Fermion Simulation
in the t-J Model

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Was glänzt, ist für den Augenblick geboren
Das Echte bleibt der Nachwelt unverloren.

JOHANN WOLFGANG VON GOETHE (1749-1832)
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Introduction

Superconductivity is a very challenging field in condensed matter physics. Thirty years ago, high-temperature superconductivity has been discovered in layered cuprates, but until today, the physics of the responsible mechanism is not understood. The theories that describe low-temperature physics can not be used for high-$T_c$ phenomena. However, it is known that high-temperature superconductivity results from hole or electron doped antiferromagnetic materials. Therefore it is interesting to examine quantum antiferromagnets in order to get a better understanding of the underlying physics. This was the motivation in constructing a low-energy effective theory for charge carriers in an antiferromagnet which was recently done [2]. The theory is derived only from symmetry considerations and not from a specific underlying microscopic model and is therefore applicable to a whole class of models. It is a systematic low-energy expansion in which every term comes with a specific low-energy coupling constant. These constants have to be determined by experiments or simulations. Determining these constants and comparing to real materials shows if the effective theory indeed describes real materials.

The aim of this thesis is to present an efficient algorithm for the determination of these coupling constants. The model that was chosen to perform the simulations is the $t$-$J$ model. It is similar to the Hubbard model which describes fermions hopping on a 2-dimensional lattice and contains on-site Coulomb repulsion. In contrast to the Hubbard model, the $t$-$J$ model completely forbids double occupation, hence the antiferromagnet can only be doped with holes in this case. However, one has to be aware of the fact that the $t$-$J$ model is much too simple to describe real materials. We start with a half-filled lattice, where the $t$-$J$ model corresponds to the Heisenberg model with coupling constant $J$, and dope it with a single hole, i.e. we remove one fermion. By measuring the energy spectrum of the hole in the antiferromagnet, the low-energy constants of the effective theory can be determined. Instead of performing a Monte Carlo simulation of the $t$-$J$ model (which was an inefficient attempt), by reformulating the problem one can trace it back to the Heisenberg model. The simulation is done by means of efficient cluster algorithms which were introduced by U.-J. Wiese in [4].

The thesis is organized as follows: In the first chapter the $t$-$J$ model is introduced. The next chapter is about the effective theory and how we can extract its parameters from the two-point correlation function. In chapter 3 this function is formulated as a path integral that can be implemented in a simulation. The algorithm is presented in the proximate chapter. The last two chapters contain the error analysis and the results for the parameter ratio $J/t = 2$. 
Chapter 1

The Model

1.1 The lattice

The antiferromagnet consists of weakly interacting layers. These interactions are not taken into account and the model describes a single two-dimensional layer. We use periodic boundary conditions and consider a square lattice of $L$ ($L$ even) sites in $x$ and $y$ direction. The lattice sites are numbered from 0 to $L - 1$ in the following way:

$$
(n_x a, n_y a) \rightarrow i = \left\{ \begin{array}{ll}
n_x + n_y L, & n_y \text{ even} \\
L - 1 - n_x + n_y L, & n_y \text{ odd} 
\end{array} \right.,
$$

such that we have two sublattices, one with even and the other with odd numbered sites. Nearest neighbor sites never belong to the same sublattice. This is illustrated in figure 1.1.

1.2 The $t$-$J$ model

To simulate the dynamics of a single hole in an anti-ferromagnet, we use the $t$-$J$ model. A main feature of the $t$-$J$ model is that double occupancy is forbidden. At half-filling, when no hole is present, it corresponds to the Heisenberg model.

1.2.1 The Hamiltonian

The $t$-$J$ model Hamiltonian reads as follows:

$$
H = P \sum_{\langle ij \rangle} h_{ij} P,
$$

$$
h_{ij} = -t \left( c_i^\dagger c_j + c_j^\dagger c_i \right) + J S_i \cdot S_j.
$$

The exchange coupling constant $J$ ($J > 0$ for an anti-ferromagnet, where anti-parallel spins are favored) is the same as in the Heisenberg model, and $t$ is the hole hopping parameter. Both $t$ and $J$ are real.

The Hamiltonian is a sum over Hamiltonians $h_{ij}$ which couple the sites $i$ and $j$. Indeed only local interactions are relevant, so we sum over nearest sites only, denoted by $\langle ij \rangle$. Note that $h_{ij}$ is symmetric under exchange of $i, j$. 

3
These Hamiltonians are projected (to avoid double occupancy). They contain fermion annihilation operators

$$c_k = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix}$$  \hspace{1cm} (1.4)$$

with standard anti-commutation relations

$$\{c_{k,s}^\dagger, c_{k',s'}^\dagger\} = 0, \quad \{c_{k,s}, c_{k',s'}\} = 0, \quad \{c_{k,s}^\dagger, c_{k',s'}\} = \delta_{kk'}\delta_{ss'}$$  \hspace{1cm} (1.5)$$

and $\bar{S}_k = c_k^\dagger \sigma c_k$ is a spin-1/2 operator, where $\sigma^1, \sigma^2, \sigma^3$ are the Pauli matrices:

$$\bar{S}_k = \frac{1}{2} \begin{pmatrix} c_{k\uparrow}^\dagger c_{k\downarrow} + c_{k\downarrow}^\dagger c_{k\uparrow} \\ i \left( -c_{k\uparrow}^\dagger c_{k\downarrow} + c_{k\downarrow}^\dagger c_{k\uparrow} \right) \\ c_{k\uparrow}^\dagger c_{k\downarrow} - c_{k\downarrow}^\dagger c_{k\uparrow} \end{pmatrix}.$$  \hspace{1cm} (1.6)$$

The total spin operator is

$$\bar{S} = \sum_k \bar{S}_k.$$  \hspace{1cm} (1.7)$$

The total charge relative to half-filling is specified by

$$Q = \sum_i (c_i^\dagger c_i - 1).$$  \hspace{1cm} (1.8)$$

The spin and the charge are conserved quantities:

$$[H, \bar{S}] = 0,$$  \hspace{1cm} (1.9)$$

$$[H, Q] = 0.$$  \hspace{1cm} (1.10)$$

Each state $|n\rangle$ can be generated from the vacuum state by creating fermions on one site after another in a certain, definite order. (Changing the order can result in a different sign due to the anti-commutation relations.) Here we start with site 0 and fill the lattice sites in the order of the labeling, for example

$$|n\rangle = c_{L-1\uparrow}^\dagger c_{L-2\uparrow}^\dagger \cdots c_{3\uparrow}^\dagger c_{2\uparrow}^\dagger c_{0\uparrow}^\dagger |0\rangle$$

We measure the third component of the spin:

$S_{L-1}^3|n\rangle = 1/2, \quad S_{L-2}^3|n\rangle = 0, \quad S_{3}^3|n\rangle = -1/2, \quad S_{2}^3|n\rangle = -1/2, \ldots, \quad S_{L-2}^3|n\rangle = 1/2, \quad S_{L-1}^3|n\rangle = -1/2.$
Thus the state can be described by a string of holes ($\ominus$, $s^3 = 0$), up-spins ($\uparrow$, $s^3 = 1/2$), and down-spins ($\downarrow$, $s^3 = -1/2$). In our example:

$$|n\rangle = |\uparrow \downarrow \cdots \uparrow\downarrow\rangle .$$

The matrix of the local Hamiltonian $h_{ij}$ in the basis of the states

$$|s_i^3s_j^3\rangle = |\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\uparrow\ominus\rangle, |\downarrow\ominus\rangle, |\ominus\uparrow\rangle, |\ominus\downarrow\rangle$$

reads as follows:

$$h_{ij} = \begin{pmatrix}
J/4 & 0 & 0 & 0 \\
0 & -J/4 & J/2 & 0 \\
0 & J/2 & -J/4 & 0 \\
0 & 0 & 0 & J/4 \\
0 & 0 & -\Sigma t & 0 \\
-\Sigma t & 0 & 0 & -\Sigma t \\
0 & 0 & 0 & -\Sigma t \\
\end{pmatrix}, \quad (1.11)
$$

where we would like to emphasize the sign $\Sigma = \pm 1$ which arises due to the anti-commutation relations. Consider for instance the matrix element for a fermion hopping from site $j$ to site $i$ on the lattice (all other matrix elements are computed analogously):

$$\langle \uparrow \ominus | h_{ij} | \uparrow \rangle = \langle \uparrow \ominus | -t \left( c_j^\dagger c_j + c_i^\dagger c_i \right) + J \vec{S}_i \cdot \vec{S}_j | \uparrow \rangle$$

$$= -t \langle \uparrow \ominus | c_i^\dagger c_j^\dagger | \uparrow \rangle$$

$$c_i^\dagger c_j^\dagger | \uparrow \rangle = -t c_i^\dagger c_j^\dagger c_{L-1,sL-1}^\dagger c_{L-2,sL-2}^\dagger \cdots c_{i+1,s_{i+1}}^\dagger c_{j+1,s_{j+1}}^\dagger c_{j-1,s_{j-1}}^\dagger \cdots c_{0,s_0}^\dagger \langle 0 \rangle$$

$$= -t c_{L-1,sL-1}^\dagger c_{L-2,sL-2}^\dagger \cdots c_{i+1,s_{i+1}}^\dagger c_{j+1,s_{j+1}}^\dagger c_{j-1,s_{j-1}}^\dagger \cdots c_{0,s_0}^\dagger | 0 \rangle$$

$$= -t \sum c_{L-1,sL-1}^\dagger c_{L-2,sL-2}^\dagger \cdots c_{i+1,s_{i+1}}^\dagger c_{j+1,s_{j+1}}^\dagger \left( 1 - c_i^\dagger c_j^\dagger \right) c_{j-1,s_{j-1}}^\dagger \cdots c_{i+1,s_{i+1}}^\dagger c_{i-1,s_{i-1}}^\dagger \cdots c_{0,s_0}^\dagger | 0 \rangle \quad (1.13)$$

$$= -t \sum c_{L-1,sL-1}^\dagger c_{L-2,sL-2}^\dagger \cdots c_{j+1,s_{j+1}}^\dagger c_{j+1,s_{j+1}}^\dagger c_{j-1,s_{j-1}}^\dagger \cdots c_{i+1,s_{i+1}}^\dagger c_{i-1,s_{i-1}}^\dagger \cdots c_{0,s_0}^\dagger | 0 \rangle$$

$$= -t \Sigma c_{L-1,sL-1}^\dagger c_{L-2,sL-2}^\dagger \cdots c_{j+1,s_{j+1}}^\dagger c_{j+1,s_{j+1}}^\dagger c_{j-1,s_{j-1}}^\dagger \cdots c_{i+1,s_{i+1}}^\dagger c_{i-1,s_{i-1}}^\dagger \cdots c_{0,s_0}^\dagger | 0 \rangle$$

$$= -t \Sigma | \uparrow \ominus \rangle$$

The operator $c_i^\dagger$ is interchanged with the other creation operators several times. One has to perform as many permutations as there are occupied sites between $i+1$ and $j-1$. In our case there is at most 1 hole on the lattice, so all sites $i+1 \ldots j-1$ have to be occupied. Therefore

$$\Sigma = (-1)^{j-i-1}. \quad (1.14)$$
In our case, for neighboring sites $i$ and $j$

$$\Sigma = 1,$$

(1.15)

because one of the sites is located on the odd sublattice, the other on the even sublattice, thus $h_{ij}$ is indeed independent of the spins on the remaining lattice and depends only on the sites $i$ and $j$.

Note: In this calculation, we used $j > i$, but the same result is valid for $j < i$ (since $h_{ij}$ is symmetric).
Chapter 2

Doping a Hole into an Antiferromagnet

2.1 Predictions from low-energy effective field theories

As pointed out in [3], antiferromagnets with a spontaneously broken $SU(2)_s$ spin symmetry have rotor spectra when considered in a finite volume. The staggered magnetization order parameter represents a slow quantum mechanical rotor with angular momentum $l \in \{0, 1, 2, \ldots\}$ and energy

$$E_l = \frac{l(l+1)}{2\Theta},$$

$$\Theta \propto L^2. \tag{2.1}$$

When a hole is doped into an antiferromagnet, the total spin changes by $1/2$ and thus the angular momentum of the rotor must be quantized in half-integer units. Systematic low-energy effective field theories have recently been constructed in [1, 2]. They make model-independent universal predictions for the entire class of lightly doped antiferromagnetic precursors of high-temperature superconductors.

The energy spectrum of holes of momentum $\vec{p}$ has been derived in [1] as

$$E_j = \frac{1}{2\Theta} \left[j(j+1) - \frac{1}{4}\right] + E(\vec{p}). \tag{2.2}$$

Minima of the hole dispersion relation $E(\vec{p})$ are located at lattice momenta $(\pm \frac{\pi}{2\sigma}, \pm \frac{\pi}{2\sigma})$ and the dispersion relation can be expanded around them:

$$E(\vec{p}) = M + \frac{\vec{p}^2}{2M'} \pm \frac{P_1P_2}{M''} + O(p^4). \tag{2.3}$$

Therefore one finds hole pockets in the form of elliptical paraboloids as shown in figure 2.1. Thus by measuring the single hole dispersion relation and measuring the hole pockets, one can determine the parameters $M$, $M'$, $M''$ of the effective theory.
2.2 The two-point correlation function

In order to measure the energy spectrum of a hole in an antiferromagnet, one has to consider the two-point correlation function

\[
G(x; t; y; t') = \langle c_x^\dagger c_y, t' \rangle = \frac{1}{Z_{Q=0}} \text{Tr}_{Q=0} \{ c_x^\dagger c_y, t' \exp(-\beta H) \}
\]

\[
= \frac{1}{Z_{Q=0}} \text{Tr}_{Q=0} \{ \exp(-tH)c_x^\dagger \exp(+tH) \exp(-t'H) \exp(+t'H) \exp(-\beta H) \}
\]

\[
= \frac{1}{Z_{Q=0}} \sum_n \langle n|c_x^\dagger \exp(-\tau H)c_y \exp(-(\beta - \tau)H)|n \rangle.
\]

(2.4)

As \([H, Q] = 0\), every charge eigenstate can be chosen as an energy eigenstate. The trace is taken over states in the \(Q = 0\) sector only, such that the doping of one hole into the antiferromagnet is considered, thus the inserted states \(|n\rangle\) are energy eigenstates at half-filling.

Starting from equation (2.4), we insert complete sets of energy eigenstates \(1 = \sum\langle m_k|m_k\rangle\) which are also charge eigenstates:

\[
G(x; t; y; t') = \frac{1}{Z_{Q=0}} \sum_{m_0, m_1} \langle m_1|c_y \rangle \langle m_0|\exp(-\tau E_{m_1})|m_1 \rangle
\]

\[
\langle m_1|c_y \rangle \langle m_0|\exp(-\beta - \tau)E_{m_0})|n \rangle.
\]

(2.5)

Due to the creation and annihilation operators, the states \(|m\rangle\) need to be in the sector \(Q = -1\). Using

\[
c_y = \sum_x c_x \exp(i\vec{p}\cdot\vec{x})
\]

(2.6)

\[
c_y^\dagger = \sum_x c_x^\dagger \exp(-i\vec{p}\cdot\vec{x}).
\]

(2.7)
we go into Fourier space:

\[ \tilde{G} (\vec{p}, t; \vec{q}, t') = \sum_{\vec{x}, \vec{y}} G (\vec{x}, t; \vec{y}, t') \exp (-i \vec{p} \vec{x}) \exp (i \vec{q} \vec{y}) \]

\[ = \frac{1}{Z_{Q=0}} \sum_{n,m} \langle n| c_p^\dagger |m \rangle \langle m| c_q |n \rangle \exp (-\tau E_m) \exp (- (\beta - \tau) E_n) . \] (2.8)

As \( \mathbf{H} \) and \( \mathbf{Q} \) are translation invariant, every energy-charge eigenstate can be chosen as a momentum eigenstate. As \( c_p^\dagger \) raises the momentum \( \vec{k}_m \) of the state \( |m \rangle \) by \( \vec{p} \), the state \( |n \rangle \) needs to have the momentum \( \vec{k}_m + \vec{p} \) in order to have a non-vanishing contribution from \( \langle n| c_p^\dagger |m \rangle \). The same criterion applies for \( \langle m| c_q |n \rangle \) with the conclusion that the state \( |n \rangle \) needs to have the momentum \( \vec{k}_m + \vec{q} \). Hence

\[ \tilde{G} (\vec{p}, \tau) = \frac{1}{Z_{Q=0}} \sum_{n,m} \left| \langle n| c_p^\dagger |m \rangle \right|^2 \exp (-\tau E_m) \exp (- (\beta - \tau) E_n) \]

\[ = \sum_{n,m} \left| \langle n| c_p^\dagger |m \rangle \right|^2 \exp (-\tau (E_m - E_n)) \exp (-\beta E_n) \sum_k \exp (-E_k \beta) \]

\[ \overset{\beta \to \infty}{\longrightarrow} \sum_m \left| \langle 0| c_p^\dagger |m \rangle \right|^2 \exp (-\tau (E_m - E_0)) . \] (2.9)

By taking the limit \( \beta \to \infty \), only the contribution from the ground state \( |0 \rangle \) is left in the numerator and in the denominator (the others are suppressed), and the energy spectrum can be extracted from the two-point correlation function in momentum space.
Chapter 3

Path Integral Formulation

The expectation value of an observable is

\[ \langle O \rangle = \frac{1}{Z} \text{Tr} (O \exp (-\beta H)) . \] (3.1)

We rewrite the \( t-J \) model Hamiltonian \( H \) as follows:

\[ H = P \sum_{x,\mu} h_{x,\mu} P \] (3.2)

\[ h_{x,\mu} = -t (c^\dagger_{x+\mu} c_{x} + c^\dagger_{x} c_{x+\mu}) + J \mathbf{S}_x \cdot \mathbf{S}_{x+\mu} \] (3.3)

where we sum over the spatial directions \( \mu = 1 \ldots d \) and \( \hat{\mu} \) is the unit vector in direction \( \mu \).

Next we decompose the Hamilton operator into \( 2d \) terms

\[ H = H_1 + H_2 + \ldots + H_{2d} \] (3.4)

\[ H_\mu = \sum_{x=(x_1, x_2, \ldots, x_d)_{x,\mu \text{ even}}} h_{x,\mu} \] (3.5)

\[ H_{\mu+d} = \sum_{x=(x_1, x_2, \ldots, x_d)_{x,\mu \text{ odd}}} h_{x,\mu} \] (3.6)

as shown in figure 3.1. Note that the individual contributions to a given \( H_i \) commute with each other, but two different \( H_i \) do not commute.

Using \( \beta = M \epsilon (\epsilon \to 0) \) such that \( M \in \mathbb{N} \), (3.7)

we write

\[ \exp (-\beta H) = \exp (-\epsilon H)^M \]

\[ = (\exp (-\epsilon H_1) \exp (-\epsilon H_2) \ldots \exp (-\epsilon H_{2d}))^M \] (3.8)

The limit \( \epsilon \to 0 \) \((M \to \infty)\) is required because \([H_i, H_j] \neq 0 \) \((i \neq j)\).

The local Hamiltonian \( h_{x,\mu} \) only affects the sites \( x \) and \( x + \hat{\mu} \), thus

\[ \exp (-\epsilon H_i) = \prod_{x=(x_1, x_2, \ldots, x_d)_{x,\mu \text{ even/odd}}} \exp (-\epsilon h_{x,\mu}) . \] (3.9)
Figure 3.1: The decomposition of the Hamiltonian in 2 dimensions. Colored edges indicate nearest neighbor coupling.

See equations (1.11), (1.15) for its matrix representation. Exponentiating this matrix gives us

\[
\exp (-\epsilon h_{x,y}) = \begin{pmatrix}
S_J & 0 & 0 \\
0 & S_t & 0 \\
0 & 0 & S_I
\end{pmatrix},
\] (3.10)

\[
S_J = \begin{pmatrix}
\exp(-\frac{\epsilon J}{4}) & 0 & 0 \\
0 & \exp(\frac{\epsilon J}{4}\cosh\frac{\epsilon L}{2}) & -\exp(\frac{\epsilon J}{4}\sinh\frac{\epsilon L}{2}) & 0 \\
0 & -\exp(\frac{\epsilon J}{4}\sinh\frac{\epsilon L}{2}) & \exp(\frac{\epsilon J}{4}\cosh\frac{\epsilon L}{2}) & 0 \\
0 & 0 & 0 & \exp(-\frac{\epsilon J}{4})
\end{pmatrix},
\] (3.11)

\[
S_t = \begin{pmatrix}
cosh \epsilon t & \sinh \epsilon t \\
\sinh \epsilon t & \cosh \epsilon t
\end{pmatrix}.
\] (3.12)

Observables can be expressed via these plaquette weights, as will be shown in the example of the fermionic path integral and the two-point correlation function.

### 3.1 Fermionic path integral

Consider the fermionic path integral in the \(Q = 0\) sector (only half-filled states):

\[
Z_{Q=0} = \text{Tr}_{Q=0} \exp (-\beta H) = \text{Tr}_{Q=0} \{ \exp (-\epsilon H_1) \exp (-\epsilon H_2) \ldots \exp (-\epsilon H_{2d}) \exp (-\epsilon H_1) \exp (-\epsilon H_2) \ldots \exp (-\epsilon H_{2d}) \\
\ldots \exp (-\epsilon H_1) \exp (-\epsilon H_2) \ldots \exp (-\epsilon H_{2d}) \} \\
= \sum_{n_0} \langle n_0 | \exp (-\epsilon H_1) \exp (-\epsilon H_2) \ldots \exp (-\epsilon H_{2d}) \\
\exp (-\epsilon H_1) \exp (-\epsilon H_2) \ldots \exp (-\epsilon H_{2d}) \\
\ldots \exp (-\epsilon H_1) \exp (-\epsilon H_2) \ldots \exp (-\epsilon H_{2d}) | n_0 \rangle,
\] (3.13)
where we sum over all half-filled states $|n_0\rangle$ (as the trace is taken in the $Q = 0$ sector). We insert complete sets of spin eigenstates $1 = \sum_{n_l} |n_l\rangle\langle n_l|$, $l = 1, \ldots, 2dM - 1$ and get:

$$Z_{Q=0} = \lim_{M \to \infty} \sum_{[n]} \exp (-S[n]) ,$$

$$\exp (-S[n]) = \langle n_0 | \exp (-\epsilon H_1) | n_1 \rangle \langle n_1 | \exp (-\epsilon H_2) | n_2 \rangle \ldots \langle n_{2d-1} | \exp (-\epsilon H_{2d}) | n_{2d} \rangle \ldots \langle n_{2d(M-1)} | \exp (-\epsilon H_1) | n_{2d(M-1)+1} \rangle \ldots \langle n_{2dM-1} | \exp (-\epsilon H_{2d}) | n_0 \rangle .$$

Consider the factors

$$\langle n_k | \exp (-\epsilon H_l) | n_{k+1} \rangle = \langle n_k | \prod_{x=(x_1,x_2,\ldots,x_d)}^{x_{\mu} \text{ even/odd}} \exp (-\epsilon h_{x,\mu}) | n_{k+1} \rangle .$$

Figure 3.2 illustrates the procedure. We start with a state $|n_0\rangle$ which interacts locally with state $|n_1\rangle$. The shaded plaquettes indicate neighbor interactions, whereof every plaquette corresponds to one entry in the matrix (3.10) (as shown in figure 3.4).

As the local Hamiltonians act on different sites, each of the factors (3.15) is a product over all plaquette weights between the two according time-slices $k$ and $k + 1$:

$$\langle n_k | \exp (-\epsilon H_l) | n_{k+1} \rangle = \prod_{x=(x_1,x_2,\ldots,x_d)}^{x_{\mu} \text{ even/odd}} \langle n_k | \exp (-\epsilon h_{x,\mu}) | n_{k+1} \rangle = \prod_{x=(x_1,x_2,\ldots,x_d)}^{x_{\mu} \text{ even/odd}} \exp (-s (\square))$$
The state \( |n_0\rangle \) is half-filled, thus every site is occupied, and in order to have only non-vanishing plaquette weights, every site in the state \( |n_1\rangle \) has to be occupied, too, and so on. Therefore all states \( |n_i\rangle \) that give a contribution to the sum are in the \( Q = 0 \) sector.

Note that the resulting sign of \( \exp(-S[n]) \) is positive for every configuration \([n]\):

See picture 3.3 for an example of a configuration and the corresponding fermion world lines. Only plaquettes of crossing fermions give a negative sign. In the given example, the number of crossing plaquettes is even. Since we have periodic boundary conditions and an even number of sites, this is the case for every configuration and thus the resulting sign is always positive. To every configuration a permutation can be assigned, as shown in picture 3.3. The sign of this permutation, which corresponds to the sign of \( \exp(-S[n]) \), is discussed below for \( d = 1 \). Here the permutation is \( \{1, 2, 3, 4, 5, 6, 7\} \rightarrow \{2, 5, 7, 3, 6, 8, 4, 1\} \). This permutation is a result of the permutations from one time-slice to the next, where fermions can be transposed on the plaquettes. Since each transposition of fermions contributes with a minus sign, the sign of \( \exp(-S[n]) \) corresponds to the sign of the permutation. This permutation can evidently be decomposed in a permutation of the fermions with spin up and down, respectively. In the example at hand, the permutation for the up-spin fermions is \( \{3, 4, 7\} \rightarrow \{7, 3, 4\} \) and for the down-spin fermions we have \( \{1, 2, 5, 6, 8\} \rightarrow \{2, 5, 6, 8, 1\} \). Fermions of the same spin do not cross, hence the only way to permute them is to wind them around the spatial boundary, therefore only cyclic permutations are possible. The offset of the cyclic permutation corresponds to the winding number of the respective spin \( \sigma \), which is defined as

\[
W_\uparrow = \frac{1}{L} \sum \{ \delta_{\square \square (\uparrow;\uparrow;\uparrow)} - \delta_{\square \square (\downarrow;\downarrow;\downarrow)} \},
\]

\[
W_\downarrow = \frac{1}{L} \sum \{ \delta_{\square \square (\downarrow;\downarrow;\downarrow)} - \delta_{\square \square (\uparrow;\uparrow;\uparrow)} \},
\]

(3.17)

all fermion hops in positive direction minus all fermion hops in negative direction, divided by the number of sites. It is easy to see that \( W_\uparrow = -W_\downarrow \) in any case. In our example, \( W_\uparrow = 1 \), the up-spin fermions are shifted one to the right, and \( W_\downarrow = -1 \), the down-spin fermions are shifted one to the left. Cyclic permutations of a set of an odd number of elements always
Figure 3.4: Plaquettes and their corresponding weights.

have a positive sign. However, if the number of up-spin fermions $N_1$ is even (and thus the number of down-spin fermions $N_1$ as well), the sign of the cyclic permutation may be even or odd, depending on the winding number. It is

$$(-1)^{(N_0+1)W_0},$$

and therefore the sign of the whole permutation is always positive:

$$(-1)^{(N_1+1)W_1}(-1)^{(N_1+1)W_1} = (-1)^{N_1W_1+N_1W_1} = 1.$$ (3.19)

3.2 The two-point correlation function

We rewrite the expression for the two-point correlation function

$$G(x,t;\bar{y},t') = \langle c_{x,t}^\dagger c_{\bar{y},t'} \rangle^{\tau=t-t} = \frac{1}{Z_{Q=0}} \frac{1}{\mathrm{Tr}_{Q=0}} \{ c_{x,t}^\dagger \exp(-\tau\mathbf{H}) c_{\bar{y}} \exp(-\beta - \tau) \}. $$ (3.20)

Using

$$\tau = k \epsilon, \beta = M \epsilon \ (\epsilon \to 0) \quad \text{such that} \ k, M \in \mathbb{N},$$ (3.21)
we follow the same steps as in the calculation of the fermionic path integral (chapter 3.1):

\[
G(\bar{x}, t; \bar{y}, t') = \frac{1}{Z_{Q=0}} \sum_{n_0} \langle n_0 | c_{\bar{x}}^\dagger (\exp(-\epsilon H_1) \exp(-\epsilon H_2) \cdots \exp(-\epsilon H_{2d}))^k c_\bar{y} (\exp(-\epsilon H_1) \exp(-\epsilon H_2) \cdots \exp(-\epsilon H_{2d}))^{M-k} | n_0 \rangle
\]

(3.22)

Again we insert complete sets of eigenstates \( n', n = |n'_0\rangle, \ldots, |n'_{2dk}\rangle, |n_{2dk}\rangle, \ldots, |n_{2dM-1}\rangle \). Additionally, we write explicitly \( c_{\bar{x}}^\dagger c_\bar{y} = \sum_{\sigma=\pm1} c_{\bar{x},\sigma}^\dagger c_{\bar{y},\sigma} \) and get:

\[
G(\bar{x}, t; \bar{y}, t') = \frac{1}{Z_{Q=0}} \lim_{M \to \infty} \sum_{\sigma=\pm1} \sum_{n,n'} \langle n_0 | c_{\bar{x},\sigma}^\dagger | n'_0 \rangle \langle n_{2dk} | c_{\bar{y},\sigma} | n_{2dk} \rangle
\]

\[
\langle n'_0 | \exp(-\epsilon H_1) | n'_1 \rangle \langle n'_1 | \exp(-\epsilon H_2) | n'_2 \rangle \cdots \langle n'_M | \exp(-\epsilon H_2d) | n'_{2dk} \rangle
\]

\[
\cdots \langle n_{2dk} | \exp(-\epsilon H_1) | n_{2dk+1} \rangle \cdots \langle n_{2dM-1} | \exp(-\epsilon H_2d) | n_0 \rangle
\]

\[
= \frac{1}{Z_{Q=0}} \lim_{M \to \infty} \sum_{\sigma=\pm1} \sum_{n,n'} \langle n_0 | c_{\bar{x},\sigma}^\dagger | n'_0 \rangle \langle n_{2dk} | c_{\bar{y},\sigma} | n_{2dk} \rangle \exp(-S[n,n'])_{IJ}
\]

(3.23)

where we sum over \( n, n' = |n_0\rangle, |n'_0\rangle, \ldots, |n'_{2dk}\rangle, |n_{2dk}\rangle, \ldots, |n_{2dM-1}\rangle \). Again we multiply over all plaquette weights.

In order to consider only plaquettes with a non-vanishing weight, there are certain restrictions on the states \( n, n' \): The trace was taken in the \( Q = 0 \) sector, hence \( |n_0\rangle \) is half-filled. In order to have a non-vanishing first factor \( \langle n_0 | c_{\bar{x},\sigma}^\dagger | n'_0 \rangle \), the state \( |n'_0\rangle \) has to correspond to \( |n_0\rangle \) except for the site \( \bar{x} \), where in the state \( |n_0\rangle \) there is a fermion with spin \( \sigma \) and in \( |n'_0\rangle \) there is a hole, and \( |n'_0\rangle \) has the charge \( Q = -1 \), since the hole is created here. The factor \( \langle n'_0 | \exp(-\epsilon H_1) | n'_1 \rangle \) is non-vanishing only if the state \( |n'_1\rangle \) has a hole in \( \bar{x} \) or \( \bar{x} + \hat{1} \), as the occupation number is conserved on every plaquette. That means the hole can hop from one site to its neighbor or stay at the same site while travelling via plaquettes from one state to the next. But when it reaches state \( |n'_{2dk}\rangle \), it must be located on site \( \bar{y} \), where the hole is annihilated.

Of course, there are restrictions not only on the hole, but on the background too. Every plaquette needs to have a non-vanishing weight in order to give a contribution to the sum. For instance, the spin must be conserved on every plaquette.

The notation of the states is chosen such that all states \( |n'_1\rangle \) are in \( Q = -1 \) and the states \( |n_i\rangle \) are in the sector \( Q = 0 \).

We rewrite the two-point correlation function as

\[
G(\bar{x}, t; \bar{y}, t') = \lim_{M \to \infty} \sum_{\sigma=\pm1} \sum_{n,n'} \frac{\exp(-S[n,\sigma])_H}{Z_{Q=0}}
\]

\[
\times \langle n_0 | c_{\bar{x},\sigma}^\dagger | n'_0 \rangle \langle n_{2dk} | c_{\bar{y},\sigma} | n_{2dk} \rangle \frac{\exp(-S[n,n'])_{IJ}}{\exp(-S[n,\sigma])_H},
\]

(3.24)

where \( n = n_1, n_2, \ldots, n_{2dk-1} \) are the same states, but with a fermion with spin \( \sigma \) instead of a
hole. So only half-filled states contribute to \( \exp(-S[n,\sigma])_H \):

\[
\exp(-S[n,\sigma])_H = \langle n_0 | \exp(-\epsilon H_1) | n_1 \rangle \langle n_1 | \exp(-\epsilon H_2) | n_2 \rangle \cdots \langle n_{2d-1} | \exp(-\epsilon H_{2d}) | n_{2d} \rangle \\
\cdots \langle n_{2d(M-1)} | \exp(-\epsilon H_1) | n_{2d(M-1)+1} \rangle \cdots \langle n_{2dM-1} | \exp(-\epsilon H_{2d}) | n_0 \rangle
\]

(3.25)

The factor \( \langle n_0 | c_{\bar{x},\sigma}^\dagger | n'_0 \rangle \langle n'_{2dk} | c_{\bar{y},\sigma} | n_{2dk} \rangle \) reduces to a simple sign:

\[
\langle n_0 | c_{\bar{x},\sigma}^\dagger | n'_0 \rangle \langle n'_{2dk} | c_{\bar{y},\sigma} | n_{2dk} \rangle = (-1)^{L-i-1}(-1)^{L-j-1} = (-1)^{i+j}
\]

(3.26)

That extra sign \((-1)^{i+j}\) is negative when \(\bar{x}\) and \(\bar{y}\) are sites from different sublattices, otherwise positive.

As the last \(2d(M-k) - 1\) matrix elements are equal in the numerator and in the denominator, \(\exp(-S[n,n'])_{ij} / \exp(-S[n,\sigma])_H\) has many vanishing terms:

\[
\frac{\exp(-S[n,n'])_{ij}}{\exp(-S[n,\sigma])_H} = \frac{\langle n'_0 | \exp(-\epsilon H_1) | n'_1 \rangle \cdots \langle n'_{2dk-2} | \exp(-\epsilon H_{2d-1}) | n'_{2dk-1} \rangle \langle n'_{2dk-2} | \exp(-\epsilon H_{2d-1}) | n_{2dk-1} \rangle \cdots \langle n_{2dM-1} | \exp(-\epsilon H_{2d}) | n_0 \rangle}{\langle n_0 | \exp(-\epsilon H_1) | n_1 \rangle \cdots \langle n_{2d-1} | \exp(-\epsilon H_{2d}) | n_{2d} \rangle}
\]

(3.27)

The \(2dk - 1\) remaining factors have a simple form, because the state \(|n_j\rangle\) differs from \(|n'_j\rangle\) only on one site. That means the numerator and the denominator consist of the same plaquette weights, except for one plaquette (the one where the hole lives). Consider, for example, the first factor. We know that the hole is located on site \(\bar{x}\). If in the state \(|n_1\rangle\) it is located in \(\bar{x} + 1\), we have

\[
\frac{\langle n'_0 | \exp(-\epsilon H_1) | n'_1 \rangle}{\langle n_0 | \exp(-\epsilon H_1) | n_1 \rangle} = \frac{\langle \sigma \sigma^\dagger | \exp(-\epsilon h_{x,1}) | \sigma \sigma^\dagger \rangle}{\langle \sigma \sigma^\dagger | \exp(-\epsilon h_{x,1}) | \sigma \sigma^\dagger \rangle}.
\]

(3.28)

Every factor is the ratio of the plaquette weight with hole and the weight of the corresponding plaquette with a fermion with spin \(\sigma\) instead of the hole.
Figure 3.6: Possible hole paths on a given background state in 1 + 1 dimensions.

Now the two-point correlation function looks as follows:

$$G(\bar{x}, t; \bar{y}, t') = \lim_{M \to \infty} \sum_{\sigma = \uparrow, \downarrow} \sum_{|n|} \frac{\exp(-S[n, \sigma])}{Z_{Q=0}} \times (-1)^{i+j} \frac{\langle n'_0 | \exp(-\epsilon H_1) | n'_1 \rangle \cdots \langle n'_{2dk-2} | \exp(-\epsilon H_{2d-1}) | n'_{2dk-1} \rangle}{\langle n'_0 | \exp(-\epsilon H_1) | n_1 \rangle \cdots \langle n'_{2dk-2} | \exp(-\epsilon H_{2d-1}) | n_{2dk-1} \rangle}$$

(3.29)

It is possible to write this as a sum over all half-filled states $|n_j\rangle$:

$$G(\bar{x}, t; \bar{y}, t') = (-1)^{i+j} \lim_{M \to \infty} \sum_{|n|} \frac{\exp(-S[n])}{Z_{Q=0}} \times \sum_{|n'|} \frac{\langle n'_0 | \exp(-\epsilon H_1) | n'_1 \rangle \cdots \langle n'_{2dk-2} | \exp(-\epsilon H_{2d-1}) | n'_{2dk-1} \rangle}{\langle n'_0 | \exp(-\epsilon H_1) | n_1 \rangle \cdots \langle n'_{2dk-2} | \exp(-\epsilon H_{2d-1}) | n_{2dk-1} \rangle}$$

(3.30)

where the sum $\sum_{|n'|}$ goes over all states $|n'|$ for which the hole is created in $|n'_0\rangle$ on site $\bar{x}$ and is annihilated in $|n'_{2dk}\rangle$ on site $\bar{y}$, and for which every $|n_j\rangle$ is equal to $|n'_j\rangle$ except for the site where the hole lives. I.e. we sum over all possible hole paths from $\bar{x}$ to $\bar{y}$ on the given background $|n|$, as shown in figure 3.6 and measure the ratio of the plaquette weights as described earlier.

Generating all possible half-filled states is not possible in a reasonable amount of time. We will use an efficient cluster algorithm for the Heisenberg model based on Monte Carlo methods which is described in the next chapter.
Chapter 4
The Algorithm

From the two-point function we can extract the energy spectrum that we are interested in. The measurement of the two-point function will be the topic of this chapter. As it is not possible to make an analytic calculation, we will use Monte Carlo methods.

4.1 Cluster algorithm for the Heisenberg model

4.1.1 Monte Carlo simulation

Consider the general expression for the expectation value of an observable:

$$\langle O \rangle = \frac{1}{Z} \sum_{[n]} O[n] \exp(-S[n]).$$  \hspace{1cm} (4.1)

A direct implementation would require to generate all possible configurations $[n]$, measure the observable on it, and average the measurements according to the Boltzmann weights $\exp(-S[n])$. However, in most cases it is only possible to sample a very small fraction of the total number of configurations.

The idea of a Monte Carlo simulation is to pick out the configurations with the largest Boltzmann weights. This is called importance sampling.

One achieves this by generating a sequence of configurations

$$[n^{(1)}] \to [n^{(2)}] \to \ldots \to [n^{(N)}]$$  \hspace{1cm} (4.2)

which form a so-called Markov chain. A Markov chain takes a system in one configuration $[m]$ and generates a new configuration of that system $[n]$ in a probabilistic manner. The probability of generating the configuration $[n]$ given configuration $[m]$ is the transition probability $P([m] \to [n])$. The transition probabilities should not vary over time, and they should depend only on the properties of the current configurations $[m]$ and $[n]$, and not on any other configurations the system has passed through. Of course the probabilities should also satisfy the constraint

$$\sum_{[n]} P([m] \to [n]) = 1 \quad \forall [m],$$  \hspace{1cm} (4.3)

since the Markov process must generate some configuration $[n]$ starting from the configuration $[m]$.
The choice of the appropriate transition step indeed is the crucial point of the Monte Carlo simulation: The Markov step should be chosen in such a way that after the system has come to equilibrium, the probability that a particular configuration \( [n] \) is chosen corresponds to its Boltzmann weight \( p[n] = Z^{-1} \exp(-S[n]) \).

Then our estimator for \( \langle O \rangle \) becomes just

\[
O_M = \sum_{i=1}^{M} O[n^{(i)}]. \tag{4.4}
\]

In order to achieve the correct Boltzmann probability for every configuration, we place two further conditions on our Markov process, the conditions of ergodicity and detailed balance. The condition of **ergodicity** is the requirement that it should be possible for the Markov process to reach any configuration of the system from any other configuration, if we apply it often enough. Then equation (4.3) is also satisfied (if additionally the transition probabilities are correctly normalized).

**Detailed balance** ensures that it is the Boltzmann probability distribution which we generate after the system has come to equilibrium, rather than any other distribution. This is shown in the next paragraph:

The condition of detailed balance reads as

\[
p[m]P([m] \rightarrow [n]) = p[n]P([n] \rightarrow [m]), \tag{4.5}
\]

where \( p[m], p[n] \) are the appropriate Boltzmann weights.

The detailed balance condition guarantees that the probability of being in a particular configuration is time-independent:

\[
p[n] \overset{(4.3)}{=} \sum_{[m]} p[n]P([n] \rightarrow [m]) \overset{(4.5)}{=} \sum_{[m]} p[m]P([m] \rightarrow [n]) \tag{4.6}
\]

The transition probabilities \( P([m] \rightarrow [n]) \) can be thought of as the elements \( P_{nm} \) of a matrix \( P \). This matrix is called the Markov matrix or the stochastic matrix of the Markov process. Likewise the probabilities can be written in a vector notation \( \mathbf{p} = (p_0, p_1, \ldots) \).

In this notation the above equation can be expressed as

\[
p_n = P_{nm} p_m, \tag{4.7}
\]

hence \( \mathbf{p} \) is an eigenvector of \( P \). If our Markov matrix satisfies the criteria of ergodicity, normalization (4.3) and detailed balance (4.5), the probabilities of the configurations stay the same from one Markov step to another, hence they are time-independent.

Note that the condition of detailed balance is sufficient for generating a time-independent probability distribution, but not necessary.

For a deeper understanding of the Monte Carlo method, the reader is referred to [8].

### 4.1.2 Cluster representation

The aim of this chapter is to find an algorithm to simulate the Heisenberg model. How can we generate a Markov chain of half-filled configurations? First we have to care about how to generate configurations that have a non-vanishing Boltzmann weight before we pay attention to the correct probabilities.
As a starting point we can choose a configuration where all the states $|n_0\rangle, |n_1\rangle, \ldots, |n_{2d-M-1}\rangle$ are equal. This ensures that all plaquette weights are non-zero. Then we have to generate a new configuration from this start configuration. However, one cannot simply choose one site on the lattice at random and flip the spin of this site, because every site belongs to two plaquettes, and both of them will have zero weight after flipping a single spin. To turn one plaquette into another one with non-vanishing weight, one has to flip the spin of two or four sites of the plaquette.

Therefore one has to flip a whole sequence of spins: We start with a random site and flip the spin on it. Then we flip the spin of a neighbor site on one of the two plaquettes such that this plaquette has a non-vanishing weight. This site again belongs to another plaquette, so we flip the spin of a neighboring site on that plaquette, etc. until we reach the site where we started the procedure and we close the path. This closed line of spins that were flipped is called a cluster and the connecting line between two successive spins is called a bond.

We can formulate some simple rules in order to have valid plaquettes after flipping: Two neighboring sites can be part of the same cluster if

a. they have parallel spins and they live on different time slices (vertical neighbors) or if

b. they have anti-parallel spins and they live on the same time slice (horizontal neighbors).

In other words: Horizontal bonds connect anti-parallel spins, and vertical bonds connect parallel spins. Furthermore every plaquette has either vertical or horizontal bonds but not both. See table 4.1 for the different plaquettes with their possible bonds.

From one state to the next, we could also flip several clusters. This is called the multi-cluster approach. For this we set the bonds on all plaquettes of the lattice and build all clusters. Every site belongs to exactly one cluster, and they cannot intersect. Then we flip each cluster with probability $1/2$. Figure 4.2 shows such a partitioning of the lattice into clusters.

With this procedure a new configuration can be generated out of an old one. However, they are not yet built with the correct probabilities. The transition probabilities have to be
chosen appropriately, such that the condition of detailed balance (4.5) is satisfied. The Boltzmann probability of a given configuration \( [m] \)

\[
p[m] = \frac{\exp(-S[m])}{Z} = \frac{1}{Z} \exp(-cH_1 | m_1 \rangle \langle m_1 | - cH_2 | m_2 \rangle \langle m_2 | \ldots - cH_{2d} | m_{2d} \rangle \langle m_{2d} | \ldots - cH_{2d(M-1)} | m_{2d(M-1)} \rangle \langle m_{2d(M-1)} | \ldots - cH_{2dM} | m_0 \rangle \langle m_0 |}{Z}
\]

(4.8)

is always positive (see section 3.2). Therefore for the cluster update one can consider only the absolute values of the plaquette weights. (Whereas in the measurement of the hole paths the sign of a plaquette weight is relevant.)

The Boltzmann probability is the product of all (normalized) plaquette weights:

\[
p_m = \prod_i p(\square_{m,i}) .
\]

(4.9)

The algorithm works as follows: We set the bonds of all plaquettes. In most of the cases, we have no choice which bond to set. However, if we have a plaquette of type II, then we choose vertical bonds with a certain probability \( p_v \), and horizontal bonds with probability \( p_h = 1 - p_v \). Then all clusters are built and each one is flipped with probability 1/2.

The transition matrix for single plaquettes is

\[
P = \frac{1}{4} \begin{pmatrix}
1 & 1 & 1 & 1 & 0 & 0 \\
1 & 1 & 1 & 1 & 0 & 0 \\
0 & 0 & 1 & 1 & p_h & p_h \\
0 & 0 & 1 & 1 & p_h & p_h
\end{pmatrix}
\]

(4.10)
The transition probability for a configuration \([m]\) into the next one \([n]\) is just the product of all plaquette transition probabilities:

\[
P_{nm} = P([m] \rightarrow [n]) = \prod_i P(\square_{m,i} \rightarrow \square_{n,i}) .
\] (4.11)

This matrix is correctly normalized:

\[
\sum_n P_{nm} = 1 .
\] (4.12)

In order to satisfy detailed balance

\[
p[m]P([m] \rightarrow [n]) = p[n]P([n] \rightarrow [m]) ,
\] (4.13)

the bond probabilities for the plaquettes of type II, \(p_v\) and \(p_h\), have to be chosen correctly. If detailed balance is satisfied for every single plaquette, then this is also the case for the whole configuration.

Consider the condition of detailed balance for a single plaquette:

\[
p(\square_{m,i}) P(\square_{m,i} \rightarrow \square_{n,i}) = p(\square_{n,i}) P(\square_{n,i} \rightarrow \square_{m,i}) .
\] (4.14)

The conditions for the transitions from and to plaquettes of all types read:

\[
\begin{align*}
\text{I} & \leftrightarrow \text{II} : \quad \exp \left( -\frac{\epsilon J}{4} \right) \times \frac{1}{4} = \exp \left( \frac{\epsilon J}{4} \right) \cosh \left( \frac{\epsilon J}{2} \right) \times \frac{p_v}{4} , \\
\text{I} & \leftrightarrow \text{III} : \quad 0 = 0 , \\
\text{II} & \leftrightarrow \text{III} : \quad \exp \left( \frac{\epsilon J}{4} \right) \cosh \left( \frac{\epsilon J}{2} \right) \times \frac{p_h}{4} = \exp \left( \frac{\epsilon J}{4} \right) \sinh \left( \frac{\epsilon J}{2} \right) \times \frac{1}{4} .
\end{align*}
\] (4.15)

We get

\[
\begin{align*}
p_v &= \frac{2}{1 + \exp \epsilon J} , \\
p_h &= \tanh \left( \frac{\epsilon J}{2} \right) .
\end{align*}
\] (4.16) (4.17)

### 4.2 Overview

Now all parts of the algorithm are collected together.

1. We choose a start configuration, for example we take all spins totally staggered or totally uniform.
2. We perform multi-cluster updates (section 4.2.1) until equilibrium is reached.
3. We measure the hole paths (section 4.2.2), then we perform multi-cluster updates. This is repeated until enough statistics is collected.
with probability $p_h = \tanh \frac{J}{T}$

with probability $p_v = \frac{2}{1 + \exp \frac{4J}{T}}$

<table>
<thead>
<tr>
<th>plaquettes</th>
<th>bonds</th>
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</table>

Figure 4.3: The choice of the bonds.

4.2.1 Multi-cluster update

One multi-cluster update consists of choosing the bonds according to the rules in 4.3, building all clusters, and flipping each one with probability 1/2.

4.2.2 Measurement of the hole paths

When we measure the two-point correlation function, we have to build all possible hole paths from one starting site.

We proceed as follows: First we choose the starting site and the time slice to start with at random. It is easy to see that $G(0, 0, 0) = 1$. There are at most two non-vanishing entries in the next time-slice. We then test if the starting site still has the same spin on the next time-slice. If so, we build the ratio of the plaquette weight with the hole on it and the corresponding plaquette weight without hole (note that the sign of a plaquette weight is relevant). This is the value of $G(0, 0, \epsilon/4)$. Proceed likewise for the neighbor site on the plaquette.

We iterate from one time-slice to the next, always retaining the sites with a non-vanishing contribution to the two-point correlation function. In the following time-slice, we loop over these sites and calculate the plaquette weight ratios. The value of $G(\bar{x}, \tau)$ is the product of the value from the previous site and this ratio.

Using the symmetries of the model, we can improve our statistics: Rotating the lattice by 90 degrees or reflecting it at the $x = y$ line does not change the Boltzmann weight. Therefore for every generated configuration we can think of the corresponding 7 configurations and measure the observable on them. Like that, we get an improved estimator of the observable. That means by calculating the two-point correlation function on a given configuration, we get 7 more estimations by simply considering the values on the corresponding points, as shown in figure 4.4.
Figure 4.4: Site $(x, y) = (3, 1)$ and its seven corresponding sites on the $8 \times 8$ lattice.
Chapter 5

Error Analysis

In the previous chapter the Monte Carlo algorithm has been presented which yields consecutive estimators of the two-point correlation function. From the Fourier transform one can extract the spectral information from which one gets the desired parameters.

However, since the estimators from a Markov chain are always correlated, the problem requires a careful error analysis.

5.1 Fitting

As shown in section 2.2, the two-point correlation function in momentum space is a sum of exponential decays. For sufficiently large times \( \tau \), only the smallest energies contribute to the sum and the others are suppressed. Thus one tries to fit the data to a function of one or two exponential decays by omitting the first time steps.

We fit the function by minimizing the squared residuals

\[
\chi^2 (\vec{p}) = \sum_{i=1}^{N} \left[ \frac{y_i - y(x_i; \vec{p})}{\sigma_i} \right]^2.
\]  

As this is a non-linear fitting problem (the fit parameters are non-linear in the model), there is no direct analytical method to solve this problem. One has to solve it numerically. Here the Levenberg-Marquardt algorithm is used, as described in [9]. In so doing, one obtains the dispersion relation of a single hole with the hole pockets centered at \((\pm \pi/2, \pm \pi/2)\). In order to determine the parameters of the effective theory, one has to perform a second fit – one fits paraboloids into the hole pockets which is a linear fitting problem, thus one can use standard linear fitting methods.

5.2 Autocorrelation and statistical errors

Consider consecutive Monte Carlo estimators of an observable

\[
A_i = A \left( [m^{(i)}] \right), \ i = 1, \ldots, N.
\]  

The error estimation for uncorrelated data

\[
S(N, A)^2 = \left\langle \left( \frac{1}{N} \sum_{i=1}^{N} A_i - \bar{A} \right)^2 \right\rangle.
\]
is not applicable - it would give a too small error.
A possibility is to use binning: We block the data by averaging neighboring pairs, i.e.

\[ A'_i = \frac{1}{2} (A_{2i-1} + A_{2i}) \]  

(5.4)

The new sample has \( N/2 \) points. Iterating this binning, after \( k \) steps we have a sample of \( N/2^k \) points, and we have

\[ S^2(sample_k) = \frac{1}{2^k} S^2(sample_0) . \]

(5.5)

If the data were uncorrelated, this quantity would be invariant. However, in our case, with increasing bin size the correlations die out and we expect a saturation at the realistic error. Binning is a standard method to determine errors for non-linear functions of observables. In our case, we’d like to estimate the parameters of the fit of the correlation function. A possible estimation results from performing the fitting procedure on the binned data and estimating the average and the variance by using the formula for uncorrelated data. However, in our case, the problem is that the bins cannot be chosen sufficiently large to average out the big fluctuations. Therefore the jackknife method is much more convenient here, where instead of the bins their complement is used such that the noise is getting smaller:

\[ A_{b,B} = \frac{1}{N - B} \left( \sum_{i=1}^{(b-1)B} A_i + \sum_{i=bB+1}^{N} A_i \right) . \]

(5.6)

Of course these bins are correlated, though in a simple and controlled way. The error estimate can be calculated as

\[ \sigma^2 = \frac{N_B - 1}{N_B} \sum_{b=1}^{N_B} \left( A_{b,B} - \frac{1}{N_B} \sum_{b'=1}^{N_B} A_{b',B} \right)^2 . \]

(5.7)
Chapter 6

Results

All simulations were performed for values $J/t = 2$ and $\beta = 80$, divided into $4 \times 1600$ time slices. Two lattices of lattice size $L = 32$ and $L = 64$ were compared.

6.1 Overview

The evaluation is performed as follows on all jackknife bins:

- Averaging the measurements of the two-point correlation function on the jackknife bin.
- Fourier transformation of the two-point correlation function into momentum space.
- Fitting a function of exponential decays on the two-point correlation function in momentum space yields the hole dispersion relation.
- Measuring the hole pockets yields the low-energy coupling constants $M, M', M''$.

These $N_B$ measurements of the low-energy coupling constants are averaged according to (5.6), (5.7).
As an example, the fitting of $G(\pi/2, \pi/2, \tau)$ is shown in figure 6.1. It shows clearly that a fit function of two exponential decays should be chosen.

In table 6.2 the results for the $L = 32$ lattice and the $L = 64$ lattice are summarized. The plots show the average of the dispersion relation on all jackknife bins, to present an estimate of the dispersion relations. However, the measurement of the holes pockets was not performed on these averaged dispersion relations, as one could think, but on all jackknife bins and evaluated according to (5.6), (5.7), as described above.

An attempt to fit the $L = 16$ lattice failed, because the lattice was simply too rough to fit a paraboloid into the hole pocket, as the discrete momenta around $(\pi/2, \pi/2)$ are not anymore in the region where the paraboloid is a good approximation. For the lattice sizes $L = 32$ and $L = 64$ it was possible. However, one has to be aware of the fact that in the effective field theory the dispersion relation was derived in an infinite volume. Finite size effects occur due to the rotor spectrum which was introduced in chapter 2. By doping a hole into an antiferromagnet of finite size, the angular momentum of the rotor changes by $1/2$, and thus we have a systematic error of $O(\Theta) \propto 1/L^2$. 

![Figure 6.1: Exponential fits.](image-url)
Figure 6.2: Dispersion relations for a $L = 32$ lattice and a $L = 64$ lattice. In the second and the third row the sections along the axes of the paraboloids are plotted.
Chapter 7

Summary and Outlook

In this thesis, an algorithm has been presented for the measurement of the two-point correlation function in the $t$-$J$ model with the aim to determine the low-energy coupling constants of the effective theory for doped antiferromagnets. The measurement of the two-point correlation function was formulated in a way that could be implemented in a Monte Carlo simulation for Heisenberg antiferromagnets, which was done by means of efficient cluster algorithms. By doping an antiferromagnet with a single hole, the low-energy constants $M, M', M''$ can be determined. Doping more than one hole into the antiferromagnet allows us to determine further constants of the effective theory.

The $t$-$J$ model is an adequate choice for the aim of this thesis, to provide numerical values for the low-energy coupling constants of the effective theory. However, to investigate the mechanism of high-temperature superconductivity, the $t$-$J$ model is a too simple model to consider. It contains only nearest-neighbor coupling. In a further step, one could include hole hopping over diagonal sites with a hopping parameter $t'$, which is the $tt'J$ model. Even with the diagonal hopping parameter, the model is still a great simplification. More complex models have to be considered.

Furthermore, there is no antiferromagnet which is superconductive when doped with a single hole. To get into the region of superconductivity, the antiferromagnet has to be doped with several holes.
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