\right|^2$, these are the terms

$$-\underbrace{\left(\Delta_s+\frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\right)}_{=\Lambda_s z}(\delta_{\nu,\uparrow}-\delta_{\nu,\downarrow})\psi_\nu(x)\cos\theta_z\sum_{\jmath}\sum_{\eta}\left|\beta_\eta(\jmath)\right|^2 \qquad \text{and}$$

$$+\ \Delta_s\left(\delta_{\nu,\uparrow}\psi_\downarrow(x)e^{-i\zeta_x}+\delta_{\nu,\downarrow}\psi_\uparrow(x)e^{i\zeta_x}\right)\sin\theta_z\sum_{\jmath}\sum_{\eta}\left|\beta_\eta(\jmath)\right|^2.$$

show no mixture They can be added to the F_H matrix, which means that a

matrix

$$F_I = \begin{pmatrix} -\Lambda_{s,Z}\cos\theta_1 & \Delta_s e^{-i\zeta_1}\sin\theta_1 & & & 0 \\ \Delta_s e^{i\zeta_1}\sin\theta_1 & \Lambda_{s,Z}\cos\theta_1 & & & \\ & & \ddots & & \\ & & & -\Lambda_{s,Z}\cos\theta_N & \Delta_s e^{-i\zeta_N}\sin\theta_N \\ 0 & & & \Delta_s e^{i\zeta_N}\sin\theta_N & \Lambda_{s,Z}\cos\theta_N \end{pmatrix}.$$

has to be defined, which always appears together with F_H. This notation is reasonable, because also a term $\beta^* F_I \beta$ exists in the same way as for the hopping part The two terms in the interaction part which are proportional to $\psi_\nu(x)$,

$$- \left(\Delta_s + \frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}\right)\psi_\nu(x)\sum_k \cos\theta_k \left(\beta^*_\uparrow(k)\beta_\uparrow(k) - \beta^*_\downarrow(k)\beta_\downarrow(k)\right) \quad \text{and}$$

$$+ \Delta_s\psi_\nu(x)\sum_k \sin\theta_k \left(\beta^*_\uparrow(k)\beta_\downarrow(k)e^{-i\zeta_k} + \beta^*_\downarrow(k)\beta_\uparrow(k)e^{i\zeta_k}\right),$$

are responsible for this

All the other terms appear in small matrices $Q^{\nu\tau}_{\eta\jmath}$, which can be combined to a big matrix $Q(\beta)$ similarly to the treatment for the $P^{\nu\tau}_{\eta\jmath}$ matrices The structure of these new matrices is as follows

$$Q^{\uparrow\downarrow}_{\uparrow\jmath} = \begin{array}{c} \\ \uparrow,\jmath \\ \downarrow,\jmath \end{array} \begin{array}{c} \begin{array}{cc} \uparrow,x & \downarrow,x \end{array} \\ \begin{pmatrix} -E_F^{(2,N)} + \cos\theta_x + \cos\theta_\jmath & -e^{-i\zeta_x}\sin\theta_x \\ -e^{i\zeta_\jmath}\sin\theta_\jmath & 0 \end{pmatrix} \end{array}$$

$$Q^{\downarrow\tau}_{\uparrow\jmath} = \begin{pmatrix} -E_F^{(2,N)} - e^{i\zeta_x}\sin\theta_x & -\cos\theta_x + \cos\theta_\jmath \\ 0 & -e^{i\zeta_\jmath}\sin\theta_\jmath \end{pmatrix}$$

$$Q^{\uparrow\tau}_{\downarrow\jmath} = \begin{pmatrix} -E_F^{(2,N)} - e^{-i\zeta_\jmath}\sin\theta_\jmath & 0 \\ \cos\theta_x - \cos\theta_\jmath & -e^{-i\zeta_x}\sin\theta_x \end{pmatrix}$$

$$Q^{\downarrow\tau}_{\downarrow\jmath} = \begin{pmatrix} -E_F^{(2,N)} & -e^{-i\zeta_\jmath}\sin\theta_\jmath \\ -e^{i\zeta_x}\sin\theta_x & -\cos\theta_x - \cos\theta_\jmath \end{pmatrix} \qquad (5\,56)$$

Now the equation (5.55) can be generalized to an expression which includes the interaction. We have found out that the system of Hartree-Fock equations has the following structure.

$$\left(E - E_F^{(2,N)}\right)\psi\,\langle\beta^*\beta\rangle = (F_H+F_I)\psi\,\langle\beta^*\beta\rangle+(\beta^*(F_H+F_I)\beta)\,\psi+P(\beta)\psi+Q(\beta)\psi \tag{5 57}$$

Single equations on the other hand, that means the whole expression on page 134, can be given in the form.

$$\begin{aligned}\langle\beta^*\ \beta\rangle\left(E - E_F^{(2,N)}\right)\psi_\nu(x) &= \langle\beta^*\cdot\beta\rangle\sum_\jmath\sum_\eta(F_H+F_I)^{\nu x}_{\eta\jmath}\psi_\eta(\jmath)\\ &+ (\beta^*(F_H+F_I)\beta)\,\psi_\nu(x)\\ &+ \sum_\jmath\sum_\eta\left(\beta^*P^{\nu x}_{\eta\jmath}\beta\right)\psi\ +\ \sum_\jmath\sum_\eta\left(\beta^*Q^{\nu x}_{\eta\jmath}\beta\right)\psi\end{aligned}$$

To write the equations in such a compact way seems to be the only possiblity to recognize the structure within the Hartree-Fock equations. After a thorough study of the matrices the finding of solutions for the energy as well as the generalization to M particles should be possible This statement offers the opportunity for further investigations.

One possibility is to perform a similar iteration as suggested on page 58 Starting with an assumption for the β-particle, the formula (5 4 5) provides equations for the wave function of the other particle, ψ On the other hand (5 4 5) is of course also true if the role of β and ψ is exchanged Therefore, ψ can be inserted into the formula, and a condition for β can be obtained. The procedure has to be repeated until self-consistency is reached

Conclusions

In the present thesis we have studied many-body effects in the persistent current problem. Starting with basic considerations we were able to derive convincing expressions for the current in normal-metal mesoscopic rings threaded by a magnetic flux. These results show the single-flux periodicity which was observed in experiments. They also correspond well to other authors' findings.

Additionally, some interesting observations which are connected with the derivation were mentioned. This includes an inhomogeneous charge distribution, which is presumably related to Friedel oscillation; it includes the parity effect, which relates Fermi statistics to flux phenomena; and it includes the period halving due to averaging processes.

When taking interaction into consideration, it turned out that the persistent current within our model is not influenced by the Coulomb repulsion. It is neither enhanced nor suppressed. This contradicts the results of many other scientists and cannot be true. Since this statement was even obtained by an exact solution of the Hartree-Fock equations, it demonstrates the weakness of the Hartree-Fock approximation and implies that it is insufficient to use simple trial wave functions.

Realizing this, some new ideas were implemented in the model. We mainly tried to improve the results by using Hubbard-Stratonovic decomposition and introducing rotated spin-quantization axes for every site. There are various possibilities to do this. Most of them led to results which are not reasonable. Eventually, we found out that the physical situation is probably described best if the following steps are performed: First of all, the usual Hubbard Hamiltonian is transformed to a path-integral description. Afterwards the Hubbard-Stratonovic decomposition is applied in order to simplify the interaction term. The resulting Hamiltonian is evaluated with the help of rotated states. Using rotated creation

operators $\tilde{c}^{\dagger}_{i,\sigma}$, these states should be in the form.

$$|\psi\rangle_{n_1,\ \ldots,n_M} = C_M \sum_{i_1,\ \ldots,i_M} \sum_{\sigma_1,\ \ldots,\sigma_M} \psi^{n_1}_{\sigma_1}(i_1) \cdot \ldots \cdot \psi^{n_M}_{\sigma_M}(i_M) \tilde{c}^{\dagger}_{i_1,\sigma_1} \cdots \tilde{c}^{\dagger}_{i_M,\sigma_M} |0\rangle,$$

and no orthogonality or normalization conditions for the single-particle wave functions should be used. After the Hartree-Fock equations are solved self-consistently one can try to minimize the obtained expression for the energy with respect to the mean fields and the angles of rotation, leading to a saddle-point approximation of the integrals.

This procedure is connected with the hope that certain spin configurations allow us to obtain lower energy values than with ordinary Bloch wave functions as used in the first part of the paper. These spin structures would of course depend on the flux through the ring. Therefore, non-trivial expressions for the persistent current would be obtained.

Unfortunately, it was not possible within this master thesis to gain such results. It turned out that the suggested procedure leads to long and cumbersome equations which have no simple analytical solutions. Even for small systems, like two particles on two sites, no solution was found. On the other hand we came to the conclusion that every trial to simplify the equations by introducing further constraints leads to results which do not describe the situation properly.

The author is also aware of the fact that in principle four integrations are still missing. These are the integrals over Matsubara time, over the mean fields, over the rotation angles and over the Grassmann numbers. The first integral could be neglected if no temperature dependence is assumed. The second and the third integral can be treated in a saddle-point approximation. However, for the last integral sophisticated methods, usually leading to determinants, are necessary.

Nevertheless, it is the opinion of the author that the present paper is a good basis for further investigations. It does not only provide the possibility to gain a deeper insight into the causes of persistent current and the problems with many-body effects. The matrix representation of the Hartree-Fock equations at the end of the last chapter can also be used to start immediately with numerical calculations per iteration. It is assumed that the given case of 2 particles and N sites can easily be generalized to M particles.

Appendix A

List of Symbols

Physical Constants

k_B	Boltzmann's constant	$k_B = 1\,381 \times 10^{23} \frac{J}{K}$
c	speed of light in vacuum	$c = 3 \times 10^8 \frac{m}{s}$
e	electrical charge of an electron	$e = 1\,602 \times 10^{-19} C$
h	Planck constant	$h = 6\,626 \times 10^{-34} Js$
$\hbar$	Planck constant, reduced	$\hbar = h/2\pi$
μ_B	Bohr's magneton	$\mu_B = 9\,247 \times 10^{-24} \frac{J}{T}$
g	Landé factor for electron	$g \approx 2$
m_e	mass of an electron	$m_e = 9\,109 \times 10^{-31} kg$
Φ_0	elementary flux quantum (Gaussian units)	$\Phi_0 = \frac{hc}{e}$

Common Physical Quantities

v_F	Fermi velocity of electrons on the ring	
μ	chemical potential of statistical system	(4 3)
T	temperature	
β	inverse temperature	$\beta = 1/k_B T$
σ	Pauli spin matrices	(1 2)
B, B_z	external magnetic field and its z-component	
A	vector potential	$\mathbf{B} = \nabla \times \mathbf{A}$
$\mathcal{H}$	any Hamiltonian	
t	hopping integral in Hubbard and Heisenberg model	(1 23), (1 24)
V	repulsive Coulomb potential for adjacent sites in Heisenberg model	(1 23)
U	on-site Coulomb repulsion in Hubbard model	(1 24)
Φ	magnetic flux through the ring	
τ	imaginary (Matsubara) time	$\tau = it$
Z	partition function in path-integral formulation	(4 5)
S	action of the system (exponent of Z)	(4 7)

Paper-Specific Physical Quantities

$b^\dagger, b$	Bose creation and annihilation operators	(1.6)
$c^\dagger, c$	Fermi creation and annihilation operators	(1.14)
$c_k^\dagger$	creation of a spinless fermion (till chap. 3) or a spinor (from chap 4 onwards) at site k	
$c_{k,\sigma}^\dagger$	creation of a spin fermion at site k	
$\tilde{c}_{k,\sigma}^\dagger$	rotated fermionic operators	(4.31)
σ, η	indicates the spin of a particle	$\sigma, \eta \in \{\uparrow, \downarrow\}$
$\hat{n}_k$	occupation number operator	$\hat{n}_k = c_{k,\uparrow}^\dagger c_{k,\uparrow} + c_{k,\downarrow}^\dagger c_{k,\downarrow}$
$\hat{s}_k$	spin projection on the z-axis	$\hat{s}_k = c_{k,\uparrow}^\dagger c_{k,\uparrow} - c_{k,\downarrow}^\dagger c_{k,\downarrow}$
N	number of sites on the ring	
M	total number of particles on the ring	
$M_\uparrow, M_\downarrow$	number of spin-up and spin-down particles	
a	distance between two sites on the ring	
L	circumference of the ring	$L = aN$
E	energy of the system	
I	persistent current in the ring	$I = -c\frac{\partial E}{\partial \Phi}$
$r(x)$	function which restricts the trapped flux onto a sufficient interval, see figure 2.6	$r(x) = \left\lvert x - \left(x + \frac{1}{2}\right)\right\rvert$
$\hat{H}_0$	hopping part of the Hamiltonian	
$\hat{V}$	interaction part of the Hamiltonian	
α_i^n	parameter for the variational wave function in the Heisenberg model	(2.7)
β_i^n	parameter for the variational wave function in the Hubbard model (sometimes also used for 2nd particle)	(3.20)
γ_i^n	parameter for the variational wave function in the Hubbard model with rotated states	(4.40)
$\psi_\sigma^n(i)$	parameter for the variational wave function in the Hubbard model with spin-sensitive states	(5.36)
$\lvert\psi\rangle_{n_1, \ldots, n_M}$	state in Fock space, determined by the quantum numbers $n_1, \ldots, n_M$	
C_M	normalization constant of a M-particle state	
$\hat{R}_k(\theta, \zeta)$	rotation matrix for the spin-quantization axis	(4.19), (E.8)
$\bar{R}_k$	combination of two rotations in (5.2)	$\bar{R}_k = \hat{R}_k^+ \hat{R}_{k+1}$
θ	spherical coordinate: colatitude	
ζ	spherical coordinate: longitude	
ϑ	difference of adjacent colatitudes	$\vartheta = \frac{1}{2}(\theta_{k+1} - \theta_k)$
Ω	unit vector in the direction of spin-quantization axis	$\Omega = \Omega(\theta, \zeta)$

Paper-Specific Physical Quantities (Continuation)

λ ..	Lagrange multiplier	
$\tau\ \nu$.	site and spin index of the parameter with respect to which derivatives are taken	
n_C . . .	quantum number of this parameter	
f . .	sometimes used for the flux phase	$f = \frac{2\pi}{N}\frac{\Phi}{\Phi_0}$
N_t	number of time-discretisation steps in a path-integral approach	
$\|\Psi\rangle$	coherent state, eigenstate of annihilation operator	$c_{k,\sigma}\|\Psi\rangle = \xi_{k,\sigma}\|\Psi\rangle$
$\xi_{k,\sigma}$	Grassmann number, eigenvalue of annihilation operator	
$\tilde{\xi}_{k,\sigma}$	rotated Grassmann number	(4 20)
$\Psi, \tilde{\Psi}$.	vector of Grassmann numbers with components $\xi_{k,\sigma}, \tilde{\xi}_{k,\sigma}$	
w ..	angle phase winding number = number of spin-rotations around the perimeter when going ones along the ring	p 89
Δ_c, Δ_s	(fictitious) mean fields over which is integrated in the Hubbard-Stratonovic decomposition, belonging to the charge and spin degree of freedom respectively	
Δ_c' ..	modification of Δ_c to avoid complex values .	$\Delta_c' = 2\mathrm{Re}(\imath\Delta_c)$
Δ_Z . ..	energy constant in Zeemann effect, not a mean field (!)	$\Delta_Z = \frac{qh^2}{m_e a^2}$
$\Lambda_{s,Z}^{(N)}$ ..	auxiliary variable for matrix equations	$\Lambda_{s,Z}^{(N)} = \Delta_s + \frac{\Delta_Z}{N^2}\frac{\Phi}{\Phi_0}$
$\Lambda_{\mathrm{hopp}}^{(N)}$ ..	auxiliary variable for matrix equations .. .	$\Lambda_{\mathrm{hopp}}^{(N)} = -2t\cos\left(\frac{2\pi\imath}{N}\frac{\Phi}{\Phi_0}\right)$
a_k .	auxiliary variables	(5 11)
$E_F^{(M,N)}$ ..	fixed (angle independent) energy contribution of the fields	(5 11)
w_1, w_2 .	auxiliary variables	(5 14)
χ .. .	phase of a wave function	
$r_{\mathrm{I\,II}}$ . .	ratio between the components of the wave function for the solutions I and II in the two-site problem	$r_{\mathrm{I,II}} = \gamma_1^{\mathrm{I,II}}/\gamma_2^{\mathrm{I,II}}$
F_{II}, F_I	matrices for a description of 2 particles (non-mixed)	sect 5 4 5
P, Q ..	matrices for a description of 2 particles (mixed)	sect. 5 4 5

Common Abbreviations

i	imaginary unit	$\mathrm{i}^2 = -1$
$\mathbb{C}$	set of complex numbers	
$\mathrm{Re}(z)/\mathrm{Im}(z)$	real/imaginary part of a complex number z	
$\mathcal{P}(M)$ .. .	set of all permutations of M integers	
$(-1)^{\mathrm{sgn}\wp}$	parity of the permutation $\wp$	$= \begin{cases} 1 \text{ if } \wp \text{ even} \\ -1 \text{ if } \wp \text{ odd} \end{cases}$
id	identical permutation	
h c.	hermitian conjugate	
$\delta_{i,j}$.	Kronecker delta of i and j	$\delta_{i,j} = \begin{cases} 1 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{cases}$
ε_{ijk} . . .	totally antisymmetric tensor	
$\mathbb{1}$ .. .	unitary operator	
$\wedge$.	logical operator AND	
$\forall x$	the statement before this symbol is valid *for all* x	
$[\cdot,\cdot]_-$	commutator of two operators .	$[\hat{A},\hat{B}]_- = \hat{A}\hat{B} - \hat{B}\hat{A}$
$[\cdot,\cdot]_+$	anticommutator of two operators	$[\hat{A},\hat{B}]_+ = \hat{A}\hat{B} + \hat{B}\hat{A}$
□ .. .	marks the end of a proof or example	
$\alpha_1 \cdots \widehat{\alpha_C} \cdots \alpha_M$	product of all α's with omission of α_C .	$= \alpha_1 \ \alpha_{C-1}\alpha_{C+1} \cdots \alpha_M$

Appendix B

The p - A - connection

The aim of this appendix is to show which effect the existence of a vector potential $\mathbf{A}(\mathbf{r}, t)$ has on the Hamiltonian and the wave function of a system in first quantization. For both expressions the changes compared to the free-electron situation are derived.

Change of the Hamiltonian

It is possible to put the effect of a magnetic field on an electric charge into the Hamiltonian of the system by substituting the expression for the momentum in the following way

$$\begin{aligned} \hat{\mathbf{p}} &\longrightarrow \hat{\mathbf{p}} - e\mathbf{A} \qquad \text{SI units,} \\ \hat{\mathbf{p}} &\longrightarrow \hat{\mathbf{p}} - \tfrac{e}{c}\mathbf{A} \qquad \text{Gaussian units,} \end{aligned} \tag{B 1}$$

where e is the elementary charge or the charge of an electron and c is the velocity of light

Proof: An explanation of the substitution goes back to analytical mechanics:[1] The Hamiltonian principle states that all processes in nature develop in such a way that the action

$$S = \int_{t_1}^{t_2} L \, \mathrm{d}t,$$

[1] the following explanation is based on Dicke *et al* [49] chap 5 and Nolting [50]

becomes an extremum. Here L is the Lagrangian of the system. According to calculus of variation, this condition is equivalent to the Euler-Lagrange equations

$$\frac{\partial L}{\partial q_i} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial q_i}\right) = 0,$$

where q_i is a (generalized) coordinate

These equations are fulfilled for conservative systems with holonom constraints In this case, a potential V exists with $m\ddot{q}_i = -\frac{\partial V}{\partial q_i}$ (Newton's law) and L can be written as

$$L = T - V \quad \text{with} \quad \begin{aligned} T &= \sum \tfrac{1}{2} m q_i^2 && \text{kinetic energy} \\ V &= V(q_i) && \ldots \text{potential energy} \end{aligned}$$

However, there is no change in the results, if instead of the potential V only a generalized potential U is available. Such a generalized potential is defined by the constraint that (generalized) forces can be obtained in the following way

$$F_j = -\frac{\partial U}{\partial q_j} + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial U}{\partial q_j}\right)$$

Then the Lagrangian can, similar to the previous case, be defined as $L = T - U$, and the Euler-Lagrange equations are still fulfilled

For a (Lorentz) force acting on a particle with a charge q in an electromagnetic field such a generalized potential exists, because

$$\begin{aligned} \mathbf{F} &= q[\mathrm{E} + \mathrm{v} \times \mathrm{B}] && \text{SI units} \\ \mathbf{F} &= q\left[\mathrm{E} + \tfrac{1}{c}(\mathrm{v} \times \mathrm{B})\right] && \text{Gaussian units} \\ \mathbf{E} &= -\nabla\phi - \tfrac{1}{c}\tfrac{\partial \mathbf{A}}{\partial t} && \downarrow \\ \mathbf{B} &= \nabla \times \mathbf{A} \end{aligned}$$

$$\begin{aligned} \Longrightarrow \quad \mathbf{F} &= q\left[-\nabla\phi - \tfrac{1}{c}\left\{\tfrac{\partial \mathbf{A}}{\partial t} - \mathrm{v} \times (\nabla \times \mathrm{A})\right\}\right] && \tfrac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} = \tfrac{\partial \mathbf{A}}{\partial t} + (\mathrm{v}\,\nabla)\mathbf{A} \\ &= q\left[-\nabla\left(\phi - \tfrac{1}{c}\mathrm{v}\mathrm{A}\right) - \tfrac{1}{c}\tfrac{\mathrm{d}\mathbf{A}}{\mathrm{d}t}\right] && \mathrm{v} \times (\nabla \times \mathrm{A}) = \nabla(\mathrm{v}\mathrm{A}) - (\mathrm{v}\nabla)\mathbf{A} \end{aligned}$$

$$\Longrightarrow \quad U \equiv q\left(\phi - \tfrac{1}{c}\mathrm{v}\mathrm{A}\right)$$

Therefore, it is

$$L = T - q\phi + \frac{q}{c}\mathrm{v} \cdot \mathrm{A}.$$

With the help of the Lagrangian, a generalized momentum can be obtained

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial T}{\partial \dot{q}_i} + \frac{q}{c} A_i$$

The Hamiltonian is the Legendre transformation of the Lagrangian, and hence:

$$\mathcal{H} = \sum_i p_i q_i - L.$$

If only skleronom holonom constraints are taken into consideration, that is if $\mathbf{r}_i(q_1, \ldots, q_s, t) = \mathbf{r}_i(q_1 \quad ., q_s)$, then

$$T = \sum_{ij} \alpha_{ij} q_i q_j \quad \Longrightarrow \quad \sum_i \frac{\partial T}{\partial \dot{q}_i} q_i = 2T$$

This leads to

$$\mathcal{H} = \sum_i \left(\frac{\partial T}{\partial q_i} + \frac{q}{c} A_i \right) q_i - \left(T - q\phi + \frac{q}{c} \mathbf{v} \cdot \mathbf{A} \right) = T + q\phi.$$

Therefore, for the movement of a particle within an electromagnetic potential $\left(\mathbf{A}, \frac{1}{c}\phi\right)$ the following two results have been obtained

1. The canonical momentum is $\mathbf{p} = m\mathbf{v} + \frac{q}{c}\mathbf{A}$ (B 2)

2. The Hamiltonian is $\mathcal{H} = \frac{\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2}{2m} + q\phi$ (B 3)

The calculation has been done in Gaussian units because this system of units is common in mesoscopics Furthermore, it is much easier to go from Gaussian units to the SI-system than the other way around. The only thing to do in this context is to omit $\frac{1}{c}$ everywhere. □

Change of the Wave Function

The modified structure of the Hamiltonian $\mathcal{H}$ compared to the case with no vector potential, influences of course also the expression for the wave function [51] Given that $\psi(\mathbf{r}, t)$ is the solution for the Schrödinger equation of a free electron with charge e, the claim is that

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}, t) \exp\left[-\frac{ie}{\hbar c} \int^{\mathbf{r}} \mathbf{A}(\mathbf{s})\, \mathrm{d}\mathbf{s} \right] \tag{B.4}$$

solves the Schrödinger equation for the Hamiltonian derived above

Proof 1: It has to be shown that

$$\mathcal{H}\Psi(\mathbf{r},t) = \mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)$$

with $\mathcal{H}$ given in (B 3) This can be done directly by rewriting the Hamiltonian in the following way.

$$\begin{aligned}\mathcal{H} &= \frac{\mathbf{p}^2}{2m} + \frac{e}{2mc}(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}) + \frac{e^2}{2mc^2}\mathbf{A}^2 - e\phi \\ &= -\frac{\hbar^2}{2m}\nabla^2 + \frac{e}{2mc}(2\mathbf{A}\cdot(-\mathrm{i}\hbar\nabla) - \mathrm{i}\hbar\nabla\cdot\mathbf{A}) + \frac{e^2}{2mc^2}\mathbf{A}^2 - e\phi \\ &= -\frac{\hbar^2}{2m}\nabla^2 + \frac{e}{2mc}2\mathbf{A}\cdot(-\mathrm{i}\hbar\nabla) + \frac{e^2}{2mc^2}\mathbf{A}^2 - e\phi \qquad \text{(B 5)}\end{aligned}$$

Two remarks explain this calculation. First, $\mathbf{p}\cdot\mathbf{A} = \mathbf{A}\cdot\mathbf{p} - \mathrm{i}\hbar\nabla\cdot\mathbf{A}$ because

$$\begin{aligned}[p_i, A_i(\mathbf{r})]\,\Psi(\mathbf{r},t) &= -\mathrm{i}\hbar\frac{\partial}{\partial x_i}A_i(\mathbf{r})\Psi(\mathbf{r},t) + \mathrm{i}\hbar A_i(\mathbf{r})\frac{\partial}{\partial x_i}\Psi(\mathbf{r},t) \\ &= -\mathrm{i}\hbar\left(\frac{\partial A_i(\mathbf{r})}{\partial x_i}\right)\Psi(\mathbf{r},t) = -\mathrm{i}\hbar\,(\nabla\cdot\mathbf{A})\,\Psi(\mathbf{r},t)\end{aligned}$$

Secondly, the Coulomb gauge $\nabla\cdot\mathbf{A} = 0$ was used Furthermore, a pure radiation field, that is $\phi = 0$, is assumed. By noting that the derivatives of the wave function (B 4) are of the form

$$\begin{aligned}\nabla\Psi(\mathbf{r},t) &= \exp\left[-\frac{\mathrm{i}e}{\hbar c}\int^{\mathbf{r}}\mathbf{A}(\mathbf{s})\,\mathrm{d}\mathbf{s}\right]\left(\nabla\psi - \frac{\mathrm{i}e}{\hbar c}\mathbf{A}\psi\right) \\ \nabla^2\Psi(\mathbf{r},t) &= \exp\left[-\frac{\mathrm{i}e}{\hbar c}\int^{\mathbf{r}}\mathbf{A}(\mathbf{s})\,\mathrm{d}\mathbf{s}\right]\left(\nabla^2\psi - \frac{2\mathrm{i}e}{\hbar c}\mathbf{A}\cdot(\nabla\psi) - \right. \\ &\qquad \left. -\frac{e^2}{\hbar^2 c}\psi\mathbf{A}^2 - \frac{\mathrm{i}e}{\hbar c}\psi\nabla\ \mathbf{A}\right) \\ \frac{\partial}{\partial t}\Psi(\mathbf{r},t) &= \exp\left[-\frac{\mathrm{i}e}{\hbar c}\int^{\mathbf{r}}\mathbf{A}(\mathbf{s})\,\mathrm{d}\mathbf{s}\right]\frac{\partial\psi}{\partial t}\end{aligned}$$

and using this expression for the calculation of $\mathcal{H}$ in (B 5) operating on $\Psi(\mathbf{r},t)$ one can easily see that the Schrodinger equation is fulfilled. □

There is another proof possible for the case that the magnetic field $\mathbf{B} = 0$ along a path of consideration We use the theory of gauge transformations in electromagnetism

$$\begin{aligned}\phi &\longrightarrow \phi' = \phi - \frac{1}{c}\frac{\partial}{\partial t}\lambda(\mathbf{r},t) \\ \mathbf{A} &\longrightarrow \mathbf{A}' = \mathbf{A} + \nabla\chi(\mathbf{r},t)\end{aligned}$$

and claim: If a wave function $\Psi(\mathbf{r},t)$ is a solution of the Schrodinger equation $\mathcal{H}\Psi(\mathbf{r},t) = E\Psi(\mathbf{r},t)$ and a gauge transformation of the proposed form is applied then simultaneously a transformation of the wave function Ψ of the form

$$\Psi(\mathbf{r},t) \longrightarrow \Psi'(\mathbf{r},t) = \Psi(\mathbf{r},t)\exp\left[-\frac{ie}{\hbar c}\chi\right]$$

is necessary for the invariance of the Schrödinger equation [32, 52]

$$\begin{aligned}
\textbf{Proof 2:}\quad \mathcal{H}'\Psi' &= \frac{1}{2m}\left(-i\hbar\nabla + \frac{e}{c}\mathbf{A}'\right)^2 \Psi'(\mathbf{r},t) \\
&= \frac{1}{2m}\left(-i\hbar\nabla + \frac{e}{c}\mathbf{A} + \frac{e}{c}\nabla\chi\right)^2 \Psi(\mathbf{r},t)\exp\left[-\frac{ie}{\hbar c}\chi\right] \\
&= \frac{1}{2m}\exp\left[-\frac{ie}{\hbar c}\chi\right]\left(-i\hbar\nabla + \frac{e}{c}\mathbf{A}\right)^2 \Psi(\mathbf{r},t) \\
&= \exp\left[-\frac{ie}{\hbar c}\chi\right]\mathcal{H}\Psi(\mathbf{r},t) = \exp\left[-\frac{ie}{\hbar c}\chi\right] E\Psi(\mathbf{r},t) \\
&= E\Psi'(\mathbf{r},t)
\end{aligned}$$

That means that the eigenfunctions of a gauged Hamiltonian are the eigenfunctions of the Hamiltonian without gauge times $\exp\left[-\frac{ie}{\hbar c}\chi\right]$ The eigenvalue E is not affected by the gauge transformation.

In regions with no magnetic field $\mathbf{A}(\mathbf{r},t)$ can be written as a gradient of a scalar field, which automatically gives zero for $\mathbf{B} = \nabla \times \mathbf{A}$ On the other hand, if $\mathbf{A}(\mathbf{r},t) = \nabla\chi(\mathbf{r},t)$ then $\mathbf{A}$ can be understood as a gauge transformation from the state of no vector potential $\mathbf{A}(\mathbf{r},t) \equiv 0$ Therefore,

$$\begin{aligned}
\Psi(\mathbf{r},t) &= \psi(\mathbf{r},t)\exp\left[-\frac{ie}{\hbar c}\chi(\mathbf{r},t)\right] = \psi(\mathbf{r},t)\exp\left[-\frac{ie}{\hbar c}\int^{\mathbf{r}}\nabla\chi(\mathbf{s},t)\,d\mathbf{s}\right] \\
&= \psi(\mathbf{r},t)\exp\left[-\frac{ie}{\hbar c}\int^{\mathbf{r}}\mathbf{A}(\mathbf{s},t)\,d\mathbf{s}\right],
\end{aligned}$$

which proves again (B 4) □

Appendix C

The Pauli Problem

In many calculations, as for instance in chapter 2 1.4, appear expressions like

$$\sum_{A=1}^{M} \sum_{\substack{i_1 \\ j_1}} \cdots \sum_{\substack{i_M \\ j_M}} \alpha_{i_1 \cdots i_M} \alpha^*_{j_1 \cdots j_M} \langle 0 | c_{j_M} \cdots c_{j_1} c^\dagger_{i_1} \cdots c^\dagger_{i_M} | 0 \rangle$$

Due to the Pauli exclusion principle two fermions with the same set of quantum numbers are not allowed to occupy the same site. This property is automatically included in the second quantized representation As soon as i_k's are equal, the operator product $c^\dagger_{i_1} \cdot \cdots \cdot c^\dagger_{i_M} | 0 \rangle$ vanishes The coefficients in front of this product are unimportant because they are multiplied by zero

However, it might be questionable what there contribution is as soon as all operators are abolished Perhaps one should reduce the expression above

$$\text{not to} \quad \sum_{i_1 \cdots i_M} \sum_{\wp \in \mathcal{P}(M)} (-1)^{\operatorname{sgn}\wp} \alpha_{i_1 \cdots i_M} \alpha^*_{\wp(i_1 \cdots i_M)}$$

$$\text{but to} \quad \sum_{i_1 \cdots i_M}{}' \sum_{\wp \in \mathcal{P}(M)} (-1)^{\operatorname{sgn}\wp} \alpha_{i_1 \cdots i_M} \alpha^*_{\wp(i_1 \cdots i_M)},$$

where the prime indicates that the summation indices should be distinct: $i_k \neq i_l$ for $k \neq l$. As a result sums would not go over the whole range of possible sites any more, what might influence their value This problem is discussed here

Normalization of many-particle states

We know that the one-particle state $|\psi\rangle_1 = \sum_{k=1}^{N} \phi_k c^\dagger_k | 0 \rangle$ is normalized. The many-particle state is constructed by a superposition of one-particle states

$$|\psi\rangle_M = \prod_{j=1}^{M} \left(\sum_{k=1}^{N} \phi_k^{(j)} c_k^\dagger \right) |0\rangle$$

Because in the primed version of products with adjoint states sums do not run over the whole range of sites any more, it could be questionable whether $|\psi\rangle_M$ is still normalized. A calculation of the example of two particles gives

$$\begin{aligned}
{}_2\langle\psi|\psi\rangle_2 &= \langle 0| \left(\sum_i \phi_i^* c_i \right) \left(\sum_j \psi_j^* c_j \right) \left(\sum_k \psi_k c_k^\dagger \right) \left(\sum_l \phi_l c_l^\dagger \right) |0\rangle \\
&= \sum_{ij,kl} \phi_i^* \psi_j^* \psi_k \phi_l \langle 0| c_i c_j c_k^\dagger c_l^\dagger |0\rangle \, (\delta_{i,l}\delta_{j,k} + \delta_{i,k}\delta_{j,l}) \\
&= \sum_{ij}{}' \phi_i^* \psi_j^* \psi_j \phi_i - \sum_{ij}{}' \phi_i^* \psi_j^* \psi_i \phi_j \underline{+ \phi_i^* \psi_i^* \psi_i \phi_i - \phi_i^* \psi_i^* \psi_i \phi_i} \\
&= \sum_{ij} \phi_i^* \psi_j^* \psi_j \phi_i - \sum_{ij} \phi_i^* \psi_j^* \psi_i \phi_j ,
\end{aligned}$$

what shows the unimportance of the prime

The same procedure is possible for an arbitrary number of particles One can fill the sums step by step, because there are always two permutations which differ only in one transposition and have the opposite sign. Therefore, it is possible to add in both sums a term with the same index for the transposed factors.

Expectation Values

$$\begin{aligned}
{}_2\langle\psi|\hat{n}_x|\psi\rangle_2 &= \sum_{ij\,kl} \phi_i^* \psi_j^* \psi_k \phi_l \langle 0| c_i c_j c_x c_x^\dagger c_k^\dagger c_l^\dagger |0\rangle \\
&\qquad (\delta_{x,k}\delta_{j,x}\delta_{i,l} - \delta_{x,k}\delta_{i,\tau}\delta_{j,l} - \delta_{x,l}\delta_{j,\tau}\delta_{i,x} + \delta_{\tau,l}\delta_{i,\tau}\delta_{j,k}) \\
&= \sum_{i/j\neq x}{}' \left(\phi_i^* \psi_x^* \psi_x \phi_i - \phi_x^* \psi_j^* \psi_x \phi_j - \phi_i^* \psi_x^* \psi_i \phi_x + \phi_x^* \psi_j^* \psi_j \phi_i \right) \\
&\qquad \underline{\pm 2 \phi_\tau^* \psi_x^* \psi_\tau \phi_\tau} \\
&= \sum_{i,j} \left(\phi_i^* \psi_x^* \psi_x \phi_i - \phi_x^* \psi_j^* \psi_x \phi_j - \phi_i^* \psi_x^* \psi_i \phi_x + \phi_\tau^* \psi_j^* \psi_j \phi_\tau \right)
\end{aligned}$$

In the same way as before we get that the missing summand in each sum can always be added, because it cancels in two sums

Hence, the answer to the Pauli problem is that in sums like

$$\sum_{i_1 \ldots i_M}{}' \sum_{p \in \mathcal{P}(M)} (-1)^{\mathrm{sgn}\, p} \alpha_{i_1 \ldots i_M} \alpha^*_{p(i_1 \ldots i_M)}$$

the prime, that is the constraint $i_k \neq i_l$ for $k \neq l$ is of no importance and the sum can be handled as if the prime / this constraint were not there.

Appendix D

Fermionic Path Integrals

The Feynman Kernel

In classical mechanics every process seems to behave in such a way that the well-known principle of least action is obeyed. It states that the classical path $\bar{q}(t)$ is that for which S is an extremum. Here, S is the action and is given by

$$S[q] = \int_{t_a}^{t_b} \mathrm{d}\, t\, L(q, q, t), \tag{D 1}$$

with $L = pq - \mathcal{H}(p, q)$ being the Lagrangian.

In quantum mechanics this principle is replaced by a **path integral** [54, 55]. That means that all paths contribute to the total amplitude, but contribute at different phases

$$\mathcal{K}(b, a) = \text{const} \cdot \sum_{\substack{\text{over all paths} \\ \text{from } a \text{ to } b}} \exp\left[\mathrm{i}\frac{S[q(t)]}{\hbar}\right] =: \int \mathcal{D}[q]\, e^{\frac{\mathrm{i}}{\hbar} S[q]} \tag{D 2}$$

Since the action is measured in units of $\hbar$, the classical limit leads, similar to above, only to the contribution of the path with extremal action. Feynman called the expression $\mathcal{K}(b, a)$ a kernel.[1] Its modulus squared, $|\mathcal{K}(b, a)|^2$, gives the probability for a particle to go from a point $a = (q_a, t_a)$ to a point $b = (q_b, t_b)$.

Proof: That this is the case can be shown by looking at the time evolution operator $U(t_b, t_a)$, which describes how a state changes in time. It is connected

[1] Sometimes it is also called "propagator"

to the kernel via

$$\left.\begin{aligned} |\psi_{t_b}\rangle &= U(t_b,t_a)\,|\psi_{t_a}\rangle \\ \psi_{t_b}(q_b) &= \int \mathrm{d}\,q_a \mathcal{K}(b,a)\psi_{t_a}(q_a) \end{aligned}\right\} \Rightarrow \mathcal{K}(q_b t_b, q_a t_a) = \langle q_b | U(t_b,t_a)\,|q_a\rangle$$

On the other hand, the properties of the time evolution operators allow the following approximation [57]

$$U(t,t_a) = \lim_{N_t\to\infty}\left(\mathbb{1} - \frac{1}{\hbar}\Delta t\mathcal{H}(t_{N_t})\right)\cdots\left(\mathbb{1} - \frac{1}{\hbar}\Delta t\mathcal{H}(t_2)\right)\left(\mathbb{1} - \frac{\mathrm{i}}{\hbar}\Delta t\mathcal{H}(t_1)\right) \quad \text{(D.3)}$$

by discretising the time in intervals of $\Delta t = \frac{t-t_a}{N_t}$ The limit can be evaluated with the help of the time order operator $\hat{T}$, leading to

$$U(t,t_a) = \hat{T}\exp\left[\frac{1}{\hbar}\int_{t_a}^{t}\mathcal{H}(t')\mathrm{d}t'\right]. \quad \text{(D 4)}$$

If the Hamiltonian $\mathcal{H}$ is independent of time, both expressions simplify to

$$U(t,t_a) = \lim_{N_t\to\infty}\left(\mathbb{1} - \frac{\frac{1}{\hbar}(t-t_a)\mathcal{H}}{N_t}\right)^{N_t} = \exp\left[-\frac{\mathrm{i}}{\hbar}(t-t_a)\mathcal{H}\right] \quad \text{(D.5)}$$

Traditionally, the Hamiltonian is a function of the momentum operator P and the coordinate operator Q Their eigenvectors satisfy the equations

$$\begin{aligned} P\,|p\rangle = p\,|p\rangle \quad &\text{and} \quad Q\,|q\rangle = q\,|q\rangle \\ \langle q|p\rangle = \frac{1}{2\pi\hbar}\mathrm{e}^{\mathrm{i}pq/\hbar} \quad &\text{and} \quad \langle p|q\rangle = \frac{1}{2\pi\hbar}\mathrm{e}^{-\mathrm{i}pq/\hbar} \end{aligned} \quad \text{(D 6)}$$

as well as a resolution of unity

$$\int_{-\infty}^{\infty}\mathrm{d}q\,|q\rangle\langle q| = \mathbb{1} \quad \text{and} \quad \int_{-\infty}^{\infty}\mathrm{d}p\,|p\rangle\langle p| = \mathbb{1}, \quad \text{(D.7)}$$

what allows two important modifications of the expression for the time evolution operator

First of all, unities might be included for each time step in (D 3) what leads to

$$U(t,t_a) = \lim_{N_t\to\infty}\left(\prod_{j=0}^{N_t}\int_{-\infty}^{\infty}\mathrm{d}q_j\right)|q_{N_t}\rangle\left(\prod_{j=1}^{N_t}\langle q_j|\mathbb{1} - \frac{1}{\hbar}\Delta t\mathcal{H}\,|q_{j-1}\rangle\right)\langle q_0| \quad \text{(D 8)}$$

Secondly, the eigenvalues of the momentum and the coordinate operator can replace the operators itself. How this happens depends usually on the order of

the operators Q and P. However, for the common case $\mathcal{H}(P,Q) = \frac{1}{2m}P^2 + V(Q)$ one does not have to care about this. By using the resolution of unity for the momentum operators $|p_j\rangle$ and with (D 6) one obtains therefore

$$U(t,t_a) = \lim_{N_t\to\infty}\left(\prod_{j=0}^{N_t}\int_{-\infty}^{\infty} dq_j\right)|q_{N_t}\rangle\left(\prod_{j=1}^{N_t}\int\frac{dp_j}{2\pi\hbar}e^{ip_j(q_j-q_{j-1})/\hbar} * \ldots \cdot * \underbrace{\left(1-\frac{1}{\hbar}\Delta t\mathcal{H}(p_j,q_j)\right)}_{\approx e^{-\frac{1}{\hbar}\Delta t\mathcal{H}(p_j,q_j)}}\right)\langle q_0|$$

$$\mathcal{K}(b,a) = \int\mathcal{D}[p]\,\mathcal{D}[q]\,\exp\left[\frac{1}{\hbar}\int_{t_a}^{t_b}(p\cdot\dot{q}-\mathcal{H}(p,q,t))\,dt\right]\Bigg|_{q_a}^{q_b}$$

Here the boundaries indicated that only such ways are allowed which start in q_a and end in q_b. The result is the same as (D 2) with the only difference that the integration is done in phase space with a Hamiltonian which depends on p and q and not with a Lagrangian which depends on q and $\dot{q}$. □

Grassmann Numbers

The description in the previous section was given in order to make it easier to understand the differences in the case of fermionic path integrals. The main alteration has its reason in the fact that the Hamiltonian in second quantization does not consist of P and Q, but of creation and annihilation operators. $c_j^\dagger$ and c_j. Therefore, the resolution of unity (D.7) has to be expressed now in terms of eigenfunctions of the new operators.

States $|\Psi\rangle$ which are eigenfunctions of all annihilation operators are called **coherent states**. If they satisfy the equations

$$c_j|\Psi\rangle = \xi_j|\Psi\rangle \quad\text{and}\quad \langle\Psi|c_j^\dagger = \langle\Psi|\xi_j^* \tag{D 9}$$

then the anticommutation relation of Fermi operators implies that their eigenvalues can not behave like ordinary numbers but must also anticommute:

$$\xi_i\xi_j + \xi_j\xi_i = 0$$

The algebra of such numbers is called **Grassmann algebra** [31, 56]

The rather strange behaviour of so-called Grassmann numbers has a lot of consequences. The most obvious one is the nilpotence of these numbers,

$$\xi_i^2 \equiv 0 \quad \forall i$$

Every Grassmann number ξ_j exists together with its conjugate ξ_j^* The most important properties for conjugation are

$$\left(\xi_j^*\right)^* = \xi_j, \quad \left(\lambda\xi_j\right)^* = \lambda^*\xi_j^* \quad \forall\, \lambda \in \mathbb{C},$$

$$\left(\xi_{j_1}\xi_{j_2} \quad \cdot\xi_{j_n}\right)^* = \xi_{j_n}^* \cdots \xi_{j_2}^*\xi_{j_1}^*.$$

The differentiation with respect to Grassmann numbers is defined similar to the complex case, except that in order for the derivative operator $\frac{\partial}{\partial\xi_j}$ to act on ξ_j, the variable ξ_j has to be anticommuted through until it is adjacent to $\frac{\partial}{\partial\xi_j}$ The same anticommutation rule applies for integration. The latter is well-defined by the conditions that the integral of an exact differential form vanishes and that the integral of a Grassmann number is normalized

$$\int \mathrm{d}\xi\, 1 = 0, \quad \int \mathrm{d}\xi\, \xi = 1. \tag{D 10}$$

Example: If one supposes that the Grassmann algebra is generated by only two Grassmann numbers ξ and ξ^* then an operator has the general form

$$A(\xi^*, \xi) = a_0 + a_1\xi + a_2\xi^* + a_3\xi^*\xi \quad \text{with } a_0, \ldots, a_3 \in \mathbb{C}$$

$\Longrightarrow$

$$\frac{\partial}{\partial\xi}A(\xi^*, \xi) = a_1 - a_3\xi^*, \qquad \frac{\partial}{\partial\xi^*}A(\xi^*, \xi) = a_2 + a_3\xi$$

$$\frac{\partial}{\partial\xi^*}\frac{\partial}{\partial\xi}A(\xi^*, \xi) = -a_3 = -\frac{\partial}{\partial\xi}\frac{\partial}{\partial\xi^*}A(\xi^*, \xi)$$

$$\int \mathrm{d}\xi\, A(\xi^*, \xi) = a_1 - a_3\xi^*, \qquad \int \mathrm{d}\xi^*\, A(\xi^*, \xi) = a_2 + a_3\xi$$

$$\int \mathrm{d}\xi^*\mathrm{d}\xi\, A(\xi^*, \xi) = -a_3 = \int \mathrm{d}\xi\mathrm{d}\xi^*\, A(\xi^*, \xi)$$

It is worth noting that differentiation and integration are identical and that the differential operators $\frac{\partial}{\partial\xi}$ and $\frac{\partial}{\partial\xi^*}$ anticommute □

Furthermore, it is natural to demand that the Grassmann numbers do not only anticommute with one another, but obey also an anticommutation relation

with fermionic operators, f e $\xi_i c_j + c_j \xi_i = 0$. Additionally, the conjugation of mixed products is handled in the way $\left(\xi_i c_j\right)^\dagger = c_j^\dagger \xi_i^*$.

With the help of all these conditions it is possible to write down an expression for the fermion coherent state [2]

$$|\Psi\rangle = \exp\left[-\sum_{j=1}^{N} \xi_j c_j^\dagger\right] |0\rangle = \prod_{j=1}^{N} \left(1 - \xi_j c_j^\dagger\right) |0\rangle \qquad \text{(D 11)}$$

Proof:

$$\begin{aligned} c_k |\Psi\rangle &= c_k \prod_j \left(1 - \xi_j c_j^\dagger\right) |0\rangle = \prod_{j \neq k} \left(1 - \xi_j c_j^\dagger\right) c_k \left(1 - \xi_k c_k^\dagger\right) |0\rangle \\ &= \prod_{j \neq k} \left(1 - \xi_j c_j^\dagger\right) \xi_k |0\rangle = \prod_{j \neq k} \left(1 - \xi_j c_j^\dagger\right) \xi_k \left(1 - \xi_k c_k^\dagger\right) |0\rangle \\ &= \xi_k \prod_j \left(1 - \xi_j c_j^\dagger\right) |0\rangle = \xi_k |\Psi\rangle \end{aligned}$$

□

Finally, these coherent states allow to give the desired expression for the resolution of unity

$$\int \left(\prod_j d\xi_j^* d\xi_j\right) e^{-\sum_j \xi_j^* \xi_j} |\Psi\rangle\langle\Psi| = \mathbb{1}_f \qquad \text{(D 12)}$$

Proof: An arbitrary many-particle state in second quantization has in this paper the form

$$\begin{aligned} |\psi\rangle_{n_1, \ldots, n_M} &= \sum_{i_1, \ldots, i_M} \alpha_{i_1}^{n_1} \cdots \alpha_{i_M}^{n_M} c_{i_1}^\dagger \cdots c_{i_M}^\dagger |0\rangle \\ {}_{n_1', \ldots, n_{M'}'}\langle\psi| &= \langle 0| \sum_{j_1, \ldots, j_{M'}} \alpha_{j_1}^{n_1'\,*} \cdots \alpha_{j_{M'}}^{n_{M'}'\,*} c_{j_1} \cdots c_{j_{M'}}, \end{aligned}$$

and the overlap of such states has already been calculated several times

$${}_{n_1', \ldots, n_{M'}'}\langle\psi|\psi\rangle_{n_1, \ldots, n_M} = \delta_{M,M'} \sum_{j_1, \ldots, j_M} \sum_{\wp \in \mathcal{P}(M)} (-1)^{\mathrm{sgn}\wp} \alpha_{j_1}^{n_1'\,*} \cdots \alpha_{j_M}^{n_M'\,*} \alpha_{j_1}^{n_{\wp(1)}} \cdots \alpha_{j_M}^{n_{\wp(M)}}$$

The result should remain unchanged when the unity is included By using (D.12) and (D 9) one obtains

[2] The motivation for such an expression, as for many other of the given definitions, comes from the treatment of boson coherent states However, a proof shows its correctness

$$
\begin{aligned}
&{}_{n'_1,\ \ldots,n'_{M'}}\langle\psi|\mathbb{1}_f|\psi\rangle_{n_1,\ \ldots,n_M} \\
&\quad = \sum_{i_1,\ \ldots,i_M}\sum_{j_1,\ \ldots,j_{M'}} \alpha_{i_1}^{n_1}\cdots\alpha_{i_M}^{n_M}\alpha_{j_1}^{n'_1\,*}\cdot\ \cdot\alpha_{j_{M'}}^{n'_{M'}\,*}\cdot\ldots \\
&\qquad \int\left(\prod_j \mathrm{d}\xi_j^*\mathrm{d}\xi_j\right)\prod_j\left(1-\xi_j^*\xi_j\right)c_{j_1}\cdots c_{j_{M'}}|\Psi\rangle\langle\Psi|c_{i_1}^\dagger\cdots c_{i_M}^\dagger \\
&\quad = \qquad \cdot\int\left(\prod_j \mathrm{d}\xi_j^*\mathrm{d}\xi_j\right)\prod_j\left(1-\xi_j^*\xi_j\right)\xi_{j_1}\cdot\ \ \xi_{j_{M'}}\xi_{i_1}^*\cdots\xi_{i_M}^*
\end{aligned}
$$

The nilpotence of Grassmann numbers and the rules for integration (D 10) imply that for a certain j

$$
\int \mathrm{d}\xi_j^*\mathrm{d}\xi_j\left(1-\xi_j^*\xi_j\right)\left\{\begin{array}{c}\xi_j\xi_j^*\\ \xi_j\\ \xi_j^*\\ 1\end{array}\right\} = \left\{\begin{array}{c}1\\0\\0\\1\end{array}\right.
$$

Hence, the integral over all N Grassmann numbers is non-vanishing only if the (unordered) sets $\{i_1,\ldots,i_M\}$ and $\{j_1,\ldots,j_{M'}\}$ are identical In this case the integration gives one Permutations are allowed and lead to the same sign as in the overlap of the two states above Thus, it is shown that the operator $\mathbb{1}_f$ really does not alter a state multiplied to the right □

Other important properties are the overlap of two coherent states

$$
\langle\Psi|\Psi'\rangle = \langle 0|\prod_{j=1}^{N}\left(1-c_j\xi_j^*\right)\left(1-\xi_j'c_j^\dagger\right)|0\rangle = \prod_{j=1}^{N}\left(1+\xi_j^*\xi_j'\right) = \mathrm{e}^{\sum_j \xi_j^*\xi_j'} \qquad \text{(D 13)}
$$

and the action of a creation operator on a coherent state

$$
c_k^\dagger|\Psi\rangle = c_k^\dagger\prod_{j\neq k}\left(1-\xi_j c_j^\dagger\right)|0\rangle = -\frac{\partial}{\partial\xi_j}\left(1-\xi_k c_k^\dagger\right)\prod_{j\neq k}\left(1-\xi_j c_j^\dagger\right)|0\rangle = -\frac{\partial}{\partial\xi_j}|\Psi\rangle \qquad \text{(D 14)}
$$

The Time Generating Function for the Fermi Case

With the experience of the previous section it is possible to write down an expression of the time ordering operator for a second quantized Hamiltonian For the sake of simplicity, we modify the expression for the unity (D 12) slightly by introducing Ψ as a vector of the Grassmann numbers $\xi_1,\ \ldots,\xi_N$ When writing

$$
\int \mathrm{d}\Psi^*\mathrm{d}\Psi\mathrm{e}^{-\Psi^*\Psi}|\Psi\rangle\langle\Psi| = \mathbb{1}_f \qquad \text{(D 15)}
$$

the integration is understood to go over all components ξ_j similarly to (D.12).

Combined with (D 3) the time ordering operator becomes

$$U(t,t_a) = \lim_{N_t\to\infty}\left(\prod_{j=0}^{N_t}\int \mathrm{d}\Psi^*(t_j)\mathrm{d}\Psi(t_j)\right)|\Psi(t_{N_t})\rangle * \ldots$$
$$\ldots * \left(\prod_{j=1}^{N_t} \mathrm{e}^{-\Psi^*(t_j)\Psi(t_j)}\langle\Psi(t_j)|\mathbb{1} - \frac{1}{\hbar}\Delta t\mathcal{H}\,|\Psi(t_{j-1})\rangle\right)\langle\Psi(t_0)|$$

The trace of this operator is important in zero temperature condensed matter theory It is called **time generating function** [57] or **vacuum persistence amplitude** [31] and has the form

$$Z = \lim_{N_t\to\infty}\left(\prod_{j=1}^{N_t}\int \mathrm{d}\Psi^*(t_j)\mathrm{d}\Psi(t_j)\right)\prod_{j=1}^{N_t}\mathrm{e}^{-\Psi^*(t_j)\Psi(t_j)}\langle\Psi(t_j)|\mathrm{e}^{-\frac{1}{\hbar}\Delta t\mathcal{H}}\,|\Psi(t_{j-1})\rangle$$

since it does not make much difference if the trace is calculated in Fock space or in the space generated by coherent states.

In order to simplify this expression further one has to think briefly about the question how $\langle\Psi|A|\Psi'\rangle$ looks like for an operator $A = A(c_k^\dagger, c_k)$ in second quantized form However, as long as this operator is normal ordered (all annihilation operators are standing to the right of all creation operators) it is easy to give the answer with the help of (D 9) and (D 13):

$$\langle\Psi|A(c_k^\dagger, c_k)\,|\Psi'\rangle = \mathrm{e}^{\Psi^*\,\Psi'}A(\xi_k^*, \xi_k')$$

Hence, we have for the time generating function in the Fermion case

$$Z = \int \mathcal{D}\Psi^*\mathcal{D}\Psi\,\exp\left[\mathrm{i}\int \mathrm{d}t\left(\Psi^*\mathrm{i}\frac{\partial}{\partial t}\Psi - \frac{1}{\hbar}\mathcal{H}(\Psi^*,\Psi)\right)\right], \qquad \text{(D.16)}$$

where it has been taken into consideration that the limit

$$\lim_{\Delta t\to 0}\frac{1}{\Delta t}\left(-\Psi^*(t_j)\Psi(t_j) + \Psi^*(t_j)\Psi(t_{j-1})\right)$$

can be understood as a derivative of Grassmann numbers

$$= -\Psi^*(t_j)\cdot\lim_{\Delta t\to 0}\frac{\Psi(t_j) - \Psi(t_j - \Delta t)}{\Delta t} = \mathrm{i}^2\Psi^*(t_j)\frac{\partial}{\partial t}\Psi(t_j)$$

Appendix E

The Structure of Rotation

The aim of this section is to find an operator representation which describes a rotation from one system of coordinates $\mathrm{x}, \mathrm{y}, \mathrm{z}$ to a new system $\hat{\mathrm{x}}, \hat{\mathrm{y}}, \hat{\mathrm{z}}$ [1]

It is possible to look at such a rotation as a transformation

$$\mathbf{r} \longrightarrow \mathbf{r}' = \hat{g}\mathbf{r}$$

of the coordinates of a fixed body when there is a change of the coordinate axis

Having got this equation the task is to determine the effect on the wave function ψ of this body. Hence, one has to find the operator $\hat{R}_g$ which changes the wave function accordingly

For this the following constraint is important A new wave function ψ' with respect to a new coordinate $\mathbf{r}'$ must be the same as the original wave function ψ at the point with the unrotated coordinates $\mathbf{r}$.

$$\psi'(\mathbf{r}') = \psi(\mathbf{r}) = \psi(\hat{g}^{-1}\mathbf{r}').$$

Combined with the relation

$$\psi'(\mathbf{r}') = \hat{R}_g\psi(\mathbf{r}')$$

this leads to

$$\hat{R}_g\psi(\mathbf{r}') = \psi(\hat{g}^{-1}\mathbf{r}') = \psi(\mathbf{r}) \qquad \text{(E.1)}$$

[1] The following derivation follows up to a certain extend the descriptions in Edmonds [58] and Davydov [59]

It is known or can easily be shown by infinitesimal rotations that such kind of changes in the wave functions caused by a rotation of the coordinate axis over an angle ϕ around $\mathbf{n}$ is realized by the operator

$$\hat{R}_g(\phi) = e^{i(\mathbf{J}\,\mathbf{n})\phi/\hbar}, \tag{E 2}$$

where $\mathbf{J}$ is the angular momentum operator.

A slightly different point of view is, that a rotation of the coordinate system is in uniquely determined by three Euler angles α, β, γ. These different angles induce the following successive procedure of rotations

1 rotation over an angle α around the z-axis

$$\hat{R}^{z}(\alpha) \quad \mathrm{x}, \mathrm{y}, \mathrm{z} \longrightarrow \mathrm{x}_1, \mathrm{y}_1, \mathrm{z}_1 = \mathrm{z}$$

2. rotation over an angle β around the y_1-axis

$$\hat{R}^{y_1}(\beta) \cdot \mathrm{x}_1, \mathrm{y}_1, \mathrm{z}_1 \longrightarrow \mathrm{x}_2, \mathrm{y}_2 = \mathrm{y}_1, \mathrm{z}_2$$

3. rotation over an angle γ around the z_2-axis

$$\hat{R}^{z_2}(\gamma) \quad \mathrm{x}_2, \mathrm{y}_2, \mathrm{z}_2 \longrightarrow \hat{\mathrm{x}}, \hat{\mathrm{y}}, \hat{\mathrm{z}} = \mathrm{z}_2$$

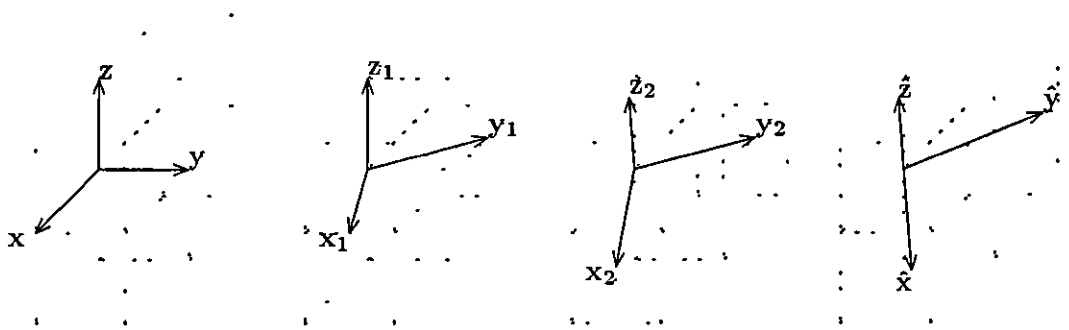


Figure E.1: *The effect of the successive procedure of rotations mentioned above is shown. Each diagram includes one rotation over an Euler angle more than the previous one.*

In the language of rotation operators this procedure can be written in the following form.

$$\hat{R}_g = \hat{R}(\alpha, \beta, \gamma) = \hat{R}^{z_2}(\gamma)\hat{R}^{y_1}(\beta)\hat{R}^{z}(\alpha).$$

For this procedure the second rotation is around an axis which follows from the first one, and the axis of the third rotation is based on the two rotations before. For practical purposes it is often more convenient to look at a fixed reference frame for these rotations. This fixed reference frame may be the coordinate system $\mathbf{x}, \mathbf{y}, \mathbf{z}$ at the beginning. This is possible because of the following relations:

$$\begin{aligned} \hat{R}^{y_1}(\beta) &= \hat{R}^{z}(\alpha)\hat{R}^{y}(\beta)\hat{R}^{z}(-\alpha) \\ \hat{R}^{z_2}(\gamma) &= \hat{R}^{y_1}(\beta)\hat{R}^{z_1}(\gamma)\hat{R}^{y_1}(-\beta) \\ &= \hat{R}^{z}(\alpha)\hat{R}^{y}(\beta)\hat{R}^{z}(\gamma)\hat{R}^{y}(-\beta)\hat{R}^{z}(-\alpha) \\ \Longrightarrow \quad \hat{R}^{z_2}(\gamma)\hat{R}^{y_1}(\beta)\hat{R}^{z}(\alpha) &= \hat{R}^{z}(\alpha)\hat{R}^{y}(\beta)\hat{R}^{z}(\alpha). \end{aligned} \tag{E.3}$$

With the help of this and equation (E.2) one can write

$$\hat{R}(\alpha,\beta,\gamma) = \mathrm{e}^{\imath \hat{J}_z \alpha/\hbar}\mathrm{e}^{\imath \hat{J}_y \beta/\hbar}\mathrm{e}^{\imath \hat{J}_z \gamma/\hbar} \tag{E 4}$$

The eigenfunctions belonging to $\mathbf{J}$ may be called as usual $|jm\rangle$ Because of the rotational invariance of $\mathbf{J}^2$ the eigenvalues $\hbar^2 j(j+1)$ are not changed when $\hat{R}(\alpha,\beta,\gamma)$ is applied Hence, the following representation is possible

$$\hat{R}(\alpha,\beta,\gamma)\,|jm\rangle = \sum_k |jk\rangle\langle jk|\hat{R}(\alpha,\beta,\gamma)\,|jm\rangle = \sum_k D^j_{mk}(\alpha,\beta,\gamma)\,|jk\rangle, \tag{E.5}$$

where the matrix elements are called **Wigner functions**, or generalized spherical functions or D-functions

The function $|jm\rangle$ could for instance be represented in spherical coordinates r, ϑ, φ and therefore with the help of the notation $\psi(\mathbf{r}) = \langle \vartheta\varphi\,|jm\rangle$ the equation (E 1) can be written in the form

$$\langle \vartheta\varphi\,|jm\rangle = \hat{R}(\alpha,\beta,\gamma)\langle \vartheta'\varphi'\,|jm\rangle = \sum_k D^j_{mk}(\alpha,\beta,\gamma)\langle \vartheta'\varphi'\,|jk\rangle \tag{E 6}$$

Coming back to the definition (E.5) for the matrix elements D^j_{mk} it is possible to calculate these terms explicitly For this thesis only the case $j = \frac{1}{2}$ is of interest [2] In this special case it is

$$\begin{aligned} D^{\frac{1}{2}}_{mk} &= \langle \tfrac{1}{2}k\,|\hat{R}(\alpha,\beta,\gamma)\,|\tfrac{1}{2}m\rangle \\ &= \langle \tfrac{1}{2}k\,|\mathrm{e}^{\imath \hat{J}_z \alpha/\hbar}\mathrm{e}^{\imath \hat{J}_y \beta/\hbar}\mathrm{e}^{\imath \hat{J}_z \gamma/\hbar}\,|\tfrac{1}{2}m\rangle \\ &= \mathrm{e}^{\imath k\alpha}\langle \tfrac{1}{2}k\,|\mathrm{e}^{\imath \hat{J}_y \beta/\hbar}\,|\tfrac{1}{2}m\rangle\mathrm{e}^{\imath m\gamma}, \end{aligned}$$

[2] A result for an arbitrary value of j can for instance be found in Edmonds [58] on page 57.

where k and m can be $\frac{1}{2}$ or $-\frac{1}{2}$.

As already mentioned in chapter 1.1 there is for the case $j = \frac{1}{2}$ a simple relationship between the spin angular momentum and the Pauli spin matrices of the form $\mathbf{J} = \frac{1}{2}\hbar\boldsymbol{\sigma}$ Hence, it is

$$\langle \tfrac{1}{2}k | e^{\imath \hat{J}_y \beta/\hbar} | \tfrac{1}{2}m \rangle = \langle \tfrac{1}{2}k | \exp\left[\frac{1}{2}\beta\sigma_y\right] | \tfrac{1}{2}m \rangle$$

A Taylor expansion and the knowledge of the relation $\sigma_y^2 = \mathbb{1}$ gives

$$\begin{aligned}
\exp\left[\frac{1}{2}\beta\sigma_y\right] &= \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{\mathrm{i}}{2}\beta\sigma_y\right)^n \\
&= \mathbb{1}\left[1 - \frac{1}{2}\left(\frac{1}{2}\beta\right) + \ldots\right] + \imath\sigma_y\left[\frac{1}{2}\beta - \frac{1}{3!}\left(\frac{1}{2}\beta\right)^3 + \ldots\right] \\
&= \mathbb{1}\cdot\cos\left(\frac{1}{2}\beta\right) + \imath\sigma_y\cdot\sin\left(\frac{1}{2}\beta\right) \\
&= \begin{pmatrix} \cos\left(\frac{1}{2}\beta\right) & \sin\left(\frac{1}{2}\beta\right) \\ -\sin\left(\frac{1}{2}\beta\right) & \cos\left(\frac{1}{2}\beta\right) \end{pmatrix} \qquad \text{because } \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \imath & 0 \end{pmatrix}
\end{aligned}$$

Putting all these results together leads to the result that $D^j_{mk}(\alpha\beta\gamma)$ consists of the following matrix elements:

$$\begin{pmatrix} e^{\frac{\imath}{2}(\alpha+\gamma)}\cos\left(\frac{1}{2}\beta\right) & e^{-\frac{\imath}{2}(\alpha-\gamma)}\sin\left(\frac{1}{2}\beta\right) \\ -e^{\frac{\imath}{2}(\alpha-\gamma)}\sin\left(\frac{1}{2}\beta\right) & e^{-\frac{\imath}{2}(\alpha+\gamma)}\cos\left(\frac{1}{2}\beta\right) \end{pmatrix} \tag{E.7}$$

The original problem was to rotate the spin quantization axis to a vector with the polar coordinates θ, ζ The question is how this can be expressed by Euler angles The easiest way to see this is to take the possibility with the fixed reference frame. The aim is to bring the z-axis in the direction of the vector The z-axis is in step two rotated along the y-axis Therefore, the coordinate system must in the first step be rotated in such a way, that the vector becomes perpendicular to the y-axis The second step is then the actual rotation of the z-axis And the third step must be a turn back of the first step That means $\alpha = \zeta$, $\beta = -\theta$ and $\gamma = -\zeta$ Hence, the rotation matrix has the following structure

$$\hat{R}(\theta,\zeta) = \begin{pmatrix} \cos\left(\frac{1}{2}\theta\right) & -e^{-\imath\zeta}\sin\left(\frac{1}{2}\theta\right) \\ e^{\imath\zeta}\sin\left(\frac{1}{2}\theta\right) & \cos\left(\frac{1}{2}\theta\right) \end{pmatrix} \tag{E 8}$$

Appendix F

The Usage of Contractions

A useful tool for dealing with long chains of creation and annihilation operators is **Wick's theorem** It gives a simple method how a product of time-ordered operators can be expressed in the form of operator products which are normal ordered The formula is

$$\begin{aligned} T\left(\hat{U}\hat{V}\hat{W}\ldots\hat{X}\hat{Y}\hat{Z}\right) &= N\left(\hat{U}\hat{V}\hat{W}\ldots\hat{X}\hat{Y}\hat{Z}\right) + N\left(\hat{U}\hat{V}\hat{W}\ldots\hat{X}\hat{Y}\hat{Z}\right) \\ &+ N\left(\hat{U}\hat{V}\hat{W}\ldots\hat{X}\hat{Y}\hat{Z}\right) + \ldots + N\left(\hat{U}\hat{V}\hat{W}\ldots\hat{X}\hat{Y}\hat{Z}\right) \\ &= N\left(\hat{U}\hat{V}\hat{W}\ldots\hat{X}\hat{Y}\hat{Z}\right) \\ &+ N\left(\text{sum over all possible pairs of contractions}\right) \end{aligned}$$

Here the following notation is used

T .... time-ordering operator $T\left(\hat{X}(t_x)\hat{Y}(t_y)\right) = \begin{cases} \hat{X}\hat{Y}, & t_x < t_y \\ -\hat{Y}\hat{X}, & t_y < t_x \end{cases}$

N .... normal-ordering operator all annihilation operators are placed to the right of all the creation operators

$\underbrace{\quad}$ indicates contractions $\hat{X}\hat{Y} = T\left(\hat{X}\hat{Y}\right) - N\left(\hat{X}\hat{Y}\right)$

Furthermore, there exists the sign convention that two contracted factors must be brought together by rearranging the order of the operators within the normal product, always keeping the standard sign convention for interchange of fermions [1]

If for the calculations of this paper the time ordering is assumed to be in the

[1] Wick's theorem is formulated in this way and proven in the book of A L Fetter and J D Walecka [60]

way $c_{k,\sigma}c^\dagger_{k',\sigma'}$ then a contraction, which is a c-number in the occupation-number Hilbert space, has the value

$$\underbrace{c_{k,\sigma}c^\dagger_{k',\sigma'}} = c_{k,\sigma}c^\dagger_{k',\sigma'} - \left(-c^\dagger_{k',\sigma'}c_{k,\sigma}\right) = [c_{k,\sigma}, c^\dagger_{k',\sigma'}]_+ = \delta_{k,k'}\delta_{\sigma,\sigma'}$$

If, on the other hand, the timer ordering is assumed to be in the way $c^\dagger_{k,\sigma}c_{k',\sigma'}$ then $\underbrace{c^\dagger_{k,\sigma}c_{k',\sigma'}} = 0$ Additionally, $\underbrace{c_{k,\sigma}c_{k',\sigma'}} = 0$ and $\underbrace{c^\dagger_{k,\sigma}c^\dagger_{k',\sigma'}} = 0$, because in these three cases the time ordered product is automatically normal ordered

The trick is to define an artificial "time ordering" as the order of the operators that is given at the beginning of a calculation. Then it is very convenient to use Wick's theorem for transformations

Example: An usual problem of this paper is to evaluate an expression like

$$\langle 0|c_{j_2}c_{j_1}c^\dagger_{k+1}c_k c^\dagger_{i_1}c^\dagger_{i_2}|0\rangle$$

This order of operator is defined to be time ordered and afterwards Wick's theorem is applied:

$$\begin{aligned}
&= \langle 0|T\left(c_{j_2}c_{j_1}c^\dagger_{k+1}c_k c^\dagger_{i_1}c^\dagger_{i_2}\right)|0\rangle \\
&= \langle 0|N\left(c_{j_2}c_{j_1}c^\dagger_{k+1}c_k c^\dagger_{i_1}c^\dagger_{i_2}\right)|0\rangle + \langle 0|N\left(\underbrace{c_{j_2}c_{j_1}}c^\dagger_{k+1}c_k c^\dagger_{i_1}c^\dagger_{i_2}\right)|0\rangle + \\
&+ \langle 0|N\left(\underbrace{c_{j_2}c_{j_1}}c^\dagger_{k+1}\underbrace{c_k c^\dagger_{i_1}}c^\dagger_{i_2}\right)|0\rangle + \langle 0|N\left(\underbrace{c_{j_2}c_{j_1}}c^\dagger_{k+1}\underbrace{c_k c^\dagger_{i_1}}c^\dagger_{i_2}\right)|0\rangle \\
&+ \langle 0|N\left(\underbrace{c_{j_2}c_{j_1}}c^\dagger_{k+1}\underbrace{c_k c^\dagger_{i_1}}c^\dagger_{i_2}\right)|0\rangle + \langle 0|N\left(\underbrace{c_{j_2}c_{j_1}}c^\dagger_{k+1}\underbrace{c_k c^\dagger_{i_1}}c^\dagger_{i_2}\right)|0\rangle + .
\end{aligned}$$

In this sum all not fully contracted terms disappear, because normal ordering brings annihilation operators to the right, and the result is zero if they operate on $|0\rangle$. Furthermore, only those of the fully contracted terms remain for which each pair of contraction consists of an annihilation operator on the left and a creation operator on the right. These four contributions have the value

$$= \delta_{j_2,i_2}\delta_{j_1,k+1}\delta_{k,i_1} - \delta_{j_2,i_1}\delta_{j_1,k+1}\delta_{k,i_2} - \delta_{j_2,k+1}\delta_{j_1,i_2}\delta_{k,i_1} + \delta_{j_2,k+1}\delta_{j_1,i_1}\delta_{k,i_2}$$

□

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