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Sign problem in the Hubbard model using Hubbard-Stratonovich transformations and application to the Hubbard-Holstein model

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Abstract

The first part of this thesis deals with the sign problem, which is a mathematical problem occuring in Monte Carlo simulations, where the integrand is used as a probability distribution and has to be nonnegative for that reason. In this thesis the Hubbard model is investigated, which has a sign problem in the repulsive case away from half filling. To improve the sign properties, two new Hubbard Stratonovich transformations are developed.
Another promising transformation will be developed in chapter 3. There the model is changed to an equivalent model at half filling and finite magnetic field. The Monte Carlo method can then be applied to every canonical partition function with fixed magnetisation separately.

The second part treats the Hubbard-Holstein model, which is the simplest model to describe the interaction between electrons and phonons in a solid. The electrons are described by a Hubbard Hamiltonian, the phonons by a harmonic oscillator and the interaction between them is assumed to be linear. Although it neglects anharmonicity effects, it is one of the most studied models in this context. In the second part of this thesis the Continuous Hubbard-Stratonovich transformation is used to calculate a formula for the partion function of this model. This formula is suitable for Determinantal Quantum Monte Carlo simulations and is discussed in its full range and some special cases.

Kurzfassung

Der erste Teil dieser Arbeit befasst sich mit dem Vorzeichenproblem. Dieses ist ein mathematisches Problem, welches bei Monte Carlo Simulationen auftritt, wo der Integrand als Wahrscheinlichkeitsverteilung interpretiert wird und deshalb nichtnegativ sein muss. In dieser Arbeit wir das Hubbard Modell untersucht, bei welchem das Vorzeichenproblem im replusiven Fall und Nicht-Halbfüllung auftritt. Um die Eigenschaften des Vorzeichens zu verbessern werden zwei neue Hubbard-Stratonovich Transformationen hergeleitet und untersucht.
Eine weitere viel versprechende Transformation wird in Abschnitt 3 entwickelt. Dort wird das Modell zuerst ersetzt durch ein äquivalentes Modell bei Halbfüllung und endlichem magnetischen Feld. Die Monte Carlo Methode kann dann für jede kanonische Zustandssumme mit konstanter Magnetisierung seperat angewendet werden.

Der zweite Teil befasst sich mit dem Hubbard-Holstein Modell, welches das einfachste Modell ist um die Wechselwirkung zwischen Elektronen und Phononen in einem Festkörper zu beschreiben. Die Elektronen werden durch einen Hubbard Hamilton Operator beschrieben, die Phononen durch einen Harmonischen Oszillator und die Wechselwirkung wird als linear angenommen. Obwohl es Effekte höherer Ordnung vernachlässigt, ist es eines der am meisten studierten Modelle in diesem Kontext.
Im zweiten Teil dieser Arbeit wird die Continuous Hubbard-Stratonovich transformation verwendet um eine Darstellung der Zustandssumme dieses Modells zu erhalten. Diese Formel ist geeignet für Determinanten Quanten Monte Carlo Simulationen und wird sowohl in voller Allgemeinheit alsauch für einige Spezialfälle betrachtet.

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1 The Hubbard Model

1.1 Introduction

Numerical calculations of quantum mechanical many-body systems are often done with Quantum Monte Carlo methods. This methods are very powerful in calculating highdimensional sums or integrals, but needs positive weights (or at least has to be dominated by positive weights) for a proper error convergence [see chapter 1.8]. Especially in fermionic systems the sign problem is, except of some special cases where it vanishes because of symmetry properties, always present because of their anticommutation relations. Fortunately the sign problem is not related to the physical problem itself, but to the mathematical model the problem is described in. With a proper transformation it is therefore possible to improve the sign problem, or to solve it at all. Finding such transformations will be the main task of the first part of this work.
The model I will look at in this thesis, is the d-dimensional Hubbard model, which has a sign-problem in the repulsive case away from halffilling. After some Hubbard Stratonovich transformations the fermionic trace can be written as a determinant, which is in this case the main origin of the sign problem. In chapter 2.1 the well known Standard HS transformation is used to look at the sign problem in a very straight forward way, just to see that only the repulsive case is the one in which the sign problem occurs. In the following chapters 2.2 - 2.4, three new HS transformations are introduced to get other representations of the Hubbard model with also other representations of the sign. In chapter 3 one kind of Fourier transforms the partition function and it turns out, that the Fourier coefficients are the canonical partition functions with constant magnetisation. One can now look at the sign of this Fourier coefficients separately in all the HS transformations introduced in chapter 2.

1.2 Definition of the Hubbard Hamiltonian

The Hubbard model was introduced by the British physicist John Hubbard in 1963, in his attempt to model electronic correlations in solids [2]. It is one of the simplest ways to approximate a solid and consists of a d-dimensional lattice, with at most one electron of every spin on every site. These electrons can move between the lattice sites and therefore, it is a good approximation for solids with highly located orbitals.
These electrons can now do the two main things electrons in solids can do namely, they hop from site to site and repulse each other.

So the basic model consists of two terms.

$$\boxed{H_{\text{basic}} = -t\sum_{i=1}^{N}\sum_{j\in\mathcal{N}_i}(c^\dagger_{i\uparrow}c_{j\uparrow} + c^\dagger_{i\downarrow}c_{j\downarrow}) + U\sum_{i=1}^{N} n_{i\uparrow}n_{i\downarrow}} \tag{1}$$

Where

- c_{is}
  is the annihilation operator, which lowers the number of electrons with spin s on site i by one.
- $c^\dagger_{is}$
  is the creation operator, which increases the number of electrons with spin s on site i by one.
- $n_{is} = c^\dagger_{is}c_{is}$
  is the number operator, which counts the number of electrons with spin s on site i.
- $\mathcal{N}_i = \{\, j \in \{1,\dots,N\} \mid j \to i \text{ possible}\,\}$
  is the set of lattice sites j, where a hopping $j \to i$ is possible.
  It is also called the set of neighbors of site i.

Thus, the terms in this basic Hamiltonian can be interpreted as follows:

- Hopping Term: $H_{\text{kin}} = -t \sum_{i=1}^{N} \sum_{j \in \mathcal{N}_i} (c_{i\uparrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{j\downarrow})$

  The operator $c_{is}^\dagger c_{js}$ annihilates an electron on site j in the first step and creates an electron on site i in the second step. Thus, altogether the operator describes the movement of an electron with spin s from site j to site i.
  $-t$ is the amount of energy which is needed for the hopping to take place.

- Coulomb Term: $H_{\text{cou}} = U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow}$

  Because there cannot be more than one electron with a specific spin on every lattice site, the number operators n_{is} can only take the values 0 and 1. Thus, the product $n_{i\uparrow} n_{i\downarrow}$ only has the value 1 if there are two electrons (one with spin $\uparrow$ and one with spin $\downarrow$) on site i and so this term describes the Coulomb attraction $(U < 0)$ or repulsion $(U > 0)$ of the two electrons.

In 1931 Hans Bethe discovered the 'Bethe ansatz' in order to calculate the eigenvalues and eigenvectors of the one-dimensional Heisenberg model analytically [3]. In 1968 E.H.Lieb and F.Y.Wu applied this ansatz to the one-dimensional Hubbard model [4], which reduces the spectral information to a set of algebraic equations (Lieb-Wu equations). The one-dimensional Hubbard model is therefore analytically solvable. With this Ansatz they calculated the ground state energy and showed a Mott metal-insulator transition at half filling. However, in more than one dimension this ansatz is not applicable and MC simulations are necessary.

This basic Hamiltonian (1) can now be expanded by additional terms, like the chemical potential or the interaction with an external magnetic field.

$$\boxed{H = -t \sum_{i=1}^{N} \sum_{j \in \mathcal{N}_i} (c_{i\uparrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{j\downarrow}) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow} + \mu \sum_{i=1}^{N} (n_{i\uparrow} + n_{i\downarrow}) + h \sum_{i=1}^{N} (n_{i\uparrow} - n_{i\downarrow})} \tag{2}$$

- Chemical Potential Term: $H_\mu = \mu \sum_{i=1}^{N} (n_{i\uparrow} + n_{i\downarrow})$

  $\sum_{i=1}^{N} (n_{i\uparrow} + n_{i\downarrow})$ counts the total number of electrons in the system and μ is the energy required to bring one electron into the system. Thus, the chemical potential term describes the total energy which is needed to bring all the existing electrons into the system.
  It increases as the number of electrons increases and by minimizing the energy, this term likes to keep the total number of electrons small.
  If one would study canonical ensembles, this term would become constant and therefore causes only an energy shift. But in this work only grandcanonical ensembles will be investigated, for which this term is nontrivial.

- Magnetic Field Term: $H_{\text{mag}} = h \sum_{i=1}^{N} (n_{i\uparrow} - n_{i\downarrow})$

  $\sum_{i=1}^{N} n_{is}$ is the total number of electrons with spin s in the system.
  Assuming a positive magnetic field $(h > 0)$, the spin $\uparrow$ electrons get repulsed and the spin $\downarrow$ electrons get attracted by the magnetic field. Vice versa for negative magnetic field $(h < 0)$.
  Thus, by minimizing the energy, the magnetic field term prefers one type of electrons to be in the system.

1.3 Particle-Hole-symmetric Hamiltonian

To make the different Hubbard-Stratonovich transformations (which will be introduced in chapter 2) applicable to the Hamiltonian (2), it has to be written in a particle-hole-symmetric form.

$$\boxed{H_{\text{cou}} + H_{\mu} = U\sum_{i=1}^{N}\left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right) + \left(\mu + \frac{U}{2}\right)\sum_{i=1}^{N}(n_{i\uparrow} + n_{i\downarrow} - 1) + N\left(\frac{U}{4} + \mu\right)} \tag{3}$$

Proof:

$$U(n_\uparrow - \tfrac{1}{2})(n_\downarrow - \tfrac{1}{2}) + (\mu + \tfrac{U}{2})(n_\uparrow + n_\downarrow - 1) + \tfrac{U}{4} + \mu =$$
$$= U(n_\uparrow n_\downarrow - \tfrac{1}{2}\cancel{(n_\uparrow + n_\downarrow)} + \cancel{\tfrac{1}{4}}) + \mu(n_\uparrow + n_\downarrow) - \cancel{\mu} + \tfrac{U}{2}(\cancel{n_\uparrow + n_\downarrow} - \cancel{1}) + \cancel{\tfrac{U}{4}} + \cancel{\mu} =$$
$$= U n_\uparrow n_\downarrow + \mu(n_\uparrow + n_\downarrow)$$

$$H_{\text{cou}} + H_{\mu} = U\sum_{i=1}^{N} n_{i\uparrow}n_{i\downarrow} + \mu\sum_{i=1}^{N}(n_{i\uparrow} + n_{i\downarrow}) =$$
$$= U\sum_{i=1}^{N}(n_{i\uparrow} - \tfrac{1}{2})(n_{i\downarrow} - \tfrac{1}{2}) + (\mu + \tfrac{U}{2})\sum_{i=1}^{N}(n_{i\uparrow} + n_{i\downarrow} - 1) + N(\tfrac{U}{4} + \mu) \qquad \blacksquare$$

1.4 Equivalence between attractive and repulsive model

The Hubbard Hamiltonian has a particle-hole symmetry, which cannot be seen easily in the original form (2). But in the form (3) this symmetry appears as one distinguishes the following two special cases:

- $\mu + \frac{U}{2} = 0$:

  This is the model where the chemical potential term in (3) vanishes. This is equivalent to the condition that exactly N particles are in the system, because then the sum $\sum_{i=1}^{N}(n_{i\uparrow} + n_{i\downarrow} - 1)$ would vanish. The name of this model, 'half filling', is because of this equivalence, although this is just a name and does not mean that the grandcanonical ensemble cannot be used.

$$\boxed{H_{\frac{1}{2}} = H_{\text{kin}} + U\sum_{i=1}^{N}\left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right) + h\sum_{i=1}^{N}(n_{i\uparrow} - n_{i\downarrow}) - N\frac{U}{4}} \tag{4}$$

- $h = 0$:

  This is the special case of the Hubbard model without magnetic field and the most common model used in this context.

$$\boxed{H_{h=0} = H_{\text{kin}} + U\sum_{i=1}^{N}\left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right) + \left(\mu + \frac{U}{2}\right)\sum_{i=1}^{N}(n_{i\uparrow} + n_{i\downarrow} - 1) + N\left(\frac{U}{4} + \mu\right)} \tag{5}$$

To show now the equivalence between these two special cases (4) and (5), one needs an additional assumption on the lattice.

Bipartite lattice:

A lattice is called bipartite, if the set of lattice points $I = \{1, \ldots, N\}$ can be separated into two disjoint sublattices I_1, I_2, with the property that for every lattice point i, all the neighbors $\mathcal{N}_i$ are in the opposite sublattice. This means that a hopping can only take place between sublattices, not within one.

For such a bipartite lattice the special cases (4) and (5) are equivalent.

$$\boxed{H_{\frac{1}{2}}(h, U) = H_{h=0}\left(\mu \to h - \frac{U}{2}\ ,\ U \to -U\right)} \tag{6}$$

Because of this equivalence one can either choose the $H_{\frac{1}{2}}$ or the $H_{h=0}$ model. Although the $H_{h=0}$ model is the common one, in this thesis only the $H_{\frac{1}{2}}$-model will be used. (Except of section 2.1)

Proof:

Another property of the lattice, beside being bipartite, is, that the hopping is symmetric. This means that the hopping $i \to j$ is possible if and only if the hopping $j \to i$ is possible. This property is not really a new assumption on the lattice, but is necessary for the Hamiltonian to be hermitean anyway.

The stated equivalence will be shown by a particle-hole transformation.
This means, the spin↓ electron creation operator is exchanged by the hole annihilation operator and the spin↑ operator stays the same. In addition, the creation operator of one of the sublattices gets a minus sign, to make sure that the kinetic term H_{kin} transforms properly.

$$\underline{d_{i\downarrow}^\dagger = \varepsilon_i \, c_{i\downarrow}} \qquad \text{with } \underline{\varepsilon_i = \begin{cases} -1 & i \in I_1 \\ +1 & i \in I_2 \end{cases}} \tag{7}$$

First it has to be checked, if the hole operators $d_{i\downarrow}^\dagger, d_{i\downarrow}$ are indeed fermionic creation and annihilation operators, which can be done easily by using the definiton (7).

$$\underline{\underline{\{d_{i\downarrow}^\dagger, d_{j\downarrow}\}}} = \varepsilon_i\varepsilon_j\{c_{i\downarrow}, c_{j\downarrow}^\dagger\} = \varepsilon_i\varepsilon_j\delta_{i,j} = \underline{\underline{\delta_{i,j}}} \tag{8}$$

The main part of the proof is to show, that the kinetic term H_{kin} stays the same after the exchange of electron and hole operators.
Looking at a hopping term $c_{i\downarrow}^\dagger c_{j\downarrow}$, the sites i and j are on different sublattices because of the bipartite lattice. Thus, by applying (7), a minus sign occurs.
Finally, with the anticommutator relation (8), the operators are brought in the right order and the minus sign vanishes again.

$$\underline{\underline{c_{i\downarrow}^\dagger c_{j\downarrow}}} = -d_{i\downarrow} d_{j\downarrow}^\dagger = \underline{\underline{d_{j\downarrow}^\dagger d_{i\downarrow}}}$$

Out of the symmetric hopping property follows, that $i \in \mathcal{N}_j \Leftrightarrow j \in \mathcal{N}_i$ and the kinetic Hamiltonian becomes

$$\underline{\underline{H_{\text{kin},\downarrow}}} = \sum_{i=1}^{N}\sum_{j\in\mathcal{N}_i} c_{i\downarrow}^\dagger c_{j\downarrow} = \sum_{i=1}^{N}\sum_{j\in\mathcal{N}_i} d_{j\downarrow}^\dagger d_{i\downarrow} = \underline{\underline{\sum_{j=1}^{N}\sum_{i\in\mathcal{N}_j} d_{j\downarrow}^\dagger d_{i\downarrow}}}$$

For the rest of the Hamiltonian (4), only the relation between the electron number operator $n_{i\downarrow} = c_{i\downarrow}^\dagger c_{i\downarrow}$ and the hole number operator $m_{i\downarrow} = d_{i\downarrow}^\dagger d_{i\downarrow}$ is needed.

$$\underline{\underline{n_{i\downarrow}}} = c_{i\downarrow}^\dagger c_{i\downarrow} = d_{i\downarrow} d_{i\downarrow}^\dagger = \underline{\underline{1 - m_{i\downarrow}}}$$

Now everything is ready to transform $H_{\frac{1}{2}}$ into $H_{h=0}$.

$$\begin{aligned}
\underline{\underline{H_{\frac{1}{2}}}} &= \sum_{i=1}^{N}\sum_{j\in\mathcal{N}_i}\left(c_{i\uparrow}^\dagger c_{j\uparrow} + c_{j\downarrow}^\dagger c_{i\downarrow}\right) + U\sum_{i=1}^{N}\left(n_{i\uparrow} - \tfrac{1}{2}\right)\left(n_{i\downarrow} - \tfrac{1}{2}\right) + h\sum_{i=1}^{N}(n_{i\uparrow} - n_{i\downarrow}) - N\tfrac{U}{4} = \\
&= \sum_{i=1}^{N}\sum_{j\in\mathcal{N}_i}\left(c_{i\uparrow}^\dagger c_{j\uparrow} + d_{j\downarrow}^\dagger d_{i\downarrow}\right) - U\sum_{i=1}^{N}\left(n_{i\uparrow} - \tfrac{1}{2}\right)\left(m_{i\downarrow} - \tfrac{1}{2}\right) + h\sum_{i=1}^{N}(n_{i\uparrow} + m_{i\downarrow} - 1) + N\left(\tfrac{-U}{4} + h\right) = \\
&= \underline{\underline{H_{h=0}(\mu \to h - \tfrac{U}{2}, U \to -U)}} \qquad \blacksquare
\end{aligned}$$

1.5 Exact Diagonalisation

In a first step the Hubbard model can be solved by calculating the full $4^N \times 4^N$ Hamilton matrix in the grandcanonical ensemble. (4^N because there are 4 possible states on every of the N lattice sites).
This is of course only possible for a small number of sites N.

To calculate the Hamilton matrix all the possible states of the system are needed.
A state-vector is given by $(n_{N\uparrow}, \dots, n_{1\uparrow}, n_{N\downarrow}, \dots, n_{1\downarrow})$, where $n_{is} \in \{0, 1\}$.

- $\underline{\underline{n_{is} = 0}}$ means, that there is no particle with spin s on site i.
- $\underline{\underline{n_{is} = 1}}$ means, that there is a particle with spin s on site i.

Because of fermions, for which the Pauli exclusion principle has to be fulfilled, 0 and 1 are the only two possibilities.

Because there are no spin-flip-terms, the matrix elements can be calculated for spin↑ and spin↓ separately.

- Hopping term:

$$\underline{\underline{\langle s_1, \dots, s_N | c_i^\dagger c_j | t_1, \dots, t_N \rangle}} = \langle s_1, \dots, s_N | \delta_{t_i,0}\, \delta_{t_j,1}\, (-1)^{\tilde{t}_j + \tilde{t}_i} | t_1, \dots, t_i = 1, \dots, t_j = 0, \dots, t_N \rangle =$$
$$= \underline{\underline{(-1)^{\tilde{t}_j + \tilde{t}_i}\, \delta_{t_i,0}\, \delta_{t_j,1}\, \delta_{s_1,t_1}\, \dots\, \delta_{s_i,1}\, \dots\, \delta_{s_j,0}\, \dots\, \delta_{s_N,t_N}}}$$

  Thus, there is only a contribution from $c_i^\dagger c_j$, if $\underline{t_i = 0}$ & $\underline{t_j = 1}$ & $\underline{s_i = 1}$ & $\underline{s_j = 0}$.

  In a physical interpretation this makes sense, because a hopping $j \to i$ is only possible if in the initial state site j is occupied and site i is empty, and in the final state site i is occupied and j is empty.

  Because of the fermionic anticommutation relations, an additional sign $(-1)^{\tilde{t}_j + \tilde{t}_i}$ occurs, where $\tilde{t}_j$ and $\tilde{t}_i$ are the number of sign-changes when $c_i^\dagger$ or rather c_j is applied.

- Diagonal terms:

$$\underline{\underline{\langle s_1, \dots, s_N | n_i | t_1, \dots, t_N \rangle}} = \langle s_1, \dots, s_N | t_i | t_1, \dots, t_N \rangle = \underline{\underline{t_i\, \delta_{s_1,t_1}\, \dots\, \delta_{s_N,t_N}}}$$

Example: Mean number of particles

As an example the mean value $< N_s >$ of the total number of particles $N_s = \sum_{i=1}^{N} n_{is}$ with a specific spin s is calculated by exact diagonalisation. Because the determinant representation of the partition function will be used later on, the systems has to be investigated in the grandcanonical ensemble. Thus, the grandcanonical ensemble for the exact diagonalisation is used here as well.

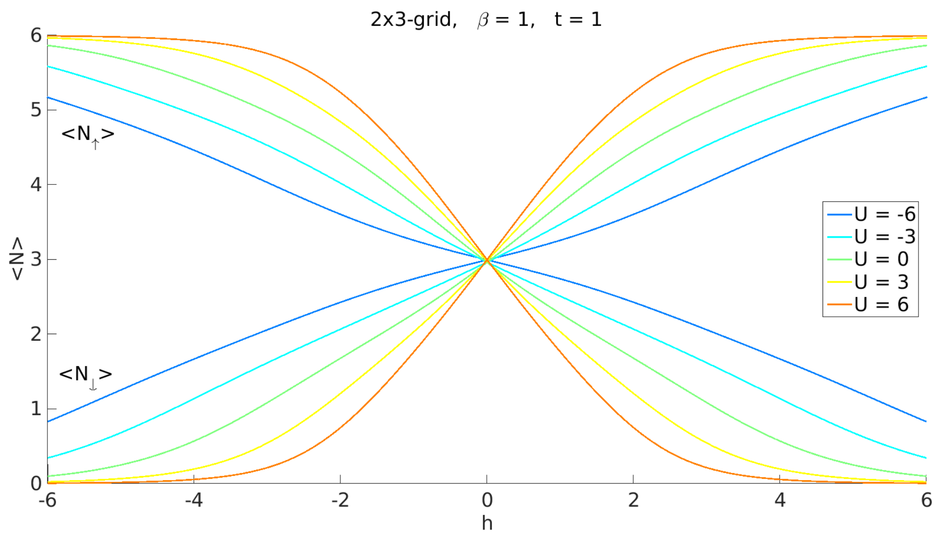


Figure 1: The mean value of the total number of electrons in the grandcanonical ensemble $< N >= \frac{1}{Z}\text{tr}(Ne^{-\beta H})$ can be seen as a function of the external magnetic field h. The plot is done for different values of the Coulomb energy U.

1.6 Hubbard-Stratonovich transformations

Because the exact diagonalisation of the Hamiltonian only works for a small number of sites N, numerical methods have to be used. In particular Determinantal Quantum Monte Carlo methods will be of interest in this thesis. Therefore, the trace of the partition function has to be written as a determinant, which will be done with the help of (69). In order to apply this theorem, the Hamiltonian has to consist of bilinear terms of the form $c_{is}^\dagger c_{js}$, which, see (5), is not true for the Coulomb term $(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$. The task is now, to write the quartic term $c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}$ in a bilinear way.
One way to achieve this, is to use the Hubbard-Stratonovich transformation and modified versions of it.

The Hubbard-Stratonovich (HS) transformation was first introduced by the Russian physicist Ruslan Stratonovich [5]. Later on it was made more popular by the British physicist John Hubbard [6].

In principle every HS transformation is based on the mathematical identity

$$\boxed{e^{x^2} = \frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{4}\sigma^2 + x\sigma} d\sigma} \tag{9}$$

which linearizes the quadratic term x^2 in the exponential at the price of a new degree of freedem σ, which couples linearly to x.

This formula is true for every $x \in \mathbb{R}$, but because the variable n_{is} in (5), which needs to be linearized, can only take values $n_{is} \in \{0, 1\}$, one can try to to replace the continuous integration by a discrete sum. This would reduce the numerical effort by magnitudes.

In the following chapter 2, a couple of different HS transformations will be presented, which differ in the sense that they are continuous or not, or how many terms of the Hamiltonian are transformed.
But all of them have in common that, because of its offdiagonal terms, they never transform the kinetic term H_{kin}. So the exponential of the partition function $Z = e^{-\beta H}$ has to be splitted up into a kinetic exponential and a diagonal rest.
Because in general $e^{A+B} = e^A e^B$ does not hold if $[A, B] \neq 0$, an approximate version of this identity is needed, namely the Trotter decomposition.

1.7 Trotter decomposition

$$\boxed{\mathrm{tr}\left(e^{A+B}\right) = \mathrm{tr}\left(\left(e^{\frac{A}{M}}e^{\frac{B}{M}}\right)^M\right) + \mathcal{O}\left(\frac{1}{M^3}\right)} \tag{10}$$

Proof:

$$\begin{aligned}
\underline{e^{\frac{A}{2M}}e^{\frac{B}{M}}e^{\frac{A}{2M}}} &= \left(1+\tfrac{A}{2M}+\tfrac{A^2}{8M^2}+\mathcal{O}(\tfrac{1}{M^3})\right)\left(1+\tfrac{B}{M}+\tfrac{B^2}{2M^2}+\mathcal{O}(\tfrac{1}{M^3})\right)\left(1+\tfrac{A}{2M}+\tfrac{A^2}{8M^2}+\mathcal{O}(\tfrac{1}{M^3})\right) = \\
&= 1+\tfrac{B}{M}+\tfrac{B^2}{2M^2}+\tfrac{A}{2M}+\tfrac{AB}{2M^2}+\tfrac{A^2}{8M^2}+\tfrac{A}{2M}+\tfrac{BA}{2M^2}+\tfrac{A^2}{4M^2}+\tfrac{A^2}{8M^2}+\mathcal{O}(\tfrac{1}{M^3}) = \\
&= \underline{1+\tfrac{A+B}{M}+\tfrac{(A+B)^2}{2M^2}+\mathcal{O}(\tfrac{1}{M^3})}
\end{aligned}$$

$$\begin{aligned}
\underline{\left(e^{\frac{A}{2M}}e^{\frac{B}{M}}e^{\frac{A}{2M}}\right)^M} &= \left(1+\tfrac{A+B}{M}+\tfrac{(A+B)^2}{2M^2}+\mathcal{O}(\tfrac{1}{M^3})\right)^M = \\
&= 1+M\tfrac{A+B}{M}+M\tfrac{(A+B)^2}{2M^2}+\tfrac{M(M-1)}{2}\,\tfrac{(A+B)^2}{M^2}+\mathcal{O}(\tfrac{1}{M^3}) = \\
&= 1+(A+B)+\tfrac{(A+B)^2}{2}+\mathcal{O}(\tfrac{1}{M^3}) = \\
&= \underline{e^{A+B}+\mathcal{O}\left(\tfrac{1}{M^3}\right)}
\end{aligned}$$

$$\begin{aligned}
\underline{\underline{\mathrm{tr}\left(e^{A+B}\right)}} &= \mathrm{tr}\left(\left(e^{\frac{A}{2M}}e^{\frac{B}{M}}e^{\frac{A}{2M}}\right)^M\right)+\mathcal{O}\left(\tfrac{1}{M^3}\right) = \qquad / \ \mathrm{tr}\left(A_1\dots A_{n-1}A_n\right) = \mathrm{tr}\left(A_nA_1\dots A_{n-1}\right) = \\
&= \underline{\underline{\mathrm{tr}\left(\left(e^{\frac{A}{M}}e^{\frac{B}{M}}\right)^M\right)+\mathcal{O}\left(\tfrac{1}{M^3}\right)}} \quad \blacksquare
\end{aligned}$$

Normally one only gets $e^{A+B} = \left(e^{\frac{A}{M}}e^{\frac{B}{M}}\right)^M + \mathcal{O}\left(\frac{1}{M^2}\right)$ with quadratic error, or the more complicated equation $e^{A+B} = \left(e^{\frac{A}{2M}}e^{\frac{B}{M}}e^{\frac{A}{2M}}\right)^M + \mathcal{O}\left(\frac{1}{M^3}\right)$ with cubic error convergence, but if the trace tr(e^{A+B}) of the exponential is needed, one order of convergence drops out for free, because of the cyclical permutability of the trace.

The Trotter decomposition (10) can now be used to split up the partition function of the Hubbard Hamiltonian (4) into diagonal and not-diagonal terms.
By using imaginary time slices $\underline{\Delta\tau = \frac{\beta}{M}}$, it has the form

$$\boxed{Z = \mathrm{tr}\left(\left(e^{-\Delta\tau(H_{\mathrm{cou}}+H_\mu+H_{\mathrm{mag}})}e^{-\Delta\tau H_{\mathrm{kin}}}\right)^M\right) + \mathcal{O}\left(\Delta\tau^3\right)}\,. \tag{11}$$

1.8 Sign problem in many-electron systems

Monte Carlo simulations are numerical instruments to calculate high-dimensional integrals in the phase space of a quantum mechanical system in polynomial time, while the phase space grows exponentially with the number of particles. The main idea is, to do not include all the points of the phase space into the calculation, but just take a representative sample, which is chosen by a certain probability distribution. Here the sign problem comes into play, because this 'probability distribution' can take negative values for fermionic systems and is therefore no longer interpretable as probability.
Fortunately, the sign problem is not really a problem of the physics itself, but of the basis of the Hilbert space in which the problem is described. That means, if the basis is chosen properly, the sign problem becomes smaller or vanishes at all. For example, in the basis the Hamiltonian is diagonal in, the weights are trivially positive. However, if such a basis is found, the problem is basically solved, because the only problem that remains is the large phase space, which can be treated by a classical MC simulation.
Unfortunately, it can also be shown that finding a basis in which the sign problem vanishes is a NP-hard problem [1]. This means, solving the sign problem equals verifying a solution for any problem in the complexity class NP.

In Quantum mechanics one is interested in the expectation value of some observable A, which is defined as

$$\langle A\rangle = \frac{\mathrm{tr}(Ae^{-\beta H})}{\mathrm{tr}(e^{-\beta H})} \tag{12}$$

with the denominator definded as the partition function

$$Z = \mathrm{tr}(e^{-\beta H}) \ .$$

The problem, in calculating this expectation values is, that the dimension of the Hilbert space grows exponentially with the number of particles. One kind of methods to face this problem are Quantum Monte Carlo simulations.
After some HS transformations or integrating out the electron degrees of freedom, the expectation value reduces in the general case to a form like

$$\langle A \rangle = \frac{\sum_x \rho(x) A(x)}{\sum_x \rho(x)} \ , \tag{13}$$

which is by no means unique, but depends on the kind of transformations and manipulations applied onto (12). So, also the sign problem, which is caused by $\rho(x)$, can be reduced by choosing the shape of (13) properly.

In a QMC algorithm a representative sample $(x_i)_i$ is drawn out of the phase space, by the probability distribution

$$P(x) = \frac{\rho(x)}{\sum_y \rho(y)} \ , \tag{14}$$

and the expectation value $\langle A \rangle$ approximated by the mean value of the sample $(A(x_i))_i$

$$\langle A \rangle \approx \langle A(x_i) \rangle \ .$$

Within this probability distribution (14), the sign problem comes into play [7]. The partition function in the denominator is, as the trace of the exponential of a selfadjoint operator, positive and its only purpose is, to normalize the probability. The function $\rho(x)$ often does not behave so nice and can take positive as well as negative values in general. If this is the case $P(x)$ can no longer be used as probability distribution and the Monte Carlo method fails.

One method to deal with this problem is, to introduce the probability distribution according to the absolute value of $\rho(x)$.

$$\tilde{P}(x) = \frac{|\rho(x)|}{\sum_y |\rho(y)|}$$

$\tilde{P}$ is positive by construction and the expectation value (13) can then be written as

$$\langle A \rangle = \frac{\langle A\ S \rangle_{\tilde{P}}}{\langle S \rangle_{\tilde{P}}} \qquad \text{with} \qquad S(x) = \begin{cases} 1 & \rho(x) > 0 \\ -1 & \rho(x) < 0 \end{cases}$$

where $\langle \cdot, \cdot \rangle_{\tilde{P}}$ means the expectation value with respect to the probability $\tilde{P}$.

This formula becomes problematic if $\langle S \rangle_{\tilde{P}}$ becomes very small, because there will be large cancellations in $\langle A\ S \rangle_{\tilde{P}}$ in this case and statistical fluctuations will have a large influence.
The behaviour of this expectation value of the sign $\langle S \rangle_{\tilde{P}}$ or rather the following quantity sign (15), will be the main question in this first part of the thesis.

$$\text{sign} = \frac{\rho^{(+)} - \rho^{(-)}}{\rho^{(+)} + \rho^{(-)}} \tag{15}$$

with $\underline{\rho^{(+)} = \sum_x \max\{\rho(x), 0\}}$ and $\underline{\rho^{(-)} = -\sum_x \min\{\rho(x), 0\}}$ the sum over all positive or negative values.

2 Different Hubbard-Stratonovich transformations

In this chapter the Hubbard model will be investigated in terms of the sign problem, either in the 'half filling' (4) $H_{\frac{1}{2}}$-hamiltonian or the equivalent 'no magnetic field' (5) $H_{h=0}$-hamiltonian. The $H_{h=0}$-hamiltonian will be used only in the section 2.1 to show that there is no sign problem in the attractive case $(U < 0)$. In the rest of section 2 as well as in section 3 the $H_{\frac{1}{2}}$-hamiltonian will be used, in which the important attractive case $(U < 0)$ is equivalent to the repulsive case $(U > 0)$ of the $H_{h=0}$-model. So the notation with negative values of U in these sections will be ment in terms of the $H_{\frac{1}{2}}$-model.
The quantity of interest will always be the fermionic partition function $Z = \exp(-\beta H)$, written in a determinant representation.
The principle of the Hubbard Stratonovich (HS) transformation was introduced in chapter 1.5. The purpose of this chapter will be to derive different variations of the HS transformation, which will only differ in the part of the Hamiltonian they transform and in the kind of discretisation they use. The idea is, to investigate this transformations in terms of the sign (15) and its shape in order to be suitable for the transformations in chapter 3. In the end no one of this transformations will solve the sign problem, but will be more or less suitable for further numerical and analytical calculations.

The first part, section 2.1, treats the well known Standard HS transformation [8]. This transformation does not have a suitable form one can use in chapter 3, but shows, that the sign problem only occurs in the repulsive case $(U > 0)$ of the $H_{h=0}$-model (5). Therefore further investigations can be restricted to this case.
In the following sections 2.2-2.4 of chapter 2, the repulsive $H_{h=0}$ model will be replaced by the equivalent attractive $H_{\frac{1}{2}}$-model (6). However, the transformations will be derived for general $U \in \mathbb{R}$ and only restricted to the important attractive case if necessary.
In section 2.2 the New HS transformation is developed for the $H_{\frac{1}{2}}$-model. It is similar to the Standard HS transformation, but additionally transforms the magnetic field. The transformation in its exact form has a quite complicated structure and is not useful for chapter 3, but its approximated version has many useful properties, like, that the determinant becomes independent of the magnetic field.
In section 2.3, the second new transformation of this thesis is developed, the New Asymmetric HS transformation. It takes all the properties which are needed for chapter 3 (h-independent determinant and discrete HS sum) and defines the transformation this way. Although this will make for example the ν-integral (50) analytically solvable, it will remain a transformation with a higher numerical effort than the previous approximated New HS transformation.
In section 2.4, with the Continuous HS transformation, another well known transformation is introduced [9]. This transformation has not a discrete σ-sum, like the previous ones, but a continuous σ-integral. The form has every advantage the approximated New HS transformation has, but the disadvantage of the continuous σ integral.

2.1 Standard HS transformation

The Standard HS transformation was invented in 1983 by J. E. Hirsch [8] and is the simplest of all HS transformations investigated here. It only transforms the Coulomb term of the Hamiltonian, so the chemical potential remains explicitely in the determinant (19), which will be not beneficial in further calculations. Nevertheless, in this Standard HS transformation the sign problem of the $H_{h=0}$ model (5) does not occur in the attractive case. So it is enough to concentrate further investigations to the repulsive case.
The reason why this Standard HS transformation is derived in the $H_{h=0}$ model, is the nice form of the partition function (19), in which one can easily see the positivity of the addends.

2.1.1 Mathematical Identity of the Standard HS transformation

Choose $\underline{\lambda \in \mathbb{C}}$, such that $\underline{\underline{\cosh(\lambda) = e^{-\frac{\Delta\tau U}{2}}}}$, (16)

which implies, that $\underline{\lambda \in \begin{cases} i(0, \frac{\pi}{2}) & \text{for} \quad U > 0 \\ (0, \infty) & \text{for} \quad U < 0 \end{cases}}$.

Then the following transformation holds.

$$e^{-\Delta\tau U\left(n_\uparrow-\frac{1}{2}\right)\left(n_\downarrow-\frac{1}{2}\right)} = \frac{1}{2}e^{\frac{\Delta\tau U}{4}} \sum_{\sigma\in\{\pm1\}} e^{\sigma\lambda(n_\uparrow+n_\downarrow-1)} \tag{17}$$

Proof:

Because of fermions the number-operators $n_\uparrow, n_\downarrow$ can only take the values $n_\uparrow, n_\downarrow \in \{0,1\}$.
So all possibilities can be investigated separately.

- $n_\uparrow \neq n_\downarrow$: $\frac{1}{2}e^{\frac{\Delta\tau U}{4}} \sum_{\sigma=\pm1} 1 = e^{\Delta\tau U \frac{1}{4}}$
  $\Rightarrow e^{\frac{\Delta\tau U}{4}} = e^{\Delta\tau U\frac{1}{4}}$
- $n_\uparrow = n_\downarrow = 1$: $\frac{1}{2}e^{\frac{\Delta\tau U}{4}} \sum_{\sigma=\pm1} e^{\sigma\lambda} = e^{-\Delta\tau U\frac{1}{4}}$
  $\Rightarrow \cosh(\lambda) = e^{-\frac{\Delta\tau U}{2}}$
- $n_\uparrow = n_\downarrow = 0$: $\frac{1}{2}e^{\frac{\Delta\tau U}{4}} \sum_{\sigma=\pm1} e^{-\sigma\lambda} = e^{-\Delta\tau U\frac{1}{4}}$
  $\Rightarrow \cosh(\lambda) = e^{-\frac{\Delta\tau U}{2}}$ ■

2.1.2 Partition function in the Standard HS transformation

The Standard HS transformation (17) can now be applied to every lattice point and every imaginary time slice of the partition function in the Trotter decomposition (11). This gives the form:

$$Z = \frac{e^{\frac{\beta NU}{2}}}{2^{NM}} \sum_{\sigma\in\{\pm1\}^{N\times M}} e^{-\lambda|\sigma|}\, \mathrm{tr}\left(\prod_{j=1}^{M}\left(e^{\sum_{i=1}^{N}\left(\sigma_{ij}\lambda-\Delta\tau(\mu+\frac{U}{2})\right)(n_{i\uparrow}+n_{i\downarrow})} e^{-\Delta\tau H_{\mathrm{kin}}}\right)\right) \tag{18}$$

with $|\sigma| = \sum_{i=1}^{N}\sum_{j=1}^{M}\sigma_{i,j}$

Proof:

Combining (11) and (5) with the additional separation of H_{cou} and H_μ (because they are diagonal), leads to the partition function

$$Z = e^{-\beta N\left(\frac{U}{4}+\mu\right)}\mathrm{tr}\left(\left(e^{-\Delta\tau U\sum_{i=1}^{N}(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})} e^{-\Delta\tau(\mu+\frac{U}{2})\sum_{i=1}^{N}(n_{i\uparrow}+n_{i\downarrow}-1)} e^{-\Delta\tau H_{\mathrm{kin}}}\right)^M\right).$$

Applying now the Standard HS transformation (17), the partition function becomes

$$\begin{aligned} Z &= e^{-\beta N\left(\frac{U}{4}+\mu\right)}\mathrm{tr}\left(\left(\prod_{i=1}^{N}\left(\frac{1}{2}e^{\frac{\Delta\tau U}{4}}\sum_{\sigma\in\{\pm1\}} e^{\sigma\lambda(n_{i\uparrow}+n_{i\downarrow}-1)}\right) e^{-\Delta\tau\left(\mu+\frac{U}{2}\right)\sum_{i=1}^{N}(n_{i\uparrow}+n_{i\downarrow}-1)} e^{-\Delta\tau H_{\mathrm{kin}}}\right)^M\right) = \\ &= \frac{e^{\frac{\beta NU}{2}}}{2^{NM}} \sum_{\sigma\in\{\pm1\}^{N\times M}} e^{-\lambda|\sigma|}\,\mathrm{tr}\left(\prod_{j=1}^{M}\left(e^{\sum_{i=1}^{N}\left(\sigma_{ij}\lambda-\Delta\tau(\mu+\frac{U}{2})\right)(n_{i\uparrow}+n_{i\downarrow})} e^{-\Delta\tau H_{\mathrm{kin}}}\right)\right). \quad ■ \end{aligned}$$

2.1.3 Determinant representation of the Standard HS transformation

In the form (18) the partition function only consists of bilinear terms in the exponent. So the spin↑ and the spin↓ exponent can be written separately in the form $\vec{c}^\dagger h \vec{c}$ with a matrix $h \in \mathbb{C}^{N\times N}$ and (69) can be applied to get a determinant representation.

$$\boxed{Z = \frac{e^{\frac{N\beta U}{2}}}{2^{NM}} \sum_{\sigma\in\{\pm1\}^{N\times M}} e^{-\lambda|\sigma|} \det\left(E + \prod_{j=1}^{M}\left(e^{\lambda G^{(j)} - \Delta\tau(\mu+\frac{U}{2})E}\; e^{t\Delta\tau h_{\mathsf{kin}}}\right)\right)^2} \tag{19}$$

with • $G^{(j)} = \begin{pmatrix} \sigma_{1j} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{Nj} \end{pmatrix}$

• $(h_{\mathsf{kin}})_{ij} = \begin{cases} 1 & j \in \mathcal{N}_i \\ 0 & \text{else} \end{cases}$

• E the $N \times N$ identity matrix

Proof:

Because of the Standard HS transformation (17) the term $n_\uparrow n_\downarrow$ is decoupled and it is possible to separate the Hamiltonian into a sum of two Hamiltonians (one for spin↑, one for spin↓). In this case, also the trace in (18) can be written as the product of the two traces acting in the subspace with a certain spin s.

$$Z = \frac{e^{\frac{\beta NU}{2}}}{2^{NM}} \sum_{\sigma\in\{\pm1\}^{N\times M}} e^{-\lambda|\sigma|} \prod_{s\in\{\pm1\}} \mathsf{tr}_s\left(\prod_{j=1}^{M}\left(e^{\sum_{i=1}^{N}\left(\sigma_{ij}\lambda - \Delta\tau(\mu+\frac{U}{2})\right)n_{is}} e^{-\Delta\tau H_{\mathsf{kin},s}}\right)\right)$$

Where $s = 1 \leftrightarrow$ spin ↑ and $s = -1 \leftrightarrow$ spin ↓.

The exponents can now be written in the form $\vec{c}_s^\dagger h \vec{c}_s$:

$$\bullet \sum_{i=1}^{N}\left(\sigma_{ij}\lambda - \Delta\tau\left(\mu + \frac{U}{2}\right)\right) n_{is} = \vec{c}_s^\dagger\left(\lambda G^{(j)} - \Delta\tau\left(\mu + \frac{U}{2}\right)E\right)\vec{c}_s \tag{20}$$

$$\bullet\; H_{\mathsf{kin,s}} = -t\sum_{i=1}^{N}\sum_{j\in\mathcal{N}_i} c_{is}^\dagger c_{js} = -t\vec{c}_s^\dagger h_{\mathsf{kin}}\vec{c}_s$$

Thus, with (69), the determinant representation of the partition function is given by

$$Z = \frac{e^{\frac{\beta NU}{4}}}{2^{NM}} \sum_{\sigma\in\{\pm1\}^{N\times M}} e^{-\lambda|\sigma|} \det\left(E + \prod_{j=1}^{M}\left(e^{\lambda G^{(j)} - \Delta\tau(\mu+\frac{U}{2})E}\; e^{\Delta\tau t h_{\mathsf{kin}}}\right)\right)^2 \quad \blacksquare$$

The formula (19) can now be investigated in terms of the sign problem. This means evaluating the distribution of the addends

$$Z_\sigma = e^{-\lambda|\sigma|} \det\left(E + \prod_{j=1}^{M}\left(e^{\lambda G^{(j)} - \Delta\tau(\mu+\frac{U}{2})E} e^{t\Delta\tau h_{\mathsf{kin}}}\right)\right)^2 \tag{21}$$

according to its value of the sign (15).

One can easily see, that for real values of λ, all the addends Z_σ are positive, thus, there is no sign problem. According to (16), this case is equivalent to the attractive case $U < 0$.

For the repulsive case of the $H_{h=0}$ model (5) away form half filling on the other hand, the sign problem does appear, and it appears in a way that it gets worse for growing β. The results can be seen in Fig.2.

In chapter 3, the form $Z = \sum_{m=-N}^{N} e^{-\beta hm}\, Z_m$ will be needed for the partition function with coefficients Z_m, not depending on the magnetic field h.
As it can be seen in (19), this is not possible for the Standard HS transformation, because the determinant depends on the magnetic field and h is not an exponential prefactor.

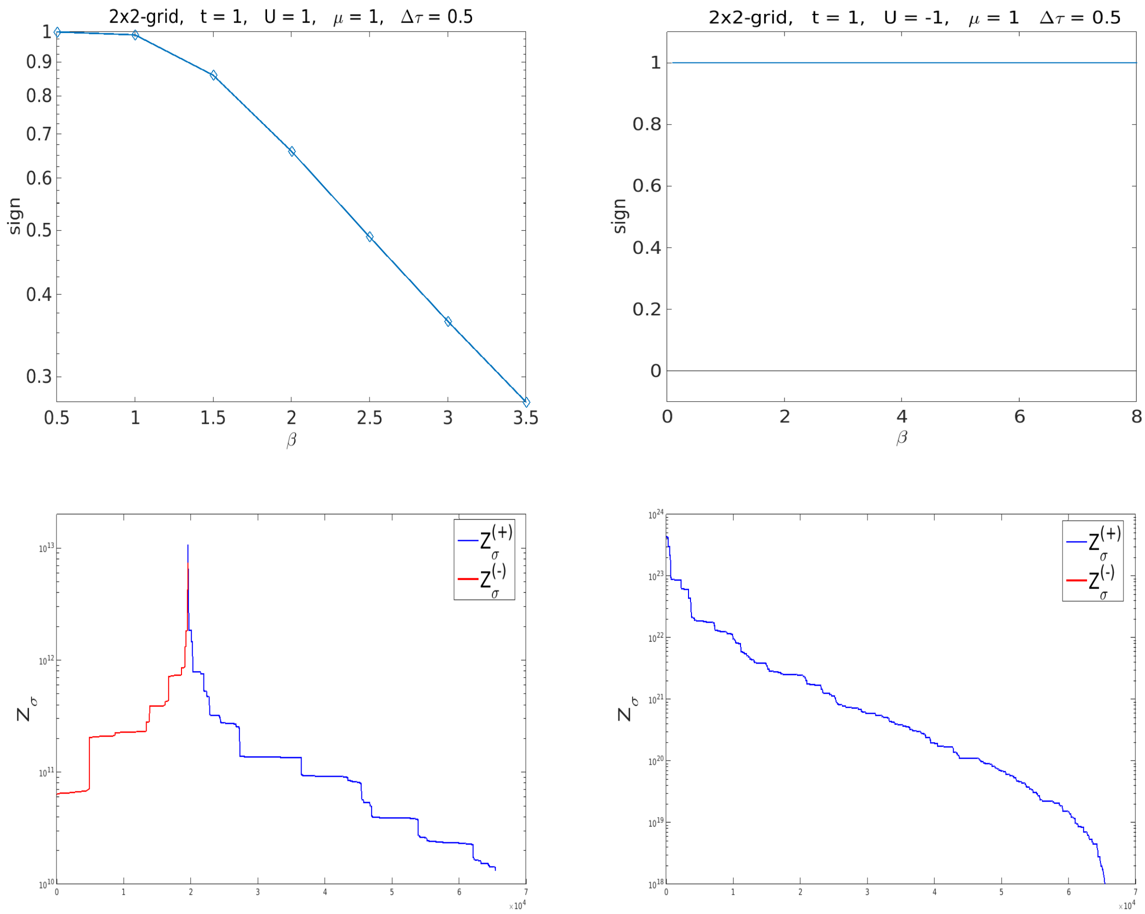


Figure 2: In the upper two plots the sign (15) of the addends (21) is plotted as a function of growing β. One sees that in the repulsive model $(U = 1)$ the sign is constantly one, while in the attractive model $(U = -1)$ the sign decreases exponentially as β increases. In the two lower plots the special value $\beta = 2$ is chosen to show the exact distribution of the addends Z_σ for all possibilties of $\sigma \in \{\pm 1\}^{N\times M}$. This means, that every σ-value corresponds to one point on the x-axis and on the y-axis the corresponding value of Z_σ is plotted. The red line means negative values and the blue line positive ones.

2.2 New HS transformation with external weight

The main result of the last section was, that no sign problem occurs in the Standard HS transformation of the $H_{h=0}$ model in the attractive case with and without chemical potential. So the remaining model to investigate is the repulsive $H_{h=0}$-model at finite chemical potential, but from here on until the end of chapter 3, the notation will be changed and the investigated model will be the equivalent (6) $H_{\frac{1}{2}}$-model (4).
For this model a new transformation will be developed.

The purpose of this New HS transformation with external weight is, to make the term $\Delta\tau(\mu + \frac{U}{2})E$

in the determinant of (19) vanish. The idea is, to go back to the Standard HS transformation (17) and transform not only the Coulomb but also the chemical potential part of the Hamiltonian. In the present case of the $H_{\frac{1}{2}}$ model this means, transforming the magnetic field part. This will be done by a second degree of freedem c in the exponent.

First of all the sign problem still occurs in this transformation and there is no progress in relation to this question. The second thing, which was unfavorable in (19), was the h-dependence of the determinant (respectively μ in the previous $H_{h=0}$ model). This problem will be solved in (27) by an approximation of the HS-coefficients.

2.2.1 Mathematical Identity of the New HS transformation

Choose $\underline{\lambda, c, D \in \mathbb{C}}$ such that:
- $\cosh(\lambda) = e^{\frac{\Delta\tau U}{2}} \cosh(\Delta\tau h)$
- $\tanh(c)\tanh(\lambda) = -\tanh(\Delta\tau h)$ (22)
- $\underline{\underline{D = \cosh(c)}}$

Because of $\cosh(\lambda) \in (0,1) \Leftrightarrow \lambda \in i(0, \frac{\pi}{2})$
$\underline{\cosh(\lambda) \in (1,\infty) \Leftrightarrow \lambda \in (0,\infty)}$

one has to calculate $e^{\frac{\Delta\tau U}{2}} \cosh(\Delta\tau h) = 1 \Rightarrow \underline{\underline{\Delta\tau U = -2\ln(\cosh(\Delta\tau h))}}$
in order to get the border line between real and complex λ-values.

In a similar fashion one gets the distribution of the values of the parameter c.

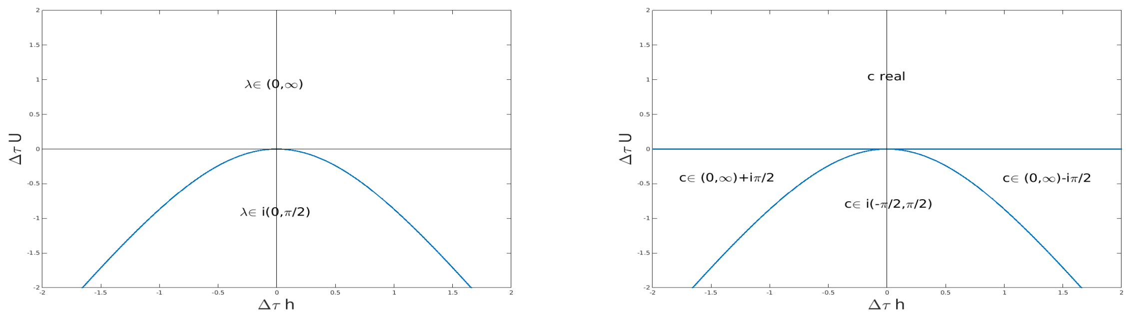


Figure 3: Possible values of the coefficients λ and c

Using these coefficients, the following transformation holds:

$$\boxed{e^{-\Delta\tau\left(U\left(n_\uparrow-\frac{1}{2}\right)\left(n_\downarrow-\frac{1}{2}\right)+h(n_\uparrow-n_\downarrow)\right)} = \frac{1}{2D} e^{-\frac{\Delta\tau U}{4}} \sum_{\sigma=\pm1} e^{\sigma(\lambda(n_\uparrow-n_\downarrow)+c)}} \tag{23}$$

Compared with (17) the additional magnetic term $h(n_\uparrow - n_\downarrow)$ on the left hand side leads to an additional parameter c in the transformed term.

<u>Proof:</u>

Because of fermions the number-operators $n_\uparrow, n_\downarrow$ can only take the values $n_\uparrow, n_\downarrow \in \{0,1\}$ and all possibilities can be investigated separately:

- $\underline{\underline{n_\uparrow = n_\downarrow}}$: $e^{-\Delta\tau\frac{U}{4}} = \frac{1}{2D} e^{-\frac{\Delta\tau U}{4}} \sum_{\sigma=\pm1} e^{\sigma c}$
  $\Rightarrow \underline{\underline{D = \cosh(c)}}$ fulfilled by assumption

- $\underline{\underline{n_\uparrow = 1 \ \wedge \ n_\downarrow = 0}}$: $e^{-\Delta\tau(-\frac{U}{4}+h)} = \frac{1}{2D} e^{-\frac{\Delta\tau U}{4}} \sum\limits_{\sigma=\pm1} e^{\sigma(c+\lambda)}$

  $\Rightarrow$ I: $\underline{e^{\Delta\tau(\frac{U}{2}-h)} = \frac{1}{D}\cosh(c+\lambda)}$

- $\underline{\underline{n_\uparrow = 0 \ \wedge \ n_\downarrow = 1}}$: $e^{-\Delta\tau\left(-\frac{U}{4}-h\right)} = \frac{1}{2D} e^{-\frac{\Delta\tau U}{4}} \sum\limits_{\sigma=\pm1} e^{\sigma(c-\lambda)}$

  $\Rightarrow$ II: $\underline{e^{\Delta\tau(\frac{U}{2}+h)} = \frac{1}{D}\cosh(c-\lambda)}$

Equations I and II should now be brought in the form of (22).
Because the two equations only differ by a sign, the calculation can be done simultaniously.

$$e^{\Delta\tau(\frac{U}{2}\mp h)} = \frac{1}{D}\cosh(c\pm\lambda)$$
$$\underline{\cosh(c)e^{\Delta\tau(\frac{U}{2}\mp h)} = \cosh(c)\cosh(\lambda) \pm \sinh(c)\sinh(\lambda)}$$

$\underline{\text{I+II}}$: $\cosh(c)e^{\Delta\tau\frac{U}{2}}\left(e^{-\Delta\tau h} + e^{\Delta\tau h}\right) = 2\cosh(c)\cosh(\lambda)$
$\underline{\underline{e^{\Delta\tau\frac{U}{2}}\cosh(\Delta\tau h) = \cosh(\lambda)}}$ fulfilled by assumption

$\underline{\text{I-II}}$: $\cosh(c)e^{\Delta\tau\frac{U}{2}}\left(e^{-\Delta\tau h} - e^{\Delta\tau h}\right) = 2\sinh(c)\sinh(\lambda)$
$-e^{\Delta\tau\frac{U}{2}}\sinh(\Delta\tau h) = \tanh(c)\sinh(\lambda) \quad / \ e^{\Delta\tau\frac{U}{2}} = \frac{\sinh(\lambda)}{\tanh(\lambda)\cosh(\Delta\tau h)}$
$\underline{\underline{-\tanh(\Delta\tau h) = \tanh(c)\tanh(\lambda)}}$ fulfilled by assumption ■

2.2.2 Partition function in the New HS transformation

In contrast to the Standard HS transformation of section 2.1, the New HS transformation (23) will now be applied to the partition function Z of the $H_{\frac{1}{2}}$ model (4).

$$\boxed{Z = \frac{1}{(2D)^{NM}} \sum_{\sigma\in\{\pm1\}^{N\times M}} e^{|\sigma|c} \, \mathrm{tr}\left(\prod_{j=1}^{M}\left(\prod_{i=1}^{N} e^{\sigma_{ij}\lambda(n_{i\uparrow}-n_{i\downarrow})} e^{-\Delta\tau H_{\mathrm{kin}}}\right)\right)} \tag{24}$$

with $\underline{\underline{|\sigma| = \sum\limits_{i=1}^{N}\sum\limits_{j=1}^{M}\sigma_{i,j}}}$

<u>Proof:</u>

In the form (11), the New HS transformation (23) can be applied to every site i and timeslice j.

$$\underline{\underline{Z}} = e^{\frac{\beta NU}{4}} \mathrm{tr}\left(\left(\prod_{i=1}^{N}\left(\frac{1}{2D}e^{-\frac{\Delta\tau U}{4}}\sum_{\sigma=\pm1} e^{\sigma(\lambda(n_{i\uparrow}-n_{i\downarrow})+c)}\right)e^{-\Delta\tau H_{\mathrm{kin}}}\right)^M\right) =$$
$$= \frac{1}{(2D)^{NM}} \sum_{\sigma\in\{\pm1\}^{N\times M}} \mathrm{tr}\left(\prod_{j=1}^{M}\left(\prod_{i=1}^{N} e^{\sigma_{ij}(\lambda(n_{i\uparrow}-n_{i\downarrow})+c)} e^{-\Delta\tau H_{\mathrm{kin}}}\right)\right) =$$
$$= \underline{\underline{\frac{1}{(2D)^{NM}} \sum_{\sigma\in\{\pm1\}^{N\times M}} e^{|\sigma|c} \, \mathrm{tr}\left(\prod_{j=1}^{M}\left(\prod_{i=1}^{N} e^{\sigma_{ij}\lambda(n_{i\uparrow}-n_{i\downarrow})} e^{-\Delta\tau H_{\mathrm{kin}}}\right)\right)}} \quad ■$$

2.2.3 Determinant representation of the New HS transformation

Analogously to the proof of (19), (69) can be used here, to write the fermionic trace as a determinant. The absolute square of the determinant in the formula (25) is only true for purely complex valued λ. For which values of $\Delta\tau, h, U$ this is true, can be seen in Fig.3. The following enumeration shows some special cases.

- $\underline{\underline{U > 0}}$: λ is never imaginary.
- $\underline{\underline{U < -2|h|}}$: λ is always imaginary.
- $\underline{\underline{-2|h| < U < 0}}$: λ becomes imaginary for sufficient small $\Delta\tau$.

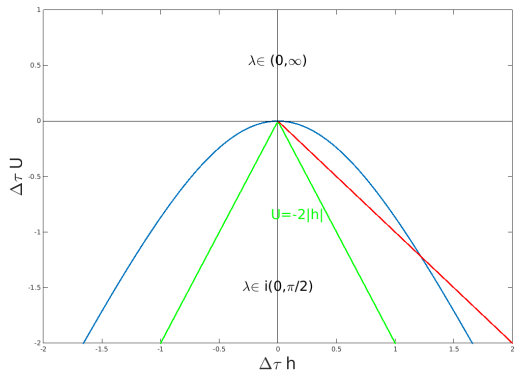


Figure 4: Possible values of the HS-coefficient λ defined in (22). The blue line is the border between real- and complex valued λ. If one changes $\Delta\tau$ at constant U and h, one moves along the red line and for sufficient small $\Delta\tau$ the value λ becomes imaginary. If the ratio between U and h is such that the red line lies below the green one, then λ is imaginary independently of $\Delta\tau$.

$$\boxed{Z = \frac{1}{(2D)^{NM}} \sum_{\sigma\in\{\pm1\}^{N\times M}} e^{|\sigma|c} \left|\det\left(E + \prod_{j=1}^{M}\left(e^{\lambda G^{(j)}} e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2} \quad (25)$$

with • $G^{(j)} = \begin{pmatrix} \sigma_{1j} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{Nj} \end{pmatrix}$

• $(h_{\text{kin}})_{ij} = \begin{cases} 1 & j \in \mathcal{N}_i \\ 0 & \text{else} \end{cases}$

• E the $N \times N$ identity matrix

Compared to (19) the sum is weighted by the factor $e^{|\sigma|c}$ and the h-dependence in the determinant is not linear, but implicitely given by $\cosh(\lambda) = e^{\frac{\Delta\tau U}{2}} \cosh(\Delta\tau h)$. This relation will be linearized in section 2.2.4.

Although the determinant of the model became the absolute square, the value of the parameter c (see Fig.3) is complex in the attractive model. So the addends become negative and the sign problem, which will be investigated in Fig.(5), occurs.

Proof:

Because there are no spin-flip-terms in the Hubbard Hamiltonian, it is possible to separate the trace in (24) into the product of two traces (one for spin↑, one for spin↓).

$$Z = \frac{1}{(2D)^{NM}} \sum_{\sigma\in\{\pm1\}^{N\times M}} e^{|\sigma|c} \prod_{s\in\{\pm1\}} \text{tr}_s \left(\prod_{j=1}^{M}\left(\prod_{i=1}^{N} e^{s\sigma_{ij}\lambda n_{is}} e^{-\Delta\tau H_{\text{kin}}}\right)\right)$$

Where $s = 1 \leftrightarrow$ spin ↑ and $s = -1 \leftrightarrow$ spin ↓

So with (20) and (69), the fermionic trace can be written as a determinant.

$$Z = \frac{1}{(2D)^{NM}} \sum_{\sigma\in\{\pm1\}^{N\times M}} e^{|\sigma|c} \prod_{s\in\{\pm1\}} \det\left(E + \prod_{j=1}^{M}\left(e^{s\lambda G^{(j)}} e^{t\Delta\tau h_{\text{kin}}}\right)\right)$$

For negative U and sufficient small magnetic field h the HS-coefficient λ becomes purely imaginary. (see Fig.4). Therefore, the product $\prod\limits_{s\in\{\pm 1\}}$ becomes the absolute square.

$$\underline{\underline{Z = \frac{1}{(2D)^{NM}} \sum_{\sigma\in\{\pm 1\}^{N\times M}} e^{|\sigma|c} \left|\det\left(E + \prod_{j=1}^{M}\left(e^{\lambda G^{(j)}} e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2}} \quad \blacksquare$$

To investigate the sign problem of this transformation one again needs to calculate all the addends, which have the form

$$Z_\sigma = e^{|\sigma|c} \left|\det\left(E + \prod_{j=1}^{M}\left(e^{\lambda G^{(j)}} e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2 . \tag{26}$$

Because of the imaginary prefactor c, the addends can become negative.

Also the form $Z = \sum_{m=-N}^{N} e^{-\beta hm}\, Z_m$ is not really given in this transformation. It became a little better, because a prefactor $e^{|\sigma|c}$ with a h-dependent factor c appeared, but this dependence is not linear, neither is the determinant independent of h.

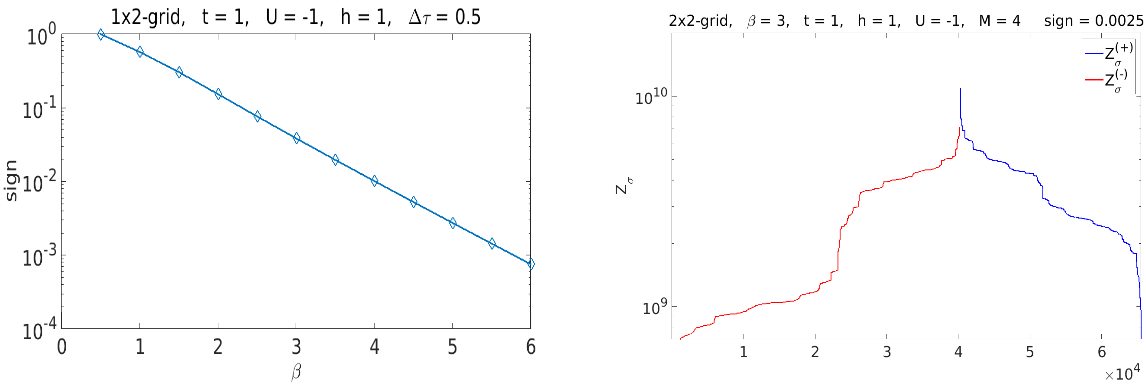


Figure 5: In the left plot the sign (15) of the addends (26) of the New HS transformation with external weights is plotted as a function of growing β. The model chosen here is the attractive $H_{\frac{1}{2}}$ model and one sees, that the sign decreases exponentially as β increases. In the right plot the special value $\beta = 3$ is chosen to show the exact distribution of the addends Z_σ for all possibilties of $\sigma \in \{\pm 1\}^{N\times M}$. This means, that every σ-value corresponds to one point on the x-axis and on the y-axis the corresponding value of Z_σ is plotted. The red line means negative values and the blue line positive ones.

2.2.4 Approximated Coefficients of the New HS transformation

One problem in (22) was the difficult h-dependence of the HS-coefficients. In order to get rid of this, one can simply expand the coefficients λ and c in orders of $\Delta\tau$. This will not solve the sign problem, but makes the determinant h-independent and the exponential prefactor linear in h.
Because the important model is the $H_{\frac{1}{2}}$ model with $U < 0$, only this one will be investigated here. So $-U$ can be replaced by the absolut value $|U|$.

- From (22), the coefficient λ is defined as $\cosh(\lambda) = e^{\frac{\Delta\tau U}{2}} \cosh(\Delta\tau h)$.
  With the expansions $\cosh(x) \approx 1 + \frac{x^2}{2}$ and $e^x \approx 1 + x$ one gets the following λ-approximation.

  $$1 + \frac{\lambda^2}{2} = (1 + \frac{\Delta\tau U}{2})\ 1$$
  $$\underline{\underline{\lambda = i\sqrt{\Delta\tau|U|} + \mathcal{O}(\Delta\tau^{\frac{3}{2}})}}$$

  Because of the possible values λ can take (see Fig.3), the positive square root is the correct one.

- Also from (22), the coefficient c is defined as $\tanh(c)\tanh(\lambda) = -\tanh(\Delta\tau h)$.
  With the expansion $\tanh(x) \approx x$ and the expansion of λ from above, one gets the following approximation for c.

$$c\lambda = -\Delta\tau h$$
$$\underline{\underline{c = -ih\sqrt{\frac{\Delta\tau}{|U|}} + \mathcal{O}(\Delta\tau^{\frac{3}{2}})}}$$

- The prefactor $D = \cosh(c)$ is approximated according to the expansion $\cosh(x) \approx 1 + \frac{x^2}{2} \approx e^{\frac{x^2}{2}}$.

$$D = e^{\frac{1}{2}h^2\frac{\Delta\tau}{U}} \Rightarrow \underline{\underline{D^M = e^{-\frac{\beta h^2}{2|U|}}}}$$

This leads for the attractive $H_{\frac{1}{2}}$-model $(U < 0)$ to a partition function of the form

$$\boxed{Z_{\frac{1}{2}} = \frac{e^{N\frac{\beta h^2}{2|U|}}}{2^{NM}} \sum_{\sigma\in\{\pm1\}^{N\times M}} e^{i|\sigma|h\sqrt{\frac{\Delta\tau}{|U|}}} \left|\det\left(E + \prod_{j=1}^{M}\left(e^{i\sqrt{\Delta\tau|U|}G^{(j)}} e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2} . \quad (27)$$

With its linear h-dependence in the exponent and h-independence of the determinant, this representation has, except of the sign problem, everything which is advantageous. There is still a h^2 in the exponent of the prefactor, which will make the integral in section 3.3 not analytically solvable, but at at least easier to compute.
The only thing left is, to check the convergence of this approximation, which is done in Fig.6.

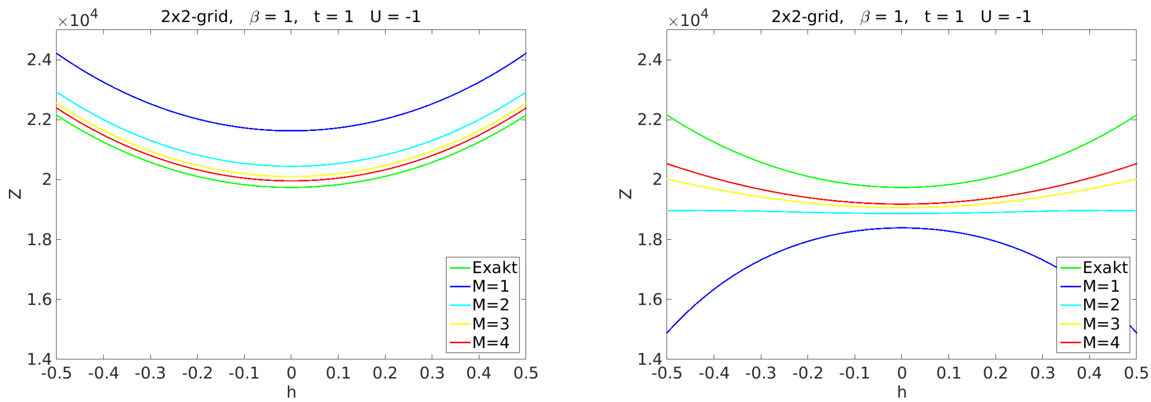


Figure 6: In the left plot the exact New HS transformation (25) and in the right plot the approximated New HS transformation (27) is plotted for the attractive $H_{\frac{1}{2}}$-model. Each plot is done for a different number of time slices M. To see the convergence of the approximation, the exact partition function is plotted as a reference in both figures. The exact New HS transformation only contains the Trotter error of (11) and the approximated transformation the additional error of the expansion of the coefficients λ, c, and D. In both cases one observes convergence.

2.3 New Asymmetric HS transformation

Beside the problem with the positivity of the addends of the New HS transformation with external weights (25), the second goal was, to make the determinant h-independent. The reason why this is desireable will be the integration over the magnetic field h in chapter 3. This integration will be of huge numerical effort, if one has to evaluate the determinant in every single integration step. The way this problem was solved in the New HS transformation, was an expansion of the HS-coefficients in terms of $\Delta\tau$ (27). Fortunately it turned out, that the first order term was h-independent and also enough to make the approximation converge. In this section the investigation of the $H_{\frac{1}{2}}$-model (4) will be continued and another way to guarantee this h-independence by construction will be presented.

The idea of this new Asymmetric HS transformation is, to enlarge the HS sum to three components. This yields to a h-independent value λ, even more, λ can be chosen almost arbitrary (see (28)). The price paid in this transformation is a prefactor D_σ, which has no simple σ-dependence like in the previous transformations. This leads in the end to the appearance (see (33)) of a complicated product of h-dependent prefactors $D_{\sigma_{ij}}$, which will be also very hard to integrate.

In terms of the sign problem, this transformation does not give any progress. For the special choice $\lambda \in \mathbb{R}$ in section 2.3.4, the determinant becomes positive (because of the absolute square), but the paramters D_σ does not show any special distribution depending on the choice of $\Delta\tau$, h and U. So the whole prefactor $\prod_j \prod_i D_{\sigma_{ij}}$ of (33) becomes an arbitrary complex valued number.

2.3.1 Mathematical Identity of the Asymmetric HS transformation

The h-dependent coefficient λ of (22) will in this Asymmetric HS transformation be made h-independent by construction. To achieve this, the sum will be enlarged to $\sigma \in \{-1, 0, 1\}$ and the prefactor D is made σ-dependent.

$$\boxed{e^{-\Delta\tau\left(U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right) + h(n_\uparrow - n_\downarrow)\right)} = e^{-\Delta\tau\frac{U}{4}} \sum_{\sigma\in\{-1,0,1\}} D_\sigma e^{i\sigma\lambda(n_\uparrow - n_\downarrow)}} \tag{28}$$

with the coefficients:
$$\lambda \in \mathbb{C} \setminus (\pi\mathbb{Z})$$
$$a = \frac{1}{i} e^{\Delta\tau\frac{U}{2}} \sinh(\Delta\tau h)$$
$$b = e^{\Delta\tau\frac{U}{2}} \cosh(\Delta\tau h)$$
$$D_- = \frac{1-b}{2(1-\cos(\lambda))} + \frac{a}{2\sin(\lambda)}$$
$$D_0 = \frac{b-\cos(\lambda)}{1-\cos(\lambda)}$$
$$D_+ = \frac{1-b}{2(1-\cos(\lambda))} - \frac{a}{2\sin(\lambda)}$$

Proof:

Because of fermions the number-operators $n_\uparrow, n_\downarrow$ can only take the values $n_\uparrow, n_\downarrow \in \{0, 1\}$
and all possibilities can be investigated separately:

- $n_\uparrow = n_\downarrow$: $e^{-\Delta\tau\frac{U}{4}} = e^{-\Delta\tau\frac{U}{4}}(D_- + D_0 + D_+)$

$$D_0 = 1 - D_- - D_+ \tag{29}$$

- $n_\uparrow = 1 \wedge n_\downarrow = 0$: $e^{-\Delta\tau\left(-\frac{U}{4}+h\right)} = e^{-\frac{\Delta\tau U}{4}}(D_- e^{-i\lambda} + D_0 + D_+ e^{i\lambda})$

$$e^{-\Delta\tau\left(-\frac{U}{2}+h\right)} = 1 - (1-e^{-i\lambda})D_- - (1-e^{i\lambda})D_+ \tag{30}$$

- $n_\uparrow = 0 \wedge n_\downarrow = 1$: $e^{-\Delta\tau\left(-\frac{U}{4}-h\right)} = e^{-\frac{\Delta\tau U}{4}}(D_- e^{i\lambda} + D_0 + D_+ e^{-i\lambda})$

$$e^{-\Delta\tau\left(-\frac{U}{2}-h\right)} = 1 - (1-e^{i\lambda})D_- - (1-e^{-i\lambda})D_+ \tag{31}$$

Where in (30) and (31) the equation (29) was used.

For the value of D_+, one multiplies (30) with $(1-e^{i\lambda})$ and (31) with $(1-e^{-i\lambda})$. Afterwards they got substracted from each other.

$$(1-e^{i\lambda})e^{-\Delta\tau\left(-\frac{U}{2}+h\right)} - (1-e^{-i\lambda})e^{-\Delta\tau\left(-\frac{U}{2}-h\right)} = (-e^{i\lambda}+e^{-i\lambda}) - D_+\left((1-e^{i\lambda})^2 - (1-e^{-i\lambda})^2\right)$$
$$(1-e^{i\lambda})(b-ia) - (1-e^{-i\lambda})(b+ia) = -2i\sin(\lambda) + 2iD_+(2\sin(\lambda) - \sin(2\lambda))$$
$$-b\sin(\lambda) - a(1-\cos(\lambda)) = -\sin(\lambda) + 2\sin(\lambda)D_+(1-\cos(\lambda))$$
$$D_+ = \frac{1-b}{2(1-\cos(\lambda))} - \frac{a}{2\sin(\lambda)}$$

For the value of D_- one multiplies (30) with $(1-e^{-i\lambda})$ and (31) with $(1-e^{i\lambda})$. Afterwards they got substracted from each other.

$$(1-e^{-i\lambda})e^{-\Delta\tau\left(-\frac{U}{2}+h\right)} - (1-e^{i\lambda})e^{-\Delta\tau\left(-\frac{U}{2}-h\right)} = (-e^{-i\lambda}+e^{i\lambda}) - D_-\left((1-e^{-i\lambda})^2-(1-e^{i\lambda})^2\right)$$
$$(1-e^{-i\lambda})(b-ia)-(1-e^{i\lambda})(b+ia) = 2i\sin(\lambda) - 2iD_-(2\sin(\lambda)-\sin(2\lambda))$$
$$b\sin(\lambda) - a(1-cos(\lambda)) = \sin(\lambda) - 2\sin(\lambda)D_-(1-\cos(\lambda))$$
$$\underline{\underline{D_- = \frac{1-b}{2(1-\cos(\lambda))} + \frac{a}{2\sin(\lambda)}}}$$

These solutions for D_+ and D_- inserted in (29) give the value for D_0, which completes the proof.

$$\underline{\underline{D_0}} = 1 - D_- - D_+ = 1 - \frac{1-b}{1-\cos(\lambda)} = \underline{\underline{\frac{b-\cos(\lambda)}{1-\cos(\lambda)}}} \quad \blacksquare$$

2.3.2 Partition function in the Asymmetric HS transformation

This Asymmetric HS transformation (28) can now be used to rewrite the partition function of the $H_{\frac{1}{2}}$-model (4). To split off the kinetic exponential $e^{-\Delta\tau H_{\text{kin}}}$ the Trotter decomposition is needed and so the form (11) is used.

$$\boxed{Z = \sum_{\sigma\in\{-1,0,1\}^{N\times M}} \text{tr}\left(\prod_{j=1}^{M}\left(\prod_{i=1}^{N}\left(D_{\sigma_{ij}} e^{i\sigma_{ij}\lambda(n_{i\uparrow}-n_{i\downarrow})}\right)e^{-\Delta\tau H_{\text{kin}}}\right)\right)} \tag{32}$$

<u>Proof:</u>

Taking (11) and applying (28) to every site i and timeslice j, leads to

$$\underline{\underline{Z}} = e^{\frac{\beta NU}{4}} \text{tr}\left(\left(\prod_{i=1}^{N}\left(e^{-\Delta\tau\frac{U}{4}}\sum_{\sigma\in\{-1,0,1\}} D_\sigma e^{i\sigma\lambda(n_{i\uparrow}-n_{i\downarrow})}\right)e^{-\Delta\tau H_{\text{kin}}}\right)^M\right) =$$
$$= \underline{\underline{\sum_{\sigma\in\{-1,0,1\}^{N\times M}} \text{tr}\left(\prod_{j=1}^{M}\left(\prod_{i=1}^{N}\left(D_{\sigma_{ij}} e^{i\sigma_{ij}\lambda(n_{i\uparrow}-n_{i\downarrow})}\right)e^{-\Delta\tau H_{\text{kin}}}\right)\right)}}. \quad \blacksquare$$

2.3.3 Determinant representation of the Asymmetric HS transformation

Analogous to the previous transformations, (69) will be used to write the trace of (32) in form of a determinant.

$$\boxed{Z = \sum_{\sigma\in\{-1,0,1\}^{N\times M}} \left(\prod_{j=1}^{M}\prod_{i=1}^{N} D_{\sigma_{ij}}\right) \prod_{s\in\{\pm1\}} \det\left(E + \prod_{j=1}^{M}\left(e^{si\lambda G^{(j)}} e^{\Delta\tau h_{\text{kin}}}\right)\right)} \tag{33}$$

with
- $G^{(j)} = \begin{pmatrix} \sigma_{1j} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{Nj} \end{pmatrix}$
- $(h_{\text{kin}})_{i,j} = \begin{cases} 1 & j \in \mathcal{N}_i \\ 0 & \text{else} \end{cases}$
- $\underline{\underline{E \text{ the } N\times N \text{ identity matrix}}}$

<u>Proof:</u>

In a first step it is possible to split up the trace in (32) into a product of two traces (one for spin↑, one for spin↓). This is possible, because the kinetic Hamiltonian consists of a sum of a spin↑ and a spin↓ part.

$$\underline{Z} = \sum_{\sigma\in\{-1,0,1\}^{N\times M}} \prod_{s\in\{\pm1\}} \mathsf{tr}_s \left(\prod_{j=1}^{M} \left(\prod_{i=1}^{N} \left(D_{\sigma_{ij}} e^{si\sigma_{ij}\lambda n_{is}} \right) e^{-\Delta\tau H_{\mathsf{kin},s}} \right) \right) =$$

$$= \underline{\sum_{\sigma\in\{-1,0,1\}^{N\times M}} \left(\prod_{j=1}^{M}\prod_{i=1}^{N} D_{\sigma_{ij}} \right) \prod_{s\in\{\pm1\}} \mathsf{tr}_s \left(\prod_{j=1}^{M} \left(\prod_{i=1}^{N} e^{si\sigma_{ij}\lambda n_{is}} e^{-\Delta\tau H_{\mathsf{kin},s}} \right) \right)}$$

Where $\underline{s = 1 \leftrightarrow \text{ spin}\uparrow}$ and $\underline{s = -1 \leftrightarrow \text{ spin}\downarrow}$

Finally with (20) and (69) the fermionic trace can be written as a determinant

$$\underline{\underline{Z_{\frac{1}{2}} = \sum_{\sigma\in\{-1,0,1\}^{N\times M}} \left(\prod_{j=1}^{M}\prod_{i=1}^{N} D_{\sigma_{ij}} \right) \prod_{s\in\{\pm1\}} \det \left(E + \prod_{j=1}^{M} \left(e^{si\lambda G^{(j)}} e^{t\Delta\tau h_{\mathsf{kin}}} \right) \right)}} \qquad \blacksquare$$

It is possible now, to choose $\lambda \in \mathbb{R}$. In this case the product $\prod_{s\in\{\pm1\}}$ becomes the absolute square of the determinant and is therefore positive. But in this transformation every part of the sum has the prefactor $\prod_j \prod_i D_{\sigma_{ij}}$ which will take also negative values in general. The quantitative investigation of the sign will be done in the following section, for a even more specific choice of λ.

2.3.4 Special representation of the Asymmetric HS transformation

Because of the free choice of the parameter λ in (28), one can choose it in a way, that the prefactors D_σ gets an easy form. So for example $\underline{\lambda = \frac{\pi}{2}}$ is a good choice, for which the partition function (33) has the form

$$\boxed{Z = \sum_{\sigma\in\{-1,0,1\}^{N\times M}} \left(\prod_{j=1}^{M}\prod_{i=1}^{N} D_{\sigma_{ij}} \right) \left| \det \left(E + \prod_{j=1}^{M} \left(e^{i\frac{\pi}{2}G^{(j)}} e^{\Delta\tau h_{\mathsf{kin}}} \right) \right) \right|^2} \tag{34}$$

with the coefficients
$$D_- = \frac{1}{2}\left(1 - e^{\frac{\Delta\tau U}{2}} (\cosh(\Delta\tau h) + i\sinh(\Delta\tau h))\right)$$
$$D_0 = e^{\frac{\Delta\tau U}{2}} \cosh(\Delta\tau h)$$
$$\underline{D_+ = \frac{1}{2}\left(1 - e^{\frac{\Delta\tau U}{2}} (\cosh(\Delta\tau h) - i\sinh(\Delta\tau h))\right)}\ .$$

The sign (15) of the addends of (33) can now be examined for every allowed value λ. The test shows the same behaviour of the sign independently of λ, namely with growing beta the sign converges to zero. In Fig.7 the convergence of the sign and the distribution of the addends is shown for the special choice $\lambda = \frac{\pi}{2}$. The addends in this case, according to (34), are given by

$$Z_\sigma = \left(\prod_{j=1}^{M}\prod_{i=1}^{N} D_{\sigma_{ij}} \right) \left| \det \left(E + \prod_{j=1}^{M} \left(e^{i\frac{\pi}{2}G^{(j)}} e^{\Delta\tau h_{\mathsf{kin}}} \right) \right) \right|^2 \tag{35}$$

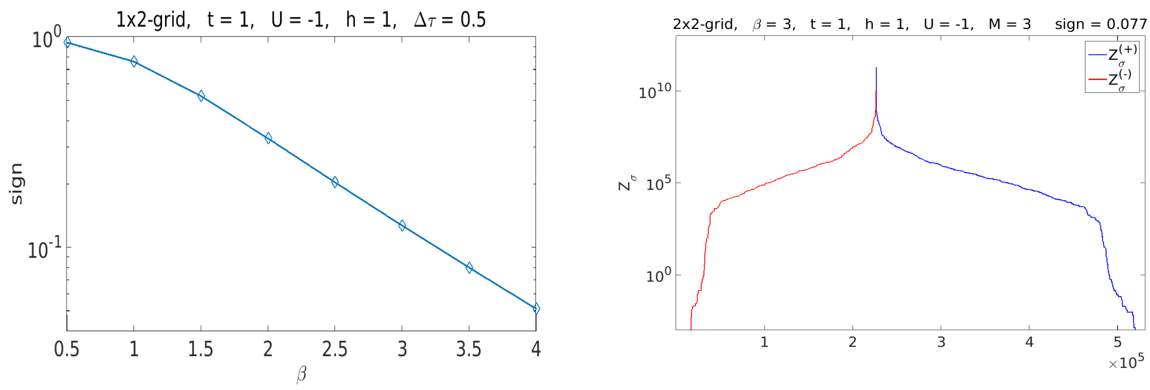


Figure 7: In the left plot the sign (15) of the addends (35) is plotted as a function of growing β. One sees that in this attractive $H_{\frac{1}{2}}$ model, the sign goes to zero exponentially as β increases. In the right plot the special value $\beta = 3$ is chosen to show the exact distribution of the addends Z_σ for all possibilties of $\sigma \in \{-1, 0, 1\}^{N\times M}$. This means, that every σ-value corresponds to one point on the x-axis and on the y-axis the corresponding value of Z_σ is plotted. The red line means negative values and the blue line positive ones.

In chapter 3, it will be tried to integrate over the magnetic field h (or in letters of chapter 3, over the complex valued magnetic field ν). The only terms h-dependent in (34) are the prefactors D_σ. So one is faced with the integral of the product of the $D_{\sigma_{ij}}$, which is analytically solvable, but will lead to a large and not easy to calculate sum (see (50)).

2.4 Continuous HS transformation

The New HS transformation in its approximated version (27) looks like the most promising form for further investigations. The sign problem was not solved there, but the h-dependence had a very simple Gaussian form, which was not enough to do the integral (43) analytically, but nevertheless easy to compute numerically.
However, another well known transformation, the Continuous HS transformation [9], is investigated as the last one of this chapter. The idea of this one is, to stay at the $H_{\frac{1}{2}}$-model (4) and make the σ-dependence continuous again, like it was in the initial idea of the HS transformation (9). In this case one does not need any prefactors D_σ like in the Asymmetric HS transformation (28) and also the coefficients λ and c become h-independent without any further approximations. The disadvantage is the continuous degree of freedem σ. While in the previous transformations only two or three values of σ had to be calculated, here the integral over the whole real line has to be evaluated or discretized.

Regardless of the huge numerical effort it will take to do the integral, it leads to a very similar form like the approximated New HS transformation (27). The linear h-dependence in the integral, as well as the quadratic dependence in the prefactor appears in both cases. Also the results of these transformations are compareable, namely the sign problem will not be solved and one gets a simple h-dependence, which is not enough to calculate the integral (43) analytically.

2.4.1 Mathematical Identity of the Continuous HS transformation

The Continuous HS transformation tries to make λ independent of h without any approximations and additional prefactors D_σ, like it was done in the New or Asymmetric HS transformation. The way this is achieved here, is choosing the σ degree of freedom continuous, which means replacing the discrete sum by an integral over σ.

$$\boxed{e^{-\Delta\tau\left(U\left(n_\uparrow-\frac{1}{2}\right)\left(n_\downarrow-\frac{1}{2}\right)+h(n_\uparrow-n_\downarrow)\right)} = \frac{1}{\sqrt{\pi}} e^{-\frac{\Delta\tau U}{4}\left(1+\frac{2h^2}{U^2}\right)} \int\limits_{-\infty}^{\infty} e^{-\sigma^2+\sigma(\lambda(n_\uparrow-n_\downarrow)+c)} d\sigma} \tag{36}$$

with the Continuous HS coefficients: $\lambda = \sqrt{2\Delta\tau U}$

$\underline{\underline{c = -h\sqrt{\frac{2\Delta\tau}{U}}}}$

Here, without further approximations, λ is not a function of h anymore.
The disadvantage is, that an σ-integration over the whole real line has to be done and not just a sum over finitely many σ-values, like in the transformations before.

Proof:

In order to prove this transformation, one uses the identity $\frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} e^{-\sigma^2+\sigma(\lambda(n_\uparrow - n_\downarrow)+c)} d\sigma = e^{\frac{(\lambda(n_\uparrow - n_\downarrow)+c)^2}{4}}$.

Thus, the coefficients λ and c have to fulfill the following equation

$$-\Delta\tau\left(U\left(n_\uparrow - \tfrac{1}{2}\right)\left(n_\downarrow - \tfrac{1}{2}\right) + h(n_\uparrow - n_\downarrow)\right) = -\frac{\Delta\tau U}{4} + \frac{1}{4}\left(\lambda^2(n_\uparrow - n_\downarrow)^2 + 2\lambda c(n_\uparrow - n_\downarrow)\right)$$

for every $n_\uparrow, n_\downarrow \in \{0, 1\}$.

By inserting all combinations, one gets three equations for the coefficients λ and c.

$\underline{\underline{n_\uparrow = n_\downarrow}}$: I: $\underline{\underline{-\Delta\tau\frac{U}{4} = -\frac{\Delta\tau U}{4}}}$

$\underline{\underline{n_\uparrow = 1 \ \wedge \ n_\downarrow = 0}}$: II: $\underline{-\Delta\tau(-\frac{U}{4} + h) = -\frac{\Delta\tau U}{4} + \frac{1}{4}(\lambda^2 + 2\lambda c)}$

$\underline{\underline{n_\uparrow = 0 \ \wedge \ n_\downarrow = 1}}$: III: $\underline{-\Delta\tau(-\frac{U}{4} - h) = -\frac{\Delta\tau U}{4} + \frac{1}{4}(\lambda^2 - 2\lambda c)}$

II+III: $\frac{\Delta\tau U}{2} = -\frac{\Delta\tau U}{2} + \frac{\lambda^2}{2} \Rightarrow \underline{\underline{\lambda = \sqrt{2\Delta\tau U}}}$

II: $\underline{\underline{c}} = \frac{4\Delta\tau(\frac{U}{2} - h) - \lambda^2}{2\lambda} = -\frac{2\Delta\tau h}{\lambda} = \underline{\underline{-h\sqrt{\frac{2\Delta\tau}{U}}}}$ ■

2.4.2 Partition function in the Continuous HS transformation

The investigated model in this section will be again the $H_{\frac{1}{2}}$-model (4). Using the Trotter decomposition and the form (11) of the partition function, allows to apply the Continuous HS transformation (36).

$$\boxed{Z = \left(\frac{e^{-\frac{\beta h^2}{U}}}{\pi^M}\right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times M}} e^{-|\sigma^2| + |\sigma| c}\, \mathrm{tr}\left(\prod_{j=1}^{M}\left(\prod_{i=1}^{N} e^{\sigma_{ij}\lambda(n_{i\uparrow} - n_{i\downarrow})} e^{-\Delta\tau H_{\mathrm{kin}}}\right)\right) d\sigma} \qquad (37)$$

with $|\sigma| = \sum\limits_{j=1}^{M}\sum\limits_{i=1}^{N} \sigma_{ij}$

$\underline{\underline{|\sigma^2| = \sum\limits_{j=1}^{M}\sum\limits_{i=1}^{N} \sigma_{ij}^2}}$

Proof:

Taking (36) and applying it on every site i and every timeslice j of (11) one ends up with

$$\underline{\underline{Z}} = e^{\frac{\beta N U}{4}} \mathrm{tr}\left(\left(\left(\prod_{i=1}^{N}\left(\frac{1}{\sqrt{\pi}} e^{-\frac{\Delta\tau U}{4}\left(1+\frac{2h^2}{U^2}\right)} \int\limits_{-\infty}^{\infty} e^{-\sigma^2+\sigma(\lambda(n_{i\uparrow} - n_{i\downarrow})+c)} d\sigma\right) e^{-\Delta\tau H_{\mathrm{kin}}}\right)^M\right) =$$

$$= \frac{e^{-\frac{\beta N h^2}{2U}}}{\pi^{\frac{NM}{2}}} \int\limits_{\mathbb{R}^{N\times M}} \mathrm{tr}\left(\prod_{j=1}^{M}\left(\prod_{i=1}^{N} e^{-\sigma_{ij}^2+\sigma_{ij}(\lambda(n_{i\uparrow} - n_{i\downarrow})+c)} e^{-\Delta\tau H_{\mathrm{kin}}}\right)\right) d\sigma =$$

$$= \underline{\underline{\left(\frac{e^{-\frac{\beta h^2}{U}}}{\pi^M}\right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times M}} e^{-|\sigma^2| + |\sigma| c}\, \mathrm{tr}\left(\prod_{j=1}^{M}\left(\prod_{i=1}^{N} e^{\sigma_{ij}\lambda(n_{i\uparrow} - n_{i\downarrow})} e^{-\Delta\tau H_{\mathrm{kin}}}\right)\right) d\sigma}}\ . \qquad ■$$

2.4.3 Determinant representation of the Continuous HS transformation

Like in the previous transformations, the identity (69) can be used to write the fermionic trace in (37) as a determinant. Also the values for λ and c are written in the interesting case $U < 0$, where $-U$ can be replaced by its absolute value.

$$\boxed{Z = \left(\frac{e^{\frac{\beta h^2}{|U|}}}{\pi^M} \right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N \times M}} e^{-|\sigma^2| + i|\sigma| h \sqrt{\frac{2\Delta\tau}{|U|}}} \left| \det \left(E + \prod_{j=1}^{M} \left(e^{i\sqrt{2\Delta\tau|U|} G^{(j)}} e^{t\Delta\tau h_{\text{kin}}} \right) \right) \right|^2 d\sigma} \qquad (38)$$

with • $G^{(j)} = \begin{pmatrix} \sigma_{1j} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{Nj} \end{pmatrix}$

• $(h_{\text{kin}})_{ij} = \begin{cases} 1 & j \in \mathcal{N}_i \\ 0 & \text{else} \end{cases}$

• E the $N \times N$ identity matrix

Proof:

Because there are no spin-flip-terms in (37), it is possible to separate the Hamiltonian into a sum of two Hamiltonians (one for spin↑, one for spin↓) and therefore, the trace into a product of two traces, acting on the respective subspaces.

$$Z = \left(\frac{e^{-\frac{\beta h^2}{U}}}{\pi^M} \right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N \times M}} e^{-|\sigma^2| + |\sigma| c} \prod_{s \in \{\pm 1\}} \text{tr}_s \left(\prod_{j=1}^{M} \left(\prod_{i=1}^{N} e^{s\sigma_{ij} \lambda n_{is}} e^{-\Delta\tau H_{\text{kin},s}} \right) \right) d\sigma$$

Where $s = 1 \leftrightarrow$ spin ↑ and $s = -1 \leftrightarrow$ spin ↓

With (20) and (69) the fermionic trace can be written in form of a determinant:

$$Z = \left(\frac{e^{-\frac{\beta h^2}{U}}}{\pi^M} \right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N \times M}} e^{-|\sigma^2| + |\sigma| c} \prod_{s \in \{\pm 1\}} \det \left(E + \prod_{j=1}^{M} \left(e^{s\lambda G^{(j)}} e^{t\Delta\tau h_{\text{kin}}} \right) \right)$$

This formula is true for every $U \in \mathbb{R}$. For the interesting case $U < 0$ the coefficients λ and c from (36) have the form $\lambda = i\sqrt{2\Delta\tau|U|}$ and $c = ih\sqrt{\frac{2\Delta\tau}{|U|}}$.
Because of this pure imaginary λ the product $\prod_{s \in \{\pm 1\}}$ becomes the absolute square.

$$Z = \left(\frac{e^{\frac{\beta h^2}{|U|}}}{\pi^M} \right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N \times M}} e^{-|\sigma^2| + i|\sigma| h \sqrt{\frac{2\Delta\tau}{|U|}}} \left| \det \left(E + \prod_{j=1}^{M} \left(e^{i\sqrt{2\Delta\tau|U|} G^{(j)}} e^{t\Delta\tau h_{\text{kin}}} \right) \right) \right|^2 d\sigma \qquad \blacksquare$$

Although the absolute square of the determinant is positive, the prefactor is imaginary in its exponent and therefore, will take negative values. The exact behaviour of the sign of the integrand

$$Z_\sigma = e^{-|\sigma^2| + i|\sigma| h \sqrt{\frac{2\Delta\tau}{|U|}}} \left| \det \left(E + \prod_{j=1}^{M} \left(e^{i\sqrt{2\Delta\tau|U|} G^{(j)}} e^{t\Delta\tau h_{\text{kin}}} \right) \right) \right|^2 \qquad (39)$$

is investigated in Fig.8.

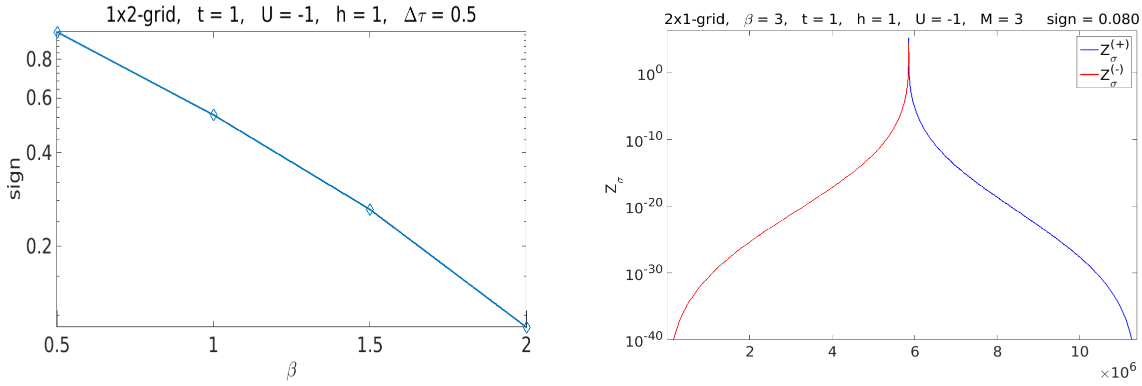


Figure 8: In the left plot the sign (15) of the addends (39) of the Continuous HS transformation is plotted as a function of growing β. Because σ is continuous in this transformation, only a representative sample of σ-values is taken, namely 21 equidistant values in the interval $[-5, 5]$ in every of the NM dimensions. One sees that in this attractive $H_{\frac{1}{2}}$ model the sign goes to zero exponentially as β increases. In the right plot the special value $\beta = 3$ is chosen to show the exact distribution of the addends Z_σ. This means, that every σ-value corresponds to one point on the x-axis and on the y-axis the corresponding value of Z_σ is plotted. The red line means negative values and the blue line positive ones.

In terms of the h-dependence this Continuous HS transformation shows the same behaviour as the approximated New HS transformation (27), namely no h-dependence in the determinant, linear in the exponential of the integrand and quadratic in the exponential of the prefactor. This simple dependency will make the integral (43) easy to compute numerically, but is not enough to give an analytic solution.

3 Partition function as a Fourier series

In chapter 2, different Hubbard-Stratonovich (HS) transformations were introduced and no one of them gave any progress in terms of the sign problem. The idea in chapter 3 is not to introduce even more variations of the HS transformation, but take the existing ones from section 2.1-2.4 and transform them to complex valued magnetic field (41). In section 2 the notation switched between the two equivalent models $H_{h=0}$ and $H_{\frac{1}{2}}$, but in this section all transformations will be investigated in the $H_{\frac{1}{2}}$-model (4). This partition function can then be written as a Fourier sum (42) and it is left to calculate the Fourier coefficients (43), which turn out to be the canonical partition functions with fixed magnetisation m. This Fourier coefficients in the different HS transformations of chapter 2 will be the quantity of interest in this chapter and investigated in terms of the sign problem.
It will turn out in the end, that the sign problem is not solved in any of the transformations, but the forms of the Fourier coefficients are quite advantageous for further numerical calculations.

3.1 Canonical partition function and imaginary magnetic field

In this first section of chapter 3 the grandcanonical partition function of the Hamiltonian (4) will be decomposed into a sum of canonical partition functions (40), each for a fixed value of the total magnetisation m of the system. In the second step the magnetic field h will be extended to imaginary values and the canonical partition functions will turn into the Fourier coefficients of the grandcanonical partition function in this case (42). These Fourier coefficients can now be represented by the inverse Fourier transformation and will be the main objects investigated in terms of the sign problem in this chapter.

The first step is to decompose the partition function Z of the Hubbard model (2) into canonical partition functions Z_m with fixed magnetizations m. This decomposition is true in its exact form $Z = \text{tr}(e^{-\beta H})$ without even the Trotter decomposition.

$$\boxed{Z(h) = \sum_{m=-N}^{N} e^{-\beta hm} Z_m} \qquad \text{with } \underline{\underline{Z_m = \text{tr}_m(e^{-\beta H(h=0)})}} \tag{40}$$

where tr_m is the trace over the Fock space of states with total magnetization $\underline{m = \sum_{i=1}^{N}(n_{i\uparrow} - n_{i\downarrow})}$.

Proof:

By looking at the trace of the Hamiltonian (4), one gets

$$\begin{aligned}
\underline{Z(h)} &= \text{tr}\left(e^{-\beta\left(U\sum_{i=1}^{N}(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})+h\sum_{i=1}^{N}(n_{i\uparrow}-n_{i\downarrow})-N\frac{U}{4}+H_{\text{kin}}\right)}\right) = \\
&= \underline{\sum_{\vec{n}_\uparrow,\vec{n}_\downarrow\in\{0,1\}^N} \langle \vec{n}_\uparrow,\vec{n}_\downarrow| \, e^{-\beta\left(U\sum_{i=1}^{N}(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})+h\sum_{i=1}^{N}(n_{i\uparrow}-n_{i\downarrow})-N\frac{U}{4}+H_{\text{kin}}\right)} \, |\vec{n}_\uparrow,\vec{n}_\downarrow\rangle} \; .
\end{aligned}$$

Because neither the Coulomb nor the kinetic part of the Hamiltonian change the total magnetization m, the commutator $[H(h=0), m]$ vanishes and the exponential can be separated.

$$\begin{aligned}
\underline{\underline{Z(h)}} &= \sum_{\vec{n}_\uparrow,\vec{n}_\downarrow\in\{0,1\}^N} \langle \vec{n}_\uparrow,\vec{n}_\downarrow| \, e^{-\beta h\sum_{i=1}^{N}(n_{i\uparrow}-n_{i\downarrow})} \, e^{-\beta\left(U\sum_{i=1}^{N}(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})-N\frac{U}{4}+H_{\text{kin}}\right)} \, |\vec{n}_\uparrow,\vec{n}_\downarrow\rangle \\
&= \sum_{m=-N}^{N} \sum_{\substack{\vec{n}_\uparrow,\vec{n}_\downarrow\in\{0,1\}^N \\ \sum_{i=1}^{N}(n_{i\uparrow}-n_{i\downarrow})=m}} e^{-\beta hm} \langle \vec{n}_\uparrow,\vec{n}_\downarrow| \, e^{-\beta\left(U\sum_{i=1}^{N}(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})-N\frac{U}{4}+H_{\text{kin}}\right)} \, |\vec{n}_\uparrow,\vec{n}_\downarrow\rangle = \\
&= \underline{\underline{\sum_{m=-N}^{N} e^{-\beta hm}\text{tr}_m\left(e^{-\beta H(h=0)}\right)}} \qquad \blacksquare
\end{aligned}$$

In this representation (40), one can see, that as a function of h, the partition function is simply a linear combination of exponentials, and therefore analytic. So it can be analytically continued throughout the whole complex plane, especially for pure imaginary numbers

$$\nu = -i\beta h. \tag{41}$$

With this imaginary magnetic field ν, a partition function $\tilde{Z}(\nu) = Z(\frac{i}{\beta}\nu)$ can be defined.

According to (40) it has the form

$$\boxed{\tilde{Z}(\nu) = \sum_{m=-N}^{N} e^{-i\nu m} Z_m} \tag{42}$$

as a discrete Fourier series with the canonical partition functions $(Z_m)_{m=-N}^{N}$ as Fourier coefficients.

The objects of interest in (42) are now the Fourier coefficients Z_m, which can be derived by inverse Fourier transformation.

$$\boxed{\forall m \in \{-N, \dots, N\}: \; Z_m = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i\nu m} \tilde{Z}(\nu) d\nu} \tag{43}$$

The function $\tilde{Z}(\nu)$ in the integrand can now be represented by any of the HS transformations of chapter 2. If the ν-dependence is simple enough, it is possible to do this integral analytically. However, this will only influence the numerical effort, but not the sign of the HS sum $\sum_{\sigma}$, which is the main question.

3.2 Standard HS transformation

The first transformation in chapter 2 was the Standard HS transformation (19). It was also the simplest one, but had the most problematic h-dependence. h appeared in the determinant and not even with an approximation one could improve this. So with this Standard HS transformation nothing more than inserting it into the definition (43) of the Fourier coefficients and investigating the sign is possible here.

Unlike the other HS transformations (section 2.2-2.4), this one was derived for the $H_{h=0}$ model. However, in a similar fashion this transformation can be applied to the $H_{\frac{1}{2}}$ model and leads to the partition function

$$\boxed{Z = \frac{1}{2^{NM}} \sum_{\sigma \in \{\pm 1\}^{N \times M}} \prod_{s \in \{\pm 1\}} \det \left(E + \prod_{j=1}^{M} \left(e^{s(\lambda G^{(j)} - \Delta\tau h E)} e^{\Delta\tau t \, h_{\mathsf{kin}}} \right) \right)} \tag{44}$$

with the coefficient λ given by $\cosh(\lambda) = e^{\frac{\Delta\tau U}{2}}$.

The Fourier coefficients Z_m from (43) with the partition function $\tilde{Z}(\nu) = Z(\frac{i}{\beta}\nu)$ in the form (44), are now given by the following expression.

$$\boxed{Z_m = \frac{1}{2^{NM+1}\pi} \sum_{\sigma \in \{\pm 1\}^{N \times M}} \int_{-\pi}^{\pi} e^{i\nu m} \prod_{s \in \{\pm 1\}} \det \left(E + \prod_{j=1}^{M} \left(e^{s(\lambda G^{(j)} - \frac{i}{M}\nu E)} e^{t\Delta\tau h_{\mathsf{kin}}} \right) \right) d\nu} \tag{45}$$

with
- $G^{(j)} = \begin{pmatrix} \sigma_{1j} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{Nj} \end{pmatrix}$
- $(h_{\mathsf{kin}})_{ij} = \begin{cases} 1 & j \in \mathcal{N}_i \\ 0 & \text{else} \end{cases}$
- E the $N \times N$ identity matrix

It would make the equation easier, if the ν-integral would become analytically solvable, but because of the ν-dependence of the determinant, this is not the case in this transformation.

However, the partition function contains the large sum $\sum_\sigma$, which should be done by Monte Carlo simulations. Therefore, the addends

$$\boxed{Z_\sigma = \int_{-\pi}^{\pi} e^{i\nu m} \prod_{s\in\{\pm 1\}} \det\left(E + \prod_{j=1}^{M} e^{s(\lambda G^{(j)} - \frac{i}{M}\nu E)} e^{t\Delta\tau h_{\text{kin}}}\right) d\nu} \tag{46}$$

have to be positive. To measure this, analogously to chapter 2 the sign (15) of the addends can be calculated. As it can be seen in Fig.9, also the results are similar to the one of chapter 2, because except of the trivial case $m = 0$, where the Fourier prefactor $e^{i\nu m}$ vanishes, all the signs converge to zero as β increases.
Fig.10 shows for the special choice $\beta = 3$ and every Fourier coefficient Z_m the distribution of the values Z_σ in detail. None of the signs dominates the other, so Monte Carlo simulations have very bad convergence properties in this case.

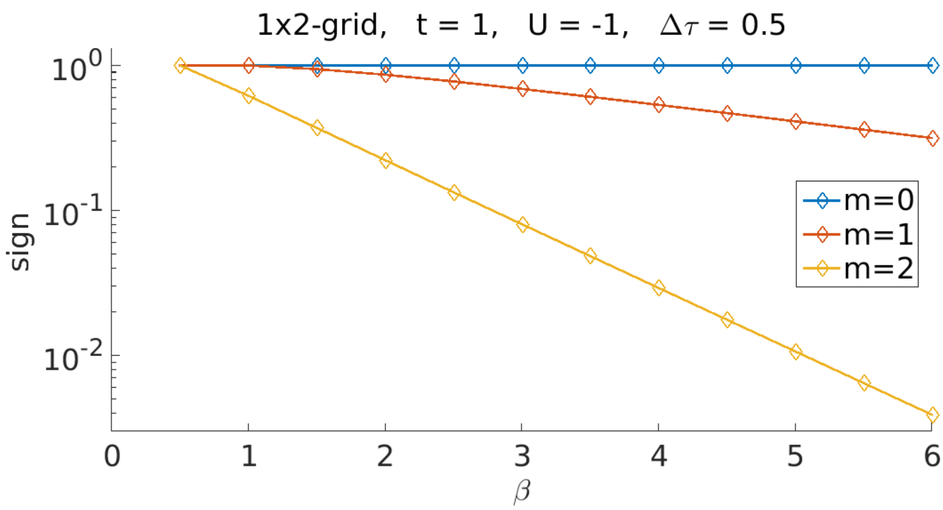


Figure 9: For the addends Z_σ of (46), the sign (15) is plotted as a function of the inverse temperatures β and for all possible magnetisations m. The plot shows, that with increasing β the sign converges to zero exponentially for every Fourier coefficient Z_m (except of $m = 0$).

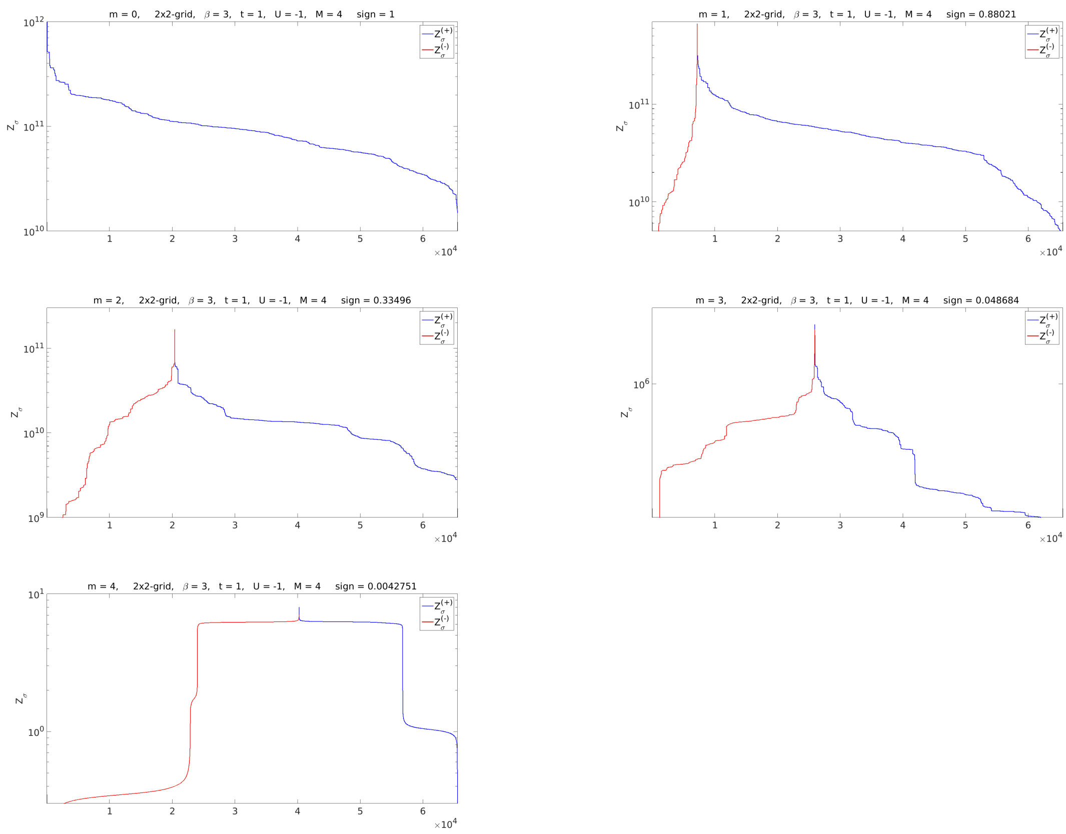


Figure 10: For the specific temperature $\beta = 3$ the distribution of the addends Z_σ is shown in detail. This means, that every σ-value corresponds to one point on the x-axis and on the y-axis the corresponding value of Z_σ is plotted. The red line means negative values and the blue line positive ones. For $m = 3, 4$ the distribution of the positive and negative values is nearly the same, which can also be seen in the value of sign, written on top of every plot. For $m = 0, 1$ the positive values dominate the negative ones indeed, but as it can be seen in Fig.9, this property vanishes for growing β, at least for $m \neq 0$.

3.3 New HS transformation with external weights

The second transformation of chapter 2 was the New HS transformation with external weights (25), which was only valid for the attractive case ($U < 0$) of the $H_{\frac{1}{2}}$-model. In this exact form, the determinant stays ν-dependent and the integral cannot be done analytically.
Fig.3 showed regions in the U-h-plane where λ and c are real or complex. A similar distribution Fig.11 exists in the U-ν-plane, which shows, for which values of U and $\Delta\tau$ the sign problem occurs.

The Fourier transformation (43) applied to the New HS transformation (25) gives the following Fourier coefficients.

$$\boxed{Z_m = \frac{1}{2^{NM+1}\pi} \sum_{\sigma \in \{\pm 1\}^{N \times M}} \int_{-\pi}^{\pi} \frac{e^{i(\nu m - |\sigma| c)}}{D^{NM}} \prod_{s \in \pm 1} \det\left(E + \prod_{j=1}^{M} \left(e^{s\lambda G^{(j)}} e^{t\Delta\tau h_{\text{kin}}} \right) \right) d\nu} \tag{47}$$

with
- $\cosh(\lambda) = e^{\frac{\Delta\tau U}{2}} \cos(\frac{\nu}{M})$
- $\tan(c)\tanh(\lambda) = \tan(\frac{\nu}{M})$
- $\underline{\underline{D = \cos(c)}}$

which are derived directly from (22), by substituting $h = \frac{i}{\beta}\nu$. Additionally, for an easier representation of the formulas, the parameter $c \to ic$ is redefined.

The values for λ are the first thing investigated here. In order to derive if λ is real or imaginary, one has to distinguish two cases.

$\cosh(\lambda) \in (0,1) \Leftrightarrow \lambda \in i(0, \frac{\pi}{2})$
$\cosh(\lambda) \in (1,\infty) \Leftrightarrow \lambda \in (0,\infty)$

Except of the case $M = 1$, $\cos(\frac{\nu}{M})$ is always positive, but smaller than 1 and for negative U also the exponential $e^{\frac{\Delta\tau U}{2}}$ is smaller than 1. So in the important attractive case, in which the sign problem occurs, the coefficient λ is always imaginary and the product $\prod_{s\in\pm1}$ of the determinant becomes the absolute square.

$$Z_m = \frac{1}{2^{NM+1}\pi} \sum_{\sigma\in\{\pm1\}^{N\times M}} \int_{-\pi}^{\pi} \frac{e^{i(\nu m-|\sigma|c)}}{D^{NM}} \left| \det\left(E + \prod_{j=1}^{M}\left(e^{\lambda G^{(j)}} e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2 d\nu$$

To get the exact interface between real- and complex valued λ, the following equation has to be fulfilled

$e^{\frac{\Delta\tau U}{2}} \cos(\frac{\nu}{M}) = 1 \Rightarrow \Delta\tau U = -2\ln(\cos(\frac{\nu}{M}))$

This gives the following distribution of the λ-values in the ν-U-plane.

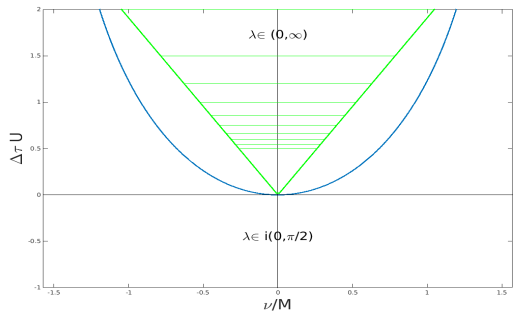


Figure 11: The blue line is the border between real- and complex valued λ. Compared to Fig.4, the whole attractive case $U < 0$ lies in the region of complex valued λ in this transformation. For the attractive case it looks like that there are also some regions with complex valued λ, but the horizontal green lines indicate (for the special case $U = 2$ and $\beta = 3$) the interval over which the ν-integral is taken. For growing M the interval becomes smaller and lies at some point completely in the region of realvalued λ.

Despite the fact that the determinant is positive, the complex valued exponential prefactor can take negative values in general. So the sign of this representation is not clear yet and has to be calculated. This is done only in the attractive case, where the addends are given by.

$$Z_\sigma = \int_{-\pi}^{\pi} \frac{e^{i(\nu m-|\sigma|c)}}{D^{NM}} \left| \det\left(E + \prod_{j=1}^{M}\left(e^{\lambda G^{(j)}} e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2 d\nu \tag{48}$$

This sign (15) of this addends is plotted in Fig.12 and has the same behaviour as the sign in the previous Standard HS transformation, namely (except of $m = 0$) it converges to zero as β becomes large. Fig.13 shows, equivalent to Fig.10, the distribution of Z_σ for every Fourier coefficient Z_m. None of the signs dominates the other and no progress in terms of the sign problem is achieved here.

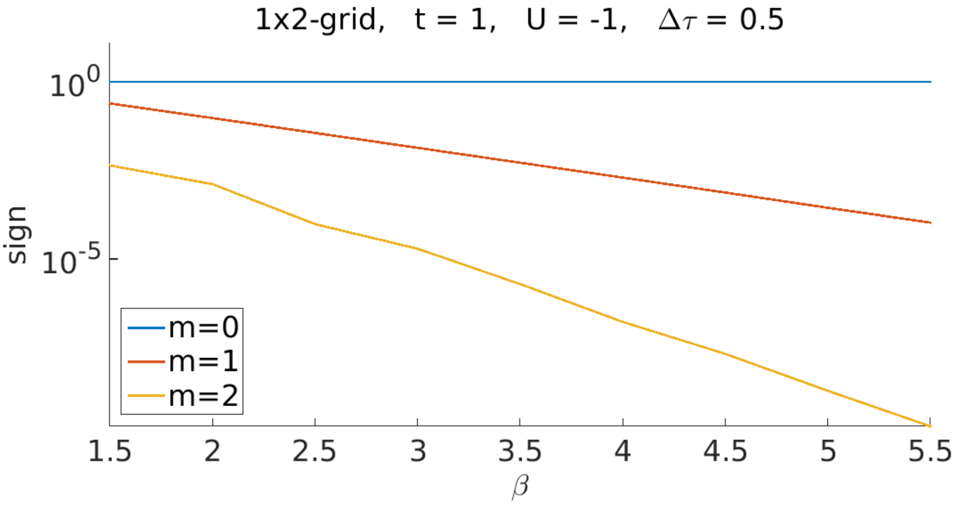


Figure 12: For the addends Z_σ of (48), the sign is plotted as a function of the inverse temperatures β for every positive magnetisation m. The plot shows, that with increasing β the sign converges to zero for every Fourier coefficient Z_m (except $m = 0$).

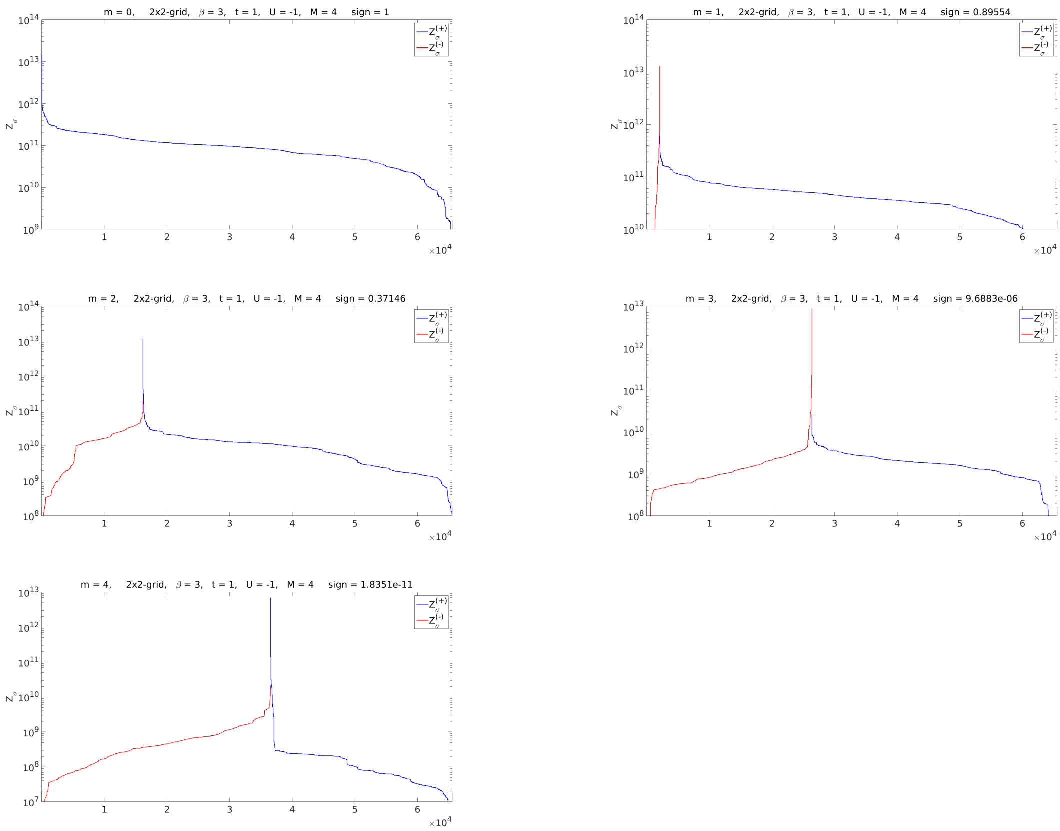


Figure 13: For the specific temperature $\beta = 3$ the distribution of the addends Z_σ of (48) is shown. This means, that every σ-value corresponds to one point on the x-axis and on the y-axis the corresponding value of Z_σ is plotted. The red line means negative values and the blue line positive ones. For $m = 3, 4$ the distribution of the positive and negative values is nearly the same, which can also be seen in the value of sign, which is written on top of every plot. For $m = 0, 1$ the positive values dominate the negative ones indeed, but as it can be seen in Fig.12, this property vanishes for increasing β, at least for $m \neq 0$.

3.4 Approximated New HS transformation

Taking $\tilde{Z}(\nu)$ in the approximated New HS transformation (27) with the variable $\nu = -i\beta h$, the Fourier coefficients (43) have the form.

$$\boxed{Z_m = \frac{1}{2^{NM+1}\pi} \sum_{\sigma\in\{\pm1\}^{N\times M}} \int_{-\pi}^{\pi} e^{\nu\left(im - \frac{|\sigma|}{\beta}\sqrt{\frac{\Delta\tau}{|U|}}\right) - \frac{N}{2\beta|U|}\nu^2} d\nu \left|\det\left(E + \prod_{j=1}^{M}\left(e^{i\sqrt{\Delta\tau|U|}G^{(j)}} e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2} \tag{49}$$

Because the Trotter error of (10) is made anyway, the New HS transformation (25) in chapter 2 was further simplified by the Approximated New HS transformation (27). Because of the ν^2-term in the exponential, the integral is still not analytically solvable, but at least the determinant does no longer appear in the integrand, which makes it much easier to compute numerically. Although this leads to a lower computational effort, it is obvious, that, because the sign problem was not solved in the original New HS transformation (47), it will not be solved in the approximation either.

It will be seen in section 3.6, that this approximated version is very similar to the one of the Continuous HS transformation, but has only a two-element sum over σ instead of the continuous integral. This reduces the size of the phase space for Monte-Carlo simulations by magnitudes.

3.5 New Asymmetric HS transformation

The first transformation, where one can do a little more, than just applying (43), is the Asymmetric HS transformation (34). Here the integration variable ν does no longer appear in the determinant, and also the ν-dependence of the prefactor is, although it is a large product, simple enough to allow an analytic solution of the integral. This looks very nice in the first glance, but the analytic solution $I_{m\sigma}$ is not that simple. It consists in general of a fivefold sum, each of order $\mathcal{O}(NM)$. This gives $\mathcal{O}\left((NM)^5\right)$ elements, which can be sometimes harder to calculate, than just accepting the error and doing the integral numerically.

However, if the integral should be done numerically, it is advantageous anyway to use the Approximated New HS transformation (49). So the main reason for this transformation is the analytic solvability of the Fourier integral.

$$\boxed{Z_m = \sum_{\sigma\in\{-1,0,1\}^{N\times M}} I_{m\sigma} \cdot \left|\det\left(E + \prod_{j=1}^{M}\left(e^{i\frac{\pi}{2}G^{(j)}} e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2} \tag{50}$$

with
$$n_m = \#\{\,(i,j)\in\{1,\dots,N\}\times\{1,\dots,M\} \mid \sigma_{ij} = -1\,\}$$
$$n_0 = \#\{\,(i,j)\in\{1,\dots,N\}\times\{1,\dots,M\} \mid \sigma_{ij} = 0\,\}$$
$$n_p = \#\{\,(i,j)\in\{1,\dots,N\}\times\{1,\dots,M\} \mid \sigma_{ij} = 1\,\}$$

$$I_{m\sigma} = \sum_{j=0}^{n_m}\sum_{k=0}^{n_m-j}\sum_{l=0}^{n_0}\sum_{s=0}^{n_p}\sum_{t=0}^{n_p-s} \frac{(-1)^{j+k+s+t}}{2^{NM+\frac{j+k+s+t}{2}}\pi} \begin{pmatrix} n_m \\ j,k \end{pmatrix} \begin{pmatrix} n_0 \\ l \end{pmatrix} \begin{pmatrix} n_p \\ s,t \end{pmatrix} \cdot e^{\frac{\Delta\tau U}{2}(j+k+n_0+s+t) + i\frac{\pi}{4}(j-k+t-s)} \frac{\sin\left(\left(m + \frac{j-k+n_0-2l+s-t}{M}\right)\pi\right)}{m + \frac{j-k+n_0-2l+s-t}{M}}$$

or

$$I_{m\sigma} = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\nu m}\left(\prod_{j=1}^{M}\prod_{i=1}^{N} D_{\sigma_{ij}}\right) d\nu$$

and the coefficients
$$D_{-1} = \frac{1}{2}\left(1 - e^{\frac{\Delta\tau U}{2}}\left(\cos(\tfrac{\nu}{M}) - \sin(\tfrac{\nu}{M})\right)\right)$$
$$D_0 = e^{\frac{\Delta\tau U}{2}}\cos(\tfrac{\nu}{M})$$
$$D_1 = \frac{1}{2}\left(1 - e^{\frac{\Delta\tau U}{2}}\left(\cos(\tfrac{\nu}{M}) + \sin(\tfrac{\nu}{M})\right)\right)$$

Proof:

$$Z_m = \frac{1}{2\pi} \sum_{\sigma\in\{-1,0,1\}^{N\times M}} \int_{-\pi}^{\pi} e^{i\nu m}\left(\prod_{j=1}^{M}\prod_{i=1}^{N} D_{\sigma_{ij}}\right) d\nu \left|\det\left(E + \prod_{j=1}^{M}\left(e^{i\frac{\pi}{2}G^{(j)}} e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2$$

To calculate this integral, first the factors D_σ of the integrand are written in a proper way.

$$\begin{aligned}
D_{-1} &= \tfrac{1}{2}\left(1-\tfrac{1}{2}e^{\frac{\Delta\tau U}{2}}\left(e^{i\frac{\nu}{M}}(1+i)+e^{-i\frac{\nu}{M}}(1-i)\right)\right)\\
D_0 &= \tfrac{1}{2}e^{\frac{\Delta\tau U}{2}}\left(e^{i\frac{\nu}{M}}+e^{-i\frac{\nu}{M}}\right)\\
D_{+1} &= \tfrac{1}{2}\left(1-\tfrac{1}{2}e^{\frac{\Delta\tau U}{2}}\left(e^{i\frac{\nu}{M}}(1-i)+e^{-i\frac{\nu}{M}}(1+i)\right)\right)
\end{aligned}$$

In the integrand above, products of these coefficients D_σ appear. In order to simplify these terms, the following multinomial formulas are used.

$$(1+a+b)^n=\sum_{j=0}^{n}\sum_{k=0}^{n-j}\begin{pmatrix} n \\ j,k \end{pmatrix} a^j b^k \quad \text{and} \quad (a+b)^n=\sum_{l=0}^{n}\begin{pmatrix} n \\ l \end{pmatrix} a^{n-l}b^l$$

- $\underline{D_{-1}^{n_m}} = \left(\tfrac{1}{2}\left(1-\tfrac{1}{2}e^{\frac{\Delta\tau U}{2}}\left(e^{i\frac{\nu}{M}}(1+i)+e^{-i\frac{\nu}{M}}(1-i)\right)\right)\right)^{n_m} =$
  $= \frac{1}{2^{n_m}}\sum_{j=0}^{n_m}\sum_{k=0}^{n_m-j}\begin{pmatrix} n_m \\ j,k \end{pmatrix}\left(-\tfrac{1}{2}e^{\frac{\Delta\tau U}{2}}e^{i\frac{\nu}{M}}(1+i)\right)^j\left(-\tfrac{1}{2}e^{\frac{\Delta\tau U}{2}}e^{-i\frac{\nu}{M}}(1-i)\right)^k =$
  $= \underline{\sum_{j=0}^{n_m}\sum_{k=0}^{n_m-j}\frac{(-1)^{j+k}}{2^{n_m+j+k}}\begin{pmatrix} n_m \\ j,k \end{pmatrix} e^{\frac{\Delta\tau U}{2}(j+k)}e^{i\frac{\nu}{M}(j-k)}(1+i)^j(1-i)^k}$
- $\underline{D_0^{n_0}} = \left(\tfrac{1}{2}e^{\frac{\Delta\tau U}{2}}\left(e^{i\frac{\nu}{M}}+e^{-i\frac{\nu}{M}}\right)\right)^{n_0} = \underline{\frac{1}{2^{n_0}}e^{\frac{\Delta\tau U}{2}n_0}\sum_{l=0}^{n_0}\begin{pmatrix} n_0 \\ l \end{pmatrix} e^{i\frac{\nu}{M}(n_0-2l)}}$
- $\underline{D_{+1}^{n_p}} = \left(\tfrac{1}{2}\left(1-\tfrac{1}{2}e^{\frac{\Delta\tau U}{2}}\left(e^{i\frac{\nu}{M}}(1-i)+e^{-i\frac{\nu}{M}}(1+i)\right)\right)\right)^{n_p} =$
  $= \frac{1}{2^{n_p}}\sum_{s=0}^{n_p}\sum_{t=0}^{n_p-s}\begin{pmatrix} n_p \\ s,t \end{pmatrix}\left(-\tfrac{1}{2}e^{\frac{\Delta\tau U}{2}}e^{i\frac{\nu}{M}}(1-i)\right)^s\left(-\tfrac{1}{2}e^{\frac{\Delta\tau U}{2}}e^{-i\frac{\nu}{M}}(1+i)\right)^t =$
  $= \underline{\sum_{s=0}^{n_p}\sum_{t=0}^{n_p-s}\frac{(-1)^{s+t}}{2^{n_p+s+t}}\begin{pmatrix} n_p \\ s,t \end{pmatrix} e^{\frac{\Delta\tau U}{2}(s+t)}e^{i\frac{\nu}{M}(s-t)}(1-i)^s(1+i)^t}$

With the integral identity $\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{iax}dx = \frac{\sin(a\pi)}{a\pi}$ the integral becomes:

$$\begin{aligned}
\underline{\underline{I_{m\sigma}}} &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\nu m}D_-^{n_m}D_0^{n_0}D_p^{n_p} =\\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\nu m}\sum_{j=0}^{n_m}\sum_{k=0}^{n_m-j}\sum_{l=0}^{n_0}\sum_{s=0}^{n_p}\sum_{t=0}^{n_p-s}\frac{(-1)^{j+k+s+t}}{2^{n_m+j+k+n_0+n_p+s+t}}\begin{pmatrix} n_m \\ j,k \end{pmatrix}\begin{pmatrix} n_0 \\ l \end{pmatrix}\begin{pmatrix} n_p \\ s,t \end{pmatrix}\cdot\\
&\qquad \cdot e^{\frac{\Delta\tau U}{2}(j+k+n_0+s+t)}e^{i\frac{\nu}{M}(j-k+n_0-2l+s-t)}(1+i)^{j+t}(1-i)^{k+s}d\nu =\\
&= \sum_{j=0}^{n_m}\sum_{k=0}^{n_m-j}\sum_{l=0}^{n_0}\sum_{s=0}^{n_p}\sum_{t=0}^{n_p-s}\frac{(-1)^{j+k+s+t}}{2^{n_m+j+k+n_0+n_p+s+t}}\begin{pmatrix} n_m \\ j,k \end{pmatrix}\begin{pmatrix} n_0 \\ l \end{pmatrix}\begin{pmatrix} n_p \\ s,t \end{pmatrix} e^{\frac{\Delta\tau U}{2}(j+k+n_0+s+t)}\cdot\\
&\qquad \cdot\left(\sqrt{2}e^{i\frac{\pi}{4}}\right)^{j+t}\left(\sqrt{2}e^{-i\frac{\pi}{4}}\right)^{k+s}\frac{\sin\left(\left(m+\frac{j-k+n_0-2l+s-t}{M}\right)\pi\right)}{\left(m+\frac{j-k+n_0-2l+s-t}{M}\right)\pi} =\\
&= \sum_{j=0}^{n_m}\sum_{k=0}^{n_m-j}\sum_{l=0}^{n_0}\sum_{s=0}^{n_p}\sum_{t=0}^{n_p-s}\frac{(-1)^{j+k+s+t}}{2^{NM+\frac{j+k+s+t}{2}}\pi}\begin{pmatrix} n_m \\ j,k \end{pmatrix}\begin{pmatrix} n_0 \\ l \end{pmatrix}\begin{pmatrix} n_p \\ s,t \end{pmatrix}\cdot\\
&\qquad \underline{\underline{\cdot e^{\frac{\Delta\tau U}{2}(j+k+n_0+s+t)+i\frac{\pi}{4}(j-k+t-s)}\frac{\sin\left(\left(m+\frac{j-k+n_0-2l+s-t}{M}\right)\pi\right)}{m+\frac{j-k+n_0-2l+s-t}{M}}}} \qquad \blacksquare
\end{aligned}$$

In terms of the sign problem, the addends Z_σ in this transformation are given by

$$\boxed{Z_\sigma = I_{m\sigma}\cdot\left|\det\left(E+\prod_{j=1}^{M}\left(e^{i\frac{\pi}{2}G^{(j)}}e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2} \tag{51}$$

and Fig.14 shows, that the sign problem still occurs.

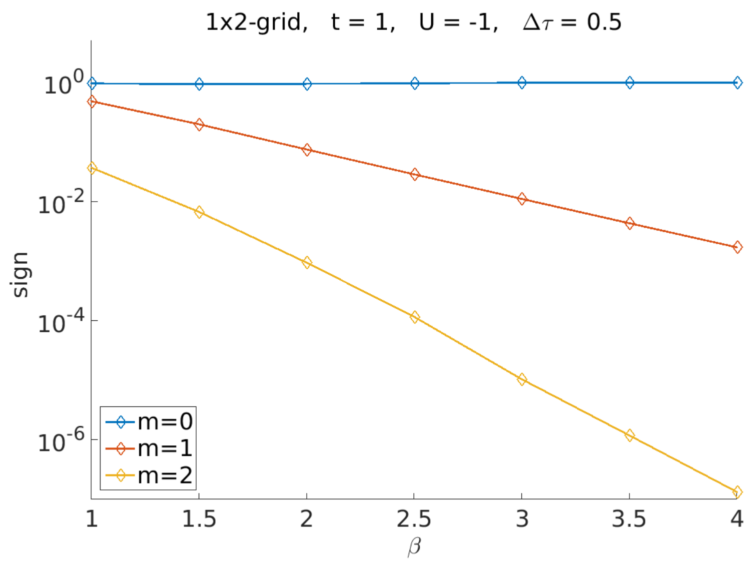


Figure 14: For the addends Z_σ of (51), the sign is plotted as a function of the inverse temperatures β for every positive magnetisation m. The plot shows, that with increasing β the sign converges to zero for every Fourier coefficient Z_m (except $m = 0$).

3.6 Continuous HS transformation

The last transformation of chapter 2, was the Continuous HS transformation (38). In this transformation in principle the same properties as in the Approximated New HS transformation (27) were found, namely a h-independent determinant and a exponential prefactor with a quadratic h-dependency. In the Approximated New HS transformation an expansion of the coefficients λ, c was the reasen for these properties, here these properties arise from a continuous degree of freedom σ. Also in this version of complex valued magnetic field, these two transformations behave similar. So the sign problem also appears in this Continuous HS transformation, like it did in the Approximated New HS transformation (49).
At the end of this section another try is given to change the interval of the Fourier integral (43) in order to change the distribution of the values of the integrals. But this did not improve things, the overall sign stayed the same.

Like in section 2.4.3, only the important attractive case $(U < 0)$ of the $H_{\frac{1}{2}}$ model is considered. Using (38), the Fourier coefficients for every fixed $m \in \{-N, \dots, N\}$ have the following form.

$$\boxed{Z_m = \frac{1}{2\pi^{\frac{NM}{2}+1}} \int\limits_{\mathbb{R}^{N\times M}} \int\limits_{-\pi}^{\pi} e^{-\frac{\nu^2 N}{2\beta|U|}} e^{\nu\left(im - \frac{|\sigma|}{\beta}\sqrt{\frac{2\Delta\tau}{|U|}}\right)} d\nu \; e^{-|\sigma^2|} \left|\det\left(E + \prod_{j=1}^{M}\left(e^{i\sqrt{2\Delta\tau|U|}G^{(j)}} e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2 d\sigma} \tag{52}$$

with $|\sigma| = \sum_{j=1}^{M}\sum_{i=1}^{N} \sigma_{ij}$

$$|\sigma^2| = \sum_{j=1}^{M}\sum_{i=1}^{N} \sigma_{ij}^2$$

$$G^{(j)} = \begin{pmatrix} \sigma_{1j} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{Nj} \end{pmatrix}$$

$$(h_{\text{kin}})_{ij} = \begin{cases} 1 & j \in \mathcal{N}_i \\ 0 & \text{else} \end{cases}$$

Proof:

The Fourier coefficient Z_m is definied in (43) and has the form

$$\underline{\underline{Z_m}} = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\nu m} \frac{1}{\pi^{\frac{NM}{2}}} e^{-\frac{\nu^2 N}{2\beta|U|}} \int_{\mathbb{R}^{N\times M}} e^{-|\sigma^2|-|\sigma|\frac{\nu}{\beta}\sqrt{\frac{2\Delta\tau}{|U|}}} \cdot \left|\det\left(E+\prod_{j=1}^{M}\left(e^{i\sqrt{2\Delta\tau|U|}G^{(j)}}e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2 d\sigma d\nu =$$

$$= \frac{1}{2\pi^{\frac{NM+2}{2}}}\int_{\mathbb{R}^{N\times M}}\int_{-\pi}^{\pi} e^{\nu\left(im-\frac{|\sigma|}{\beta}\sqrt{\frac{2\Delta\tau}{|U|}}\right)-\frac{N}{2\beta|U|}\nu^2} d\nu\, e^{-|\sigma^2|} \cdot \underline{\underline{\left|\det\left(E+\prod_{j=1}^{M}\left(e^{i\sqrt{2\Delta\tau|U|}G^{(j)}}e^{t\Delta\tau h_{\text{kin}}}\right)\right)\right|^2 d\sigma}}\ . \qquad \blacksquare$$

To apply a Monte Carlo method, the positiveness of the integrand has to be verified. The $e^{-|\sigma|^2}$ as well as the absolute square of the determinant are always positive values, the only thing left to check, is the integral

$$\boxed{I_\sigma = \int_{-\pi}^{\pi} e^{-\frac{\nu^2 N}{2\beta|U|}} e^{\nu\left(im-\frac{|\sigma|}{\beta}\sqrt{\frac{2\Delta\tau}{|U|}}\right)} d\nu}\ , \tag{53}$$

which is done in Fig.15.

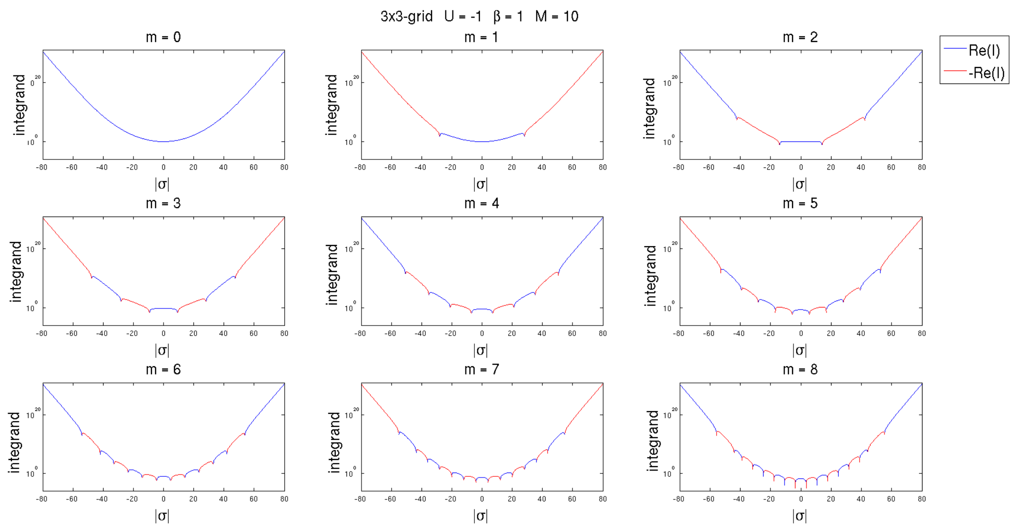


Figure 15: The values of the Fourier integral (53) can be seen for every magnetisation m separately. Unfortunatly, they can get negative and grow exponentially with $|\sigma|$. Because the whole integral is interpreted as a partition function with constant magnetisation, it has to be positive. So the negative part (drawn in red) has to be dominated by the positive part (drawn in blue). This is possible, because the integral gets multiplicated with $e^{-|\sigma^2|}$ which gets small for large σ and also because of the many realisations with small $|\sigma|$ and not that many for big $|\sigma|$.

To get a complete calculation of the sign of (52), not only the Fourier integral (53) has to be considered, like it is done in Fig.15, but the whole integrand is needed. This means, that also the values $e^{-|\sigma|^2}$ and $|\det(\dots)|^2$ have to be multiplied, before judging whether the integrand is positive or not. Because the determinant is not a function of $|\sigma|$ anymore, but of every single value σ_{ij}, the numerical effort increases rapidly. So this cannot be done for the 3×3-grid and $M=10$ Trotter timeslices any more. One has to reduce both values in order to show the whole distribution of the integrands. In Fig.16 this is done for a 2×1-grid and a $M=2$ Trotter timeslices.

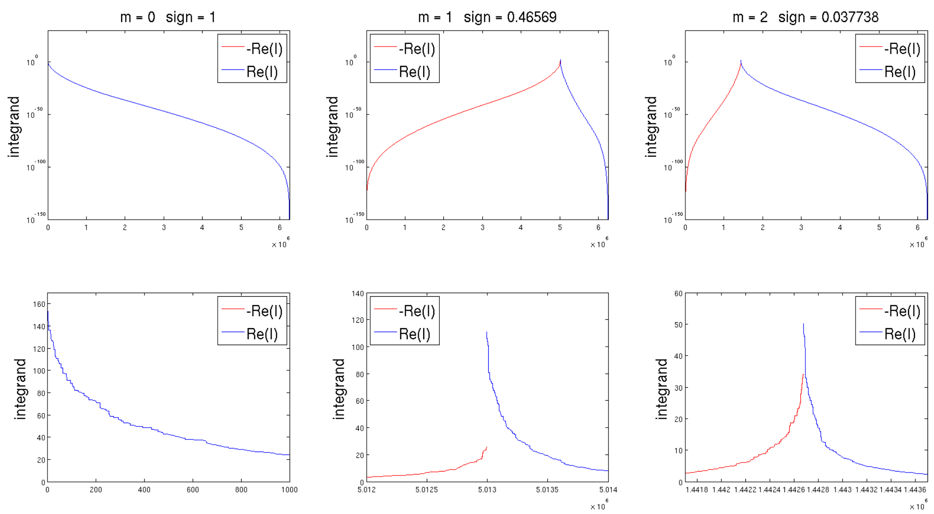


Figure 16: The values of the whole integrand of (52), including the Fourier integral (53), the exponential $e^{-|\sigma|^2}$ and the determinant $|\det(\dots)|^2$ can be seen for a small 2×1-grid and $M = 2$ timeslices. Like in figure 15 $\beta = 1$ is used, which gives Trotter timeslices $\Delta\tau = 0.5$. Every σ-value corresponds to one point on the x-axis and on the y-axis the corresponding value of Z_σ is plotted. The red line means negative values and the blue line positive ones and so one sees that positive as well as negative values appear. The important quantitative value sign (15), which describes the ratio between the difference and the sum of the positive and negative values, is calculated for every magnetization m. Always two plots (one above the other) belong to the same setting. The plot below is just zoomed into the region of the largest values.

Another tuning parameter, one can use to improve the sign, is given by the interval $[\nu_0, \nu_0 + 2\pi]$ over which the Fourier transformation is done. Different values of ν_0 can be tried, in order to make the integrand positive.

As an example, the case $\underline{\nu_0 = 0}$ is tried here. It can be seen in the following Fig.17, that the Fourier integral keeps its positive and negative values, but shifted them to more negative values of $|\sigma|$. One can think, that this could improve things, because the negative values get damped by $e^{-|\sigma^2|}$, but Fig.18 shows, that the value of sign does not change.

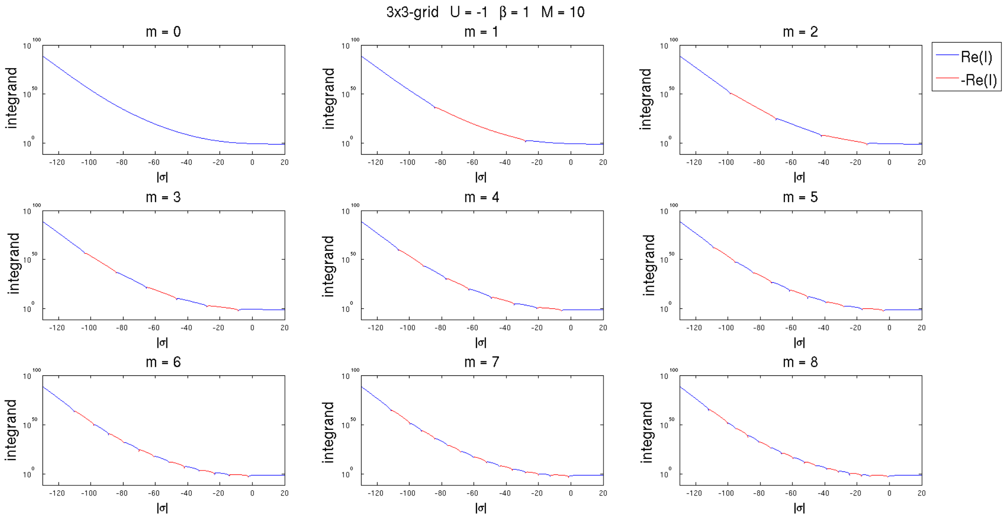


Figure 17: The values of the Fourier integral (15) over a shifted interval $\int_0^{2\pi} d\nu$ can be seen in these plots. Every σ-value corresponds to one point on the x-axis and on the y-axis the corresponding value of Z_σ is plotted. The red line means negative values and the blue line positive ones, which shows that the integrand becomes negative, but grows exponentially just on the negative side of $|\sigma|$. Unfortunately this does not improve things at all, like it can be seen in Fig.18.

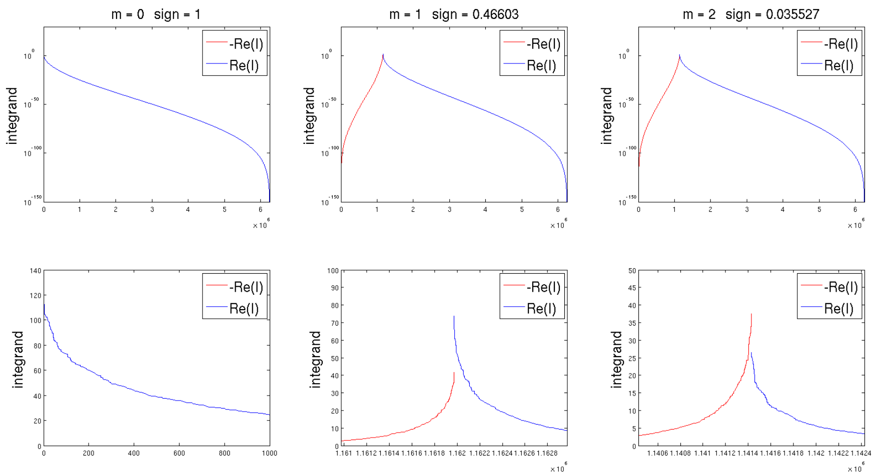


Figure 18: In this figure the values of the whole integrand of (52), including the shifted Fourier integral $\int_0^{2\pi} d\nu$, the exponential $e^{-|\sigma|^2}$ and the determinant $|\det(\dots)|^2$ are plotted for a small 2×1-grid and $M = 2$ timeslices. Like in figure 17 $\beta = 1$ is used, which gives Trotter timeslices $\Delta\tau = 0.5$. Every σ-value corresponds to one point on the x-axis and on the y-axis the corresponding value of Z_σ is plotted. The red line means negative values and the blue line positive ones. Analogously to Fig.16, one sees, that again positive as well as negative values appear. Always two plots (one above the other) belong to the same setting, the plot below is just zoomed into the region of the largest values.

The idea in chapter 3 was, to treat the partition function as a function of complex valued magnetic field and derive formulas for its Fourier coefficients. The hope was, that the sign of the Fourier coefficients has better properties, than the sign of the partition function itself. But in the same fashion the sign vanished in chapter 2, all the considered transformations in chapter 3 led to a sign which goes to zero as beta increases.

II The Hubbard-Holstein model and new transformations

4 Introduction

In this second part of the thesis the Hubbard model, which only treats electrons, is enlarged by phonons. With harmonic oscillating phonons and a linear coupling to the electrons one ends up with the Hubbard-Holstein (HH) model. The HH model is one of the simplest ways to combine the electron-electron as well as the electron-phonon interaction in a solid. Although it has a quite simple structure, it is a very reliable model in a variety of physical problems and therefore of great interest in analytical and numerical studies. For large electron-phonon coupling, two electrons pair together and form a bipolaron [10, 11, 12], which can be important, for example in the appearance of supercoductivity [13, 14].
The Hubbard-Holstein model became even more important, as in 1994 the one-electron spectral functions for a one-dimensional continuum model, including electron-phonon coupling, were calculated exactly [15].

In chapter 5 the Continuous HS transformation of section 2.4 is applied to the HH model by using an effective chemical potential which is shifted by the coupling constant of the electrons and phonons. This transformation does not change the Gaussian behaviour of the phonon part and so the phonon trace can still be calculated analytically. This leads to a form of the partition function with an arbitrary number of Trotter time slices (59), which is a generalisation of the commonly used limit case $\Delta\tau \to 0$. In section A.4-A.6, extensions of this chapter are made.
In A.4 the partition function is calculated without the above-mentioned Continuous HS transformation and the phonon trace is integrated out directly.
In A.5 it was tried to rewrite the partition function of chapter 5 in the Standard HS transformation. This means after the Continuous HS transformation was applied and the phonon trace was integrated out, I tried to undo the Continuous HS transformation again and write it in the form of a Standard HS transformation (section 2.1) with site dependend parameters. It turned out that after the transformation number operators of different timeslices are coupled to each other and it was not possible to end up with an effective Hubbard model onto which the Standard HS transformation could be applied.
In A.6 the two ways of writing the partition function (with or without the Continuous HS transformation) are compared for a small system.

The common way to treat the phonon degree of freedom in the HH model, is to integrate it out analytically straight away. The idea of this thesis will be, to apply the Continuous HS transformation of chapter 2.4 first and integrate out the phonons afterwards. This leads to an improved version of the partition function, which can be compared in chapter 5 and 6. However, in both versions the integral over the phonon degree of freedom causes a coupling between different Trotter timeslices. The analytic solution of this multidimensional gaussian integral is one of the main results of this part and done in two different ways [Appendix A.2 and A.3]. The numerical effort to calculate the partition function, raises rapidely by introducing the Continuous HS transformation. Therefore in chapter 7, it is tried to replace the continuous transformation again by the discrete one, but unfortunately this did not work out in the end. So in this favorable form of the HH model in the Continuous HS transformation, one is faced with an integral of dimension N (number of sites) times M (number of Trotter timeslices).

The Hamiltonian of the Hubbard model without external magnetic field is given by (2).

$$H = -t\sum_{i=1}^{N}\sum_{j\in\mathcal{N}_i}(c_{i\uparrow}^{\dagger}c_{j\uparrow} + c_{i\downarrow}^{\dagger}c_{j\downarrow}) + U\sum_{i=1}^{N} n_{i\uparrow}n_{i\downarrow} + \mu\sum_{i=1}^{N}(n_{i\uparrow} + n_{i\downarrow})$$

Additionally to the Hubbard model, phonons are introduced, which are described by a harmonic oscillator and couple linearly to the electrons on every site i, with a coupling constant α.

Thus, the Hamiltonian of the Hubbard-Holstein model looks like

$$\boxed{H = \sum_{i=1}^{N}\left(-t\sum_{j\in\mathcal{N}_i}(c_{i\uparrow}^{\dagger}c_{j\uparrow} + c_{i\downarrow}^{\dagger}c_{j\downarrow}) + Un_{i\uparrow}n_{i\downarrow} + (\mu - \alpha x_i)(n_{i\uparrow} + n_{i\downarrow}) + \frac{p_i^2}{2m} + \frac{m\omega^2 x_i^2}{2}\right)} \quad . \tag{54}$$

To make the notation easier, consider the appearing parameters in atomic units.

- $t \to \frac{t}{E_h}$
- $U \to \frac{U}{E_h}$
- $\mu \to \frac{\mu}{E_h}$
- $\alpha \to \frac{\alpha}{\frac{E_h}{a_0}}$
- $x \to \frac{x}{a_0}$
- $\omega \to \frac{\omega}{\frac{E_h}{\hbar}}$
- $p \to \frac{p}{\frac{\hbar}{a_0}}$
- $\beta \to E_h \beta$

with

- a_0 atomic radius
- m electron mass
- $\hbar$ planck's constant
- $E_h = \frac{\hbar^2}{m a_0^2}$ Hartree energy

in which the Hamiltonian (54) has the simpler form

$$\boxed{H = \sum_{i=1}^{N} \left(-t \sum_{j \in \mathcal{N}_i} (c_{i\uparrow}^{\dagger} c_{j\uparrow} + c_{i\downarrow}^{\dagger} c_{j\downarrow}) + U n_{i\uparrow} n_{i\downarrow} + (\mu - \alpha x_i)(n_{i\uparrow} + n_{i\downarrow}) + \frac{p_i^2}{2} + \frac{\omega^2 x_i^2}{2} \right)} . \quad (55)$$

For a shorter notation define the following Hamiltonians.

$$H_{\text{cou}} = U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow}$$
$$H_{\mu,\alpha} = \sum_{i=1}^{N} (\mu - \alpha x_i)(n_{i\uparrow} + n_{i\downarrow})$$
$$H_{\text{kin}} = -t \sum_{i=1}^{N} \sum_{j \in \mathcal{N}_i} (c_{i\uparrow}^{\dagger} c_{j\uparrow} + c_{i\downarrow}^{\dagger} c_{j\downarrow})$$
$$H_{\text{osc}} = \sum_{i=1}^{N} \left(\frac{p_i^2}{2} + \frac{\omega^2 x_i^2}{2} \right)$$

5 HH model in the Continuous HS transformation

In chapter 4 the Hubbard Holstein (HH) model was introduced as an expansion of the Hubbard model, which additionally includes the interactions between electrons and phonons. The coupling constant α in (55), acts like a shift of the chemical potential. Therefore, a HS transformation similar to section 2.4 can be applied here. This will lead to a coupling of the HS-coefficients in between the timeslices, but not in between sites (59).
To write the partition function in section 5.2 in the form of the Continuous HS transformation, the condition (57) is needed, so the investigations in this chapter are restricted to models in which this condition is fulfilled. The attractive model ($U < 0$) is valid anyway and the repulsive model ($U > 0$) only for sufficient small coupling constants α.
The HH model in the form of the Continuous HS transformation is very common in determinantal quantum Monte Carlo methods, but mostly written in the limit case $\Delta\tau \to 0$ [16, 17]. Our result will be slightly more general, by allowing also finite values of $\Delta\tau$, which will also be the main result of this chapter (59). The main advantage of this formula is, that espcially the phonon parameters α and ω no longer appear inside the determinant. Therefore one can easily differentiate with respect to them or simply use different values for this paramters.
In section 5.5 the limiting case $U \to 0$ of this formula is taken. This limit is not obvious, because in the Hubbard-Stratonovich transformation itself one has to exclude $U = 0$, but in the end it turns out that the limit exists and leads to a result, which only couples neighboring timeslices anymore.

5.1 Continuous HS transformation

In section 2.4.1 the Continuous HS transformation was calculated for the $H_{\frac{1}{2}}$ model (4). Because the electronic part of the HH Hamiltonian is the one of the $H_{h=0}$ model (5) and the fact that these models are equivalent (according to (6)), a similar transformation exists for this model.
Basically the Continuous HS transformation can be done either in the initial form (2) or in the particle-hole symmetric form (3) of the Hamiltonian. Both transformations lead to the same result (58), so the shorter one is presented here.

$$\boxed{e^{-\Delta\tau(Un_\uparrow n_\downarrow+\mu(n_\uparrow+n_\downarrow))} = \frac{1}{\sqrt{\pi}} e^{\frac{\Delta\tau U}{2}(\frac{\mu}{U}-\frac{1}{2})^2} \int\limits_{-\infty}^{\infty} e^{-\sigma^2+\sigma\lambda(n_\uparrow+n_\downarrow+\frac{\mu}{U}-\frac{1}{2})} d\sigma} \tag{56}$$

with the HS coefficients: $\underline{\underline{\lambda = \sqrt{-2\Delta\tau U}}}$

Proof:

Using the identity $\int\limits_{-\infty}^{\infty} e^{-x^2+bx}dx = \sqrt{\pi}e^{\frac{b^2}{4}}$, the right hand side becomes $e^{\frac{\Delta\tau U}{2}\left(\frac{\mu}{U}-\frac{1}{2}\right)^2} e^{\frac{1}{4}\lambda^2(n_\uparrow+n_\downarrow+\frac{\mu}{U}-\frac{1}{2})^2}$, and so the equation, which has to be fulfilled for every $n_\uparrow, n_\downarrow \in \{0,1\}$, is

$$-\Delta\tau\left(Un_\uparrow n_\downarrow + \mu(n_\uparrow+n_\downarrow)\right) = -\frac{\Delta\tau U}{2}(n_\uparrow+n_\downarrow)(n_\uparrow+n_\downarrow+2(\frac{\mu}{U}-\frac{1}{2}))\ .$$

Simply testing all possibilities of $n_\uparrow$ and $n_\downarrow$, gives the needed result.

$\underline{\underline{n_\uparrow = n_\downarrow = 0}}$: $\underline{\underline{0 = 0}}$ fulfilled

$\underline{\underline{n_\uparrow = n_\downarrow = 1}}$: $\underline{\underline{-\Delta\tau(U+2\mu) = -\Delta\tau U(2+2(\frac{\mu}{U}-\frac{1}{2}))}}$ fulfilled

$\underline{\underline{n_\uparrow \neq n_\downarrow}}$: $\underline{\underline{-\Delta\tau\mu = -\frac{\Delta\tau U}{2}(1+2(\frac{\mu}{U}-\frac{1}{2}))}}$ fulfilled ■

5.2 Hubbard-Holstein partition function in the HS transformation

The HS transformation (56) can now be used to rewrite the partition function $Z = \text{tr}\left(e^{-\beta H}\right)$ of the HH Hamiltonian (55) in form of a determinant. The value μ in (56) is chosen to be the shifted chemical potential $\mu - \alpha\hat{x}_i$.

To make the HS transformation applicable at all, the Trotter decomposition (10) is used for the exponential $e^{-\beta H}$.
In order to exchange the integration regarding to x and σ, the condition

$$\boxed{\omega^2 > \frac{\alpha^2}{U}} \tag{57}$$

will be needed, which is anyway fulfilled for the attractive model $U < 0$.

$$\boxed{Z = \left(\frac{e^{\beta U c^2}}{\pi^M}\right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times M}} e^{-|\sigma|^2+|\sigma|\lambda c}\ \mathrm{tr}\left(\prod_{j=1}^{M} e^{\sum\limits_{i=1}^{N}\left(\sigma_{ij}\lambda(n_{i\uparrow}+n_{i\downarrow})-\alpha x_i\left(\Delta\tau c+\frac{\sigma_{ij}\lambda}{U}\right)+\frac{\Delta\tau\alpha^2}{2U}x_i^2\right)} e^{-\Delta\tau(H_{\mathsf{kin}}+H_{\mathsf{osc}})}\right) d\sigma} \tag{58}$$

with $c = \frac{\mu}{U} - \frac{1}{2}$

Proof:

The partition function in the Trotter decomposition (10) leads to a form where the Continuous HS transformation (56) can be applied. It looks like, that this could cause problems, because the chemical potential has to be replaced by the opertor valued $\mu - \alpha\hat{x}_i$. But the spatial trace can be carried out in front, and the operator $\hat{x}_i$ becomes the spatial integration variable x_i.

$$\underline{Z} = \mathrm{tr}\left(\left(e^{-\Delta\tau\sum\limits_{i=1}^{N}(Un_{i\uparrow}n_{i\downarrow}+(\mu-\alpha x_i)(n_{i\uparrow}+n_{i\downarrow}))} e^{-\Delta\tau(H_{\mathsf{kin}}+H_{\mathsf{osc}})}\right)^M\right) =$$
$$= \mathrm{tr}\left(\left(\left(\prod_{i=1}^{N}\frac{1}{\sqrt{\pi}}e^{\frac{\Delta\tau U}{2}\left(\frac{\mu-\alpha x_i}{U}-\frac{1}{2}\right)^2}\int\limits_{-\infty}^{\infty} e^{-\sigma^2+\sigma\lambda(n_{i\uparrow}+n_{i\downarrow}+\frac{\mu-\alpha x_i}{U}-\frac{1}{2})}d\sigma\right) e^{-\Delta\tau(H_{\mathsf{kin}}+H_{\mathsf{osc}})}\right)^M\right)$$

Using the definition of c (58) the exponent can be simplified and ordered in terms of n_{is} and x_i.

$$\frac{\Delta\tau U}{2}\left(\frac{\mu-\alpha x_i}{U}-\frac{1}{2}\right)^2 - \sigma^2 + \sigma\lambda(n_{i\uparrow}+n_{i\downarrow}+\frac{\mu-\alpha x_i}{U}-\frac{1}{2}) =$$
$$= \frac{\Delta\tau U}{2}\left(c^2 + \frac{\alpha^2 x_i^2}{U^2} - 2c\frac{\alpha x_i}{U}\right) - \sigma^2 + \sigma\lambda(n_{i\uparrow}+n_{i\downarrow}+c-\frac{\alpha x_i}{U}) =$$
$$= \sigma\lambda(n_{i\uparrow}+n_{i\downarrow}) - \alpha x_i\left(\Delta\tau c + \frac{\sigma\lambda}{U}\right) + \frac{\Delta\tau\alpha^2}{2U}x_i^2 + \frac{\Delta\tau U}{2}c^2 - \sigma^2 + \sigma\lambda c$$

In the next step, the integration over σ should be exchanged with the phonon trace, which contains the phonon integral over x. This is mathematically only allowed, if the integrals still converge after the exchange. The integral over x becomes a Gaussian integral with a prefactor $-\frac{\Delta\tau}{2}(\omega^2 - \frac{\alpha^2}{U})$ of the quadratic term x^2. To ensure convergence, this value has to be negative and so the condition (57) is necessary.

$$Z = \left(\frac{e^{\beta U c^2}}{\pi^M}\right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times M}} e^{-|\sigma|^2+|\sigma|\lambda c}\ \mathrm{tr}\left(\prod_{j=1}^{M} e^{\sum\limits_{i=1}^{N}\left(\sigma_{ij}\lambda(n_{i\uparrow}+n_{i\downarrow})-\alpha x_i\left(\Delta\tau c+\frac{\sigma_{ij}\lambda}{U}\right)+\frac{\Delta\tau\alpha^2}{2U}x_i^2\right)} e^{-\Delta\tau(H_{\mathsf{kin}}+H_{\mathsf{osc}})}\right) d\sigma \qquad \blacksquare$$

5.3 Determinant representation of the Continuous HS transformation

In the HH model the situation is now a bit more complicated, than in the previous Hubbard model (37), because the trace is not only the fermionic sum over all possible occupations, but also the integral over all phonen states x. Fortunately this phonon integral can be done analytically and for the electrons the determinant representation of the trace (69) can be used again.
This finally leads to the following partition function.

$$\boxed{\begin{aligned} Z = \left(\frac{e^{\frac{\beta U^2 c^2 \omega^2}{U\omega^2-\alpha^2}}}{\pi^M(\Omega^M-1)(1-\Omega^{-M})}\right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times M}} e^{-\sum\limits_{i=1}^{N}\vec{\sigma}_i^T\left(E+\frac{\alpha^2\Delta\tau^2}{2U(1-\Omega^{-M})\sqrt{a^2-1}}R\right)\vec{\sigma}_i+|\sigma|\frac{\lambda c U\omega^2}{U\omega^2-\alpha^2}}\ \cdot \\ \cdot\det\left(E+\prod_{j=1}^{M}\left(e^{\lambda G^{(j)}}e^{t\Delta\tau h_{\mathsf{kin}}}\right)\right)^2 d\sigma \end{aligned}} \tag{59}$$

with • $a = \frac{\Delta\tau^2}{2}(\omega^2 - \frac{\alpha^2}{U}) + 1$
• $\Omega = a + \sqrt{a^2 - 1}$
• $R_{ij} = \Omega^{-|i-j|} + \Omega^{-M+|i-j|}$

Like in (58), this representation is only true for models which fulfill the condition (57).

Proof:

Because there are no spin-flip-terms in the Hubbard-Holstein Hamiltonian (54) and because the transformation (56) brakes up the coupling between x_i and n_i as well as the coupling $n_\uparrow$ and $n_\downarrow$, it is possible to separate the partition function (58) into a product of three exponentials (spin↑, spin↓ and phonons).

$$Z = \left(\frac{e^{\beta U c^2}}{\pi^M}\right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times M}} e^{-|\sigma^2|+|\sigma|\lambda c} \, \text{tr} \left(\prod_{s\in\{\uparrow,\downarrow\}} \prod_{j=1}^{M} \left(e^{\sum\limits_{i=1}^{N} \sigma_{ij}\lambda n_{is}} e^{-\Delta\tau H_{\text{kin},s}} \right) \cdot \right.$$
$$\left. \cdot \prod_{j=1}^{M} \left(e^{\sum\limits_{i=1}^{N} \left(\frac{\Delta\tau\alpha^2}{2U} x_i^2 - \alpha x_i \left(\Delta\tau c + \frac{\sigma_{ij}\lambda}{U} \right) \right)} e^{-\Delta\tau H_{\text{osc}}} \right) \right) d\sigma$$

Now the trace is has a form tr$(O_\uparrow O_\downarrow O_{\text{phonon}})$, where all three operators only act in their respective subspaces. So the trace can be replaced by the product of the three subtraces tr$_\uparrow$, tr$_\downarrow$, tr$_{\text{phonon}}$ as well.

$$Z = \left(\frac{e^{\beta U c^2}}{\pi^M}\right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times M}} e^{-|\sigma^2|+|\sigma|\lambda c} \prod_{s\in\{\uparrow,\downarrow\}} \text{tr}_s \left(\prod_{j=1}^{M} \left(e^{\sum\limits_{i=1}^{N} \sigma_{ij}\lambda n_{is}} e^{-\Delta\tau H_{\text{kin},s}} \right) \right) \cdot$$
$$\cdot \text{tr}_{\text{phonon}} \left(\prod_{j=1}^{M} \left(e^{\sum\limits_{i=1}^{N} \left(\frac{\Delta\tau\alpha^2}{2U} x_i^2 - \alpha x_i \left(\Delta\tau c + \frac{\sigma_{ij}\lambda}{U} \right) \right)} e^{-\Delta\tau H_{\text{osc}}} \right) \right) d\sigma$$

Using the representation of the fermionic trace as a determinant (69) together with the matrix form of the exponent (20), the electron trace tr$_s$ can be written as a determinant.

$$Z = \left(\frac{e^{\beta U c^2}}{\pi^M}\right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times M}} e^{-|\sigma^2|+|\sigma|\lambda c} \det \left(E + \prod_{j=1}^{M} \left(e^{\lambda G^{(j)}} e^{t\Delta\tau h_{\text{kin}}} \right) \right)^2 \cdot$$
$$\cdot \, \text{tr}_{\text{phonon}} \left(\prod_{j=1}^{M} \left(e^{\sum\limits_{i=1}^{N} \left(\frac{\Delta\tau\alpha^2}{2U} x_i^2 - \alpha x_i \left(\Delta\tau c + \frac{\sigma_{ij}\lambda}{U} \right) \right)} e^{-\Delta\tau H_{\text{osc}}} \right) \right) d\sigma \qquad (60)$$

Until here, just the trace of the electron states is rewritten and the partition function looks similar to the one of the Hubbard model (38) with the additional phonon trace. This phonon trace (integral over spatial coordinates) can be done analytically and will cause a coupling between σ-values of different timeslices j.

$$\text{tr}_{\text{phonon}} \left(\prod_{j=1}^{M} \left(e^{\sum\limits_{i=1}^{N} \left(\frac{\Delta\tau\alpha^2}{2U} x_i^2 - \alpha x_i \left(\Delta\tau c + \frac{\sigma_{ij}\lambda}{U} \right) \right)} e^{-\Delta\tau H_{\text{osc}}} \right) \right) =$$
$$= \int\limits_{\mathbb{R}^N} \langle \vec{x}^{(1)} | \prod_{j=1}^{M} \left(e^{\sum\limits_{i=1}^{N} \left(\frac{\Delta\tau\alpha^2}{2U} x_i^2 - \alpha x_i \left(\Delta\tau c + \frac{\sigma_{ij}\lambda}{U} \right) \right)} e^{-\Delta\tau \sum\limits_{i=1}^{N} \left(\frac{p_i^2}{2} + \frac{\omega^2 x_i^2}{2} \right)} \right) | \vec{x}^{(1)} \rangle \, d\vec{x}^{(1)} =$$
$$= \int\limits_{\mathbb{R}^{N\times M}} \prod_{j=1}^{M} \left(\langle \vec{x}^{(j)} | \, e^{\sum\limits_{i=1}^{N} \left(-\frac{\Delta\tau}{2}(\omega^2 - \frac{\alpha^2}{U}) x_i^2 - \alpha x_i \left(\Delta\tau c + \frac{\sigma_{ij}\lambda}{U} \right) \right)} e^{-\frac{\Delta\tau}{2} \sum\limits_{i=1}^{N} p_i^2} | \vec{x}^{(j+1)} \rangle \right) d\vec{x} =$$
$$= \int\limits_{\mathbb{R}^{N\times M}} \prod_{j=1}^{M} \left(e^{\sum\limits_{i=1}^{N} \left(-\frac{\Delta\tau}{2}(\omega^2 - \frac{\alpha^2}{U}) x_i^{(j)2} - \alpha x_i^{(j)} \left(\Delta\tau c + \frac{\sigma_{ij}\lambda}{U} \right) \right)} \langle \vec{x}^{(j)} | \, e^{-\frac{\Delta\tau}{2} \sum\limits_{i=1}^{N} p_i^2} | \vec{x}^{(j+1)} \rangle \right) d\vec{x}$$

By inserting a full set of momentum basis vectors $|\vec{p}\rangle$ and the identity $\langle \vec{p} \mid \vec{x} \rangle = \frac{1}{(2\pi)^{\frac{N}{2}}} e^{-i\langle \vec{p}, \vec{x} \rangle}$, one can evaluate the corresponding terms in the equation above.

$$\langle \vec{x}| \, e^{-\frac{\Delta\tau}{2} \sum\limits_{i=1}^{N} \hat{p}_i^2} |\vec{y}\rangle = \int\limits_{\mathbb{R}^N} \langle \vec{x}| \, e^{-\frac{\Delta\tau}{2} \sum\limits_{i=1}^{N} \hat{p}_i^2} |\vec{p}\rangle \langle \vec{p} \mid \vec{y}\rangle \, d\vec{p} = \frac{1}{(2\pi)^N} \int\limits_{\mathbb{R}^N} e^{i\langle \vec{p}, \vec{x}-\vec{y}\rangle} e^{-\frac{\Delta\tau}{2}|\vec{p}|^2} d\vec{p}$$

The $\vec{p}$ integral inserted above, became Gaussian and can be integrated out analytically again.

$$\underline{\langle \vec{x}| \, e^{-\frac{\Delta\tau}{2} \sum\limits_{i=1}^{N} \hat{p}_i^2} |\vec{y}\rangle = \left(\frac{1}{2\pi\Delta\tau}\right)^{\frac{N}{2}} e^{-\frac{1}{2\Delta\tau}(\vec{x}-\vec{y})^2}} \tag{61}$$

This solution can now be used to simplify the phonen trace, where now the spatial integral will become Gaussian. There is no coupling between the sites i and so the trace can be written as a product of traces acting only on a single site. Because of the coupling between $\vec{x}$ and $\vec{y}$ in (61), this separation is not possible for the time slices j. So this Gaussian does not further reduce to a product of one-dimensional Gaussians, but stays M-dimensional and therefore, needs the more complicated identity (75) to be solved.

$$\begin{aligned}
&\underline{\mathrm{tr}_{\text{phonon}} \left(\prod_{j=1}^{M} \left(e^{\sum\limits_{i=1}^{N} \left(\frac{\Delta\tau\alpha^2}{2U} x_i^2 - \alpha x_i (\Delta\tau c + \frac{\sigma_{ij}\lambda}{U}) \right)} e^{-\Delta\tau H_{\text{osc}}} \right) \right)} = \\
&= \left(\frac{1}{2\pi\Delta\tau}\right)^{\frac{NM}{2}} \int\limits_{\mathbb{R}^{N\times M}} \prod_{j=1}^{M} \left(e^{\sum\limits_{i=1}^{N} \left(-\frac{\Delta\tau}{2}(\omega^2 - \frac{\alpha^2}{U}) x_i^{(j)2} - \alpha x_i^{(j)} \left(\Delta\tau c + \frac{\sigma_{ij}\lambda}{U}\right)\right)} e^{-\frac{1}{2\Delta\tau}\left(\vec{x}^{(j)} - \vec{x}^{(j+1)}\right)^2} \right) d\vec{x} = \\
&= \left(\frac{1}{2\pi\Delta\tau}\right)^{\frac{NM}{2}} \prod_{i=1}^{N} \int\limits_{\mathbb{R}^M} \left(e^{\sum\limits_{j=1}^{M} \left(-\left(\frac{\Delta\tau}{2}(\omega^2 - \frac{\alpha^2}{U}) + \frac{1}{\Delta\tau}\right) x^{(j)2} - \alpha x^{(j)} \left(\Delta\tau c + \frac{\sigma_{ij}\lambda}{U}\right) + \frac{1}{\Delta\tau} x^{(j)} x^{(j+1)} \right)} \right) d\vec{x} \\
&= \underline{\left(\frac{1}{2\pi}\right)^{\frac{NM}{2}} \prod_{i=1}^{N} \int\limits_{\mathbb{R}^M} \left(e^{\sum\limits_{j=1}^{M} \left(-\left(\frac{\Delta\tau^2}{2}(\omega^2 - \frac{\alpha^2}{U}) + 1\right) x^{(j)2} - \alpha\sqrt{\Delta\tau} x^{(j)} \left(\Delta\tau c + \frac{\sigma_{ij}\lambda}{U}\right) + x^{(j)} x^{(j+1)} \right)} \right) d\vec{x}}
\end{aligned} \tag{62}$$

Where in the last equation the substitution $\vec{x} \rightarrow \sqrt{\Delta\tau}\vec{x}$ was made.

The anyalytic calculation of this integral is done in the Appendix (75) or rather (83), with the coefficients Ω and R are given in (59). At this point also the condition (57) is needed to ensure that $a > 1$.

$$\begin{aligned}
&\underline{\mathrm{tr}_{\text{phonon}} \left(\prod_{j=1}^{M} \left(e^{\sum\limits_{i=1}^{N} \left(\frac{\Delta\tau\alpha^2}{2U} x_i^2 - \alpha x_i (\Delta\tau c + \frac{\sigma_{ij}\lambda}{U}) \right)} e^{-\Delta\tau H_{\text{osc}}} \right) \right)} = \\
&= \left(\tfrac{1}{2\pi}\right)^{\frac{NM}{2}} \left(\tfrac{(2\pi)^M}{(\Omega^M - 1)(1 - \Omega^{-M})} \right)^{\frac{N}{2}} \prod_{i=1}^{N} \exp\left(\frac{\frac{\alpha^2\Delta\tau\lambda^2}{U^2} \vec{\sigma}_i^T R \vec{\sigma}_i}{4(1-\Omega^{-M})\sqrt{a^2-1}} + \frac{\alpha\Delta\tau^{\frac{3}{2}} c\left(2\frac{\alpha\sqrt{\Delta\tau}\lambda}{U}|\vec{\sigma}_i| + M\alpha\Delta\tau^{\frac{3}{2}} c\right)}{2(a-1)} \right) = \\
&= \underline{\left(\tfrac{1}{(\Omega^M - 1)(1 - \Omega^{-M})} \right)^{\frac{N}{2}} e^{\frac{\alpha^2 c\left(2\frac{\lambda}{U}|\sigma| + N\beta c\right)}{2(\omega^2 - \frac{\alpha^2}{U})}} \exp\left(\frac{\alpha^2\Delta\tau^2}{2U(\Omega^{-M} - 1)\sqrt{a^2-1}} \sum_{i=1}^{N} \vec{\sigma}_i^T R \vec{\sigma}_i \right)}
\end{aligned}$$

This is now the analytic expression of the phonon trace, which was needed in (60). Plugging it in, leads to the asserted representation of the partition function.

$$\begin{aligned}
\underline{\underline{Z}} = &\left(\tfrac{e^{\beta U c^2}}{\pi^M} \right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times M}} e^{-|\sigma^2| + |\sigma|\lambda c} \det\left(E + \prod_{j=1}^{M} \left(e^{\lambda G^{(j)}} e^{t\Delta\tau h_{\text{kin}}} \right) \right)^2 \cdot \\
&\cdot \left(\tfrac{1}{(\Omega^M - 1)(1 - \Omega^{-M})} \right)^{\frac{N}{2}} e^{\frac{\alpha^2 c\left(2\frac{\lambda}{U}|\sigma| + N\beta c\right)}{2(\omega^2 - \frac{\alpha^2}{U})}} \exp\left(\frac{\alpha^2\Delta\tau^2}{2U(\Omega^{-M} - 1)\sqrt{a^2-1}} \sum_{i=1}^{N} \vec{\sigma}_i^T R \vec{\sigma}_i \right) d\sigma = \\
= &\left(\frac{e^{\frac{\beta U^2 c^2 \omega^2}{U\omega^2 - \alpha^2}}}{\pi^M (\Omega^M - 1)(1 - \Omega^{-M})} \right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times M}} \exp\left(-\sum_{i=1}^{N} \vec{\sigma}_i^T \left(E + \frac{\alpha^2\Delta\tau^2}{2U(1 - \Omega^{-M})\sqrt{a^2-1}} R \right) \vec{\sigma}_i + |\sigma| \frac{\lambda c U \omega^2}{U\omega^2 - \alpha^2} \right) \cdot
\end{aligned}$$

$$\cdot\det\left(E+\prod_{j=1}^{M}\left(e^{\lambda G^{(j)}}e^{t\Delta\tau h_{\text{kin}}}\right)\right)^2 d\sigma \qquad \blacksquare$$

5.4 Determinant representation with Fourier transformed HS parameter

A decisive part of the proof of (59), was the calculation of the multi-dimensional Gaussian integral in (62). For this, the identity (75) was used, which was calculated mainly by inverting the matrix B (77) directly. This Gaussian integral can also be calculated by using Fourier transformation (84), which leads to a different representation of the partition function.

$$Z=\left(\frac{e^{\frac{\beta U^2c^2\omega^2}{U\omega^2-\alpha^2}}}{\pi^M(\Omega^M-1)(1-\Omega^{-M})}\right)^{\frac{N}{2}}\int\limits_{\mathbb{R}^{N\times M}} e^{\sum\limits_{i=1}^{N}\left(-\sum\limits_{k=1}^{M}|\tilde\sigma_{ik}|^2\left(M+\frac{\beta\alpha^2\Delta\tau}{2U\left(a-\cos\left(2\pi\frac{k}{M}\right)\right)}\right)+\tilde\sigma_{iM}\frac{M\lambda cU\omega^2}{U\omega^2-\alpha^2}\right)}\cdot$$
$$\cdot\det\left(E+\prod_{j=1}^{M}\left(e^{\lambda\sum\limits_{k=1}^{M}e^{-2\pi i\frac{jk}{M}}\tilde G^{(k)}}e^{t\Delta\tau h_{\text{kin}}}\right)\right)^2 d\sigma \qquad (63)$$

with • $a=\frac{\Delta\tau^2}{2}(\omega^2-\frac{\alpha^2}{U})+1$
• $\Omega=a+\sqrt{a^2-1}$
• $\forall l\in\{1,\dots,N\},j\in\{1,\dots,M\}:\tilde\sigma_{lj}=\frac{1}{M}\sum\limits_{k=1}^{M}e^{2\pi i\frac{kj}{M}}\sigma_{lk}$

Like in the previous representation, also here the constant a has to be greater than 1 and so the condition (57) is necessary to make this representation valid.

Proof:

The first part is the same as in the proof of (59). Only in the calculation of $\text{tr}_{\text{phonon}}(\dots)$, the different way of doing the integral comes into play.

$$\text{tr}_{\text{phonon}}\left(\prod_{j=1}^{M}\left(e^{\sum\limits_{i=1}^{N}\left(\frac{\Delta\tau\alpha^2}{2U}x_i^2-\alpha x_i\left(\Delta\tau c+\frac{\sigma_{ij}\lambda}{U}\right)\right)}e^{-\Delta\tau H_{\text{osc}}}\right)\right)=$$

$$=\left(\frac{1}{2\pi}\right)^{\frac{NM}{2}}\prod_{i=1}^{N}\sqrt{\frac{(2\pi)^M}{(\Omega^M-1)(1-\Omega^{-M})}}e^{\frac{M\alpha^2\Delta\tau^3c^2}{4(a-1)}+\frac{M\alpha\Delta\tau^{\frac{3}{2}}c\alpha\sqrt{\Delta\tau}\frac{\lambda}{U}\tilde\sigma_{iM}}{2(a-1)}+\frac{M}{4}\sum\limits_{k=1}^{M}\frac{\frac{\alpha^2\Delta\tau\lambda^2}{U^2}|\tilde\sigma_{ik}|^2}{a-\cos\left(2\pi\frac{k}{M}\right)}}=$$
$$=\left(\frac{e^{\frac{\beta\alpha^2c^2U}{U\omega^2-\alpha^2}}}{(\Omega^M-1)(1-\Omega^{-M})}\right)^{\frac{N}{2}}e^{\sum\limits_{i=1}^{N}\left(\frac{M\alpha^2c\lambda\tilde\sigma_{iM}}{U\omega^2-\alpha^2}-\sum\limits_{k=1}^{M}\frac{\beta\alpha^2\Delta\tau|\tilde\sigma_{ik}|^2}{2U\left(a-\cos\left(2\pi\frac{k}{M}\right)\right)}\right)}$$

This can now be inserted in (60) and leads to the following partition function.

$$\underline{\underline{Z}}=\left(\frac{e^{\beta Uc^2}}{\pi^M}\right)^{\frac{N}{2}}\int\limits_{\mathbb{R}^{N\times M}}e^{-|\sigma^2|+|\sigma|\lambda c}\det\left(E+\prod_{j=1}^{M}\left(e^{\lambda G^{(j)}}e^{t\Delta\tau h_{\text{kin}}}\right)\right)^2\cdot$$
$$\cdot\left(\frac{e^{\frac{\beta\alpha^2c^2U}{U\omega^2-\alpha^2}}}{(\Omega^M-1)(1-\Omega^{-M})}\right)^{\frac{N}{2}}e^{\sum\limits_{i=1}^{N}\left(\frac{M\alpha^2c\lambda\tilde\sigma_{iM}}{U\omega^2-\alpha^2}-\sum\limits_{k=1}^{M}\frac{\beta\alpha^2\Delta\tau|\tilde\sigma_{ik}|^2}{2U\left(a-\cos\left(2\pi\frac{k}{M}\right)\right)}\right)}d\sigma=$$
$$=\left(\frac{e^{\frac{\beta U^2c^2\omega^2}{U\omega^2-\alpha^2}}}{\pi^M(\Omega^M-1)(1-\Omega^{-M})}\right)^{\frac{N}{2}}\int\limits_{\mathbb{R}^{N\times M}}e^{\sum\limits_{i=1}^{N}\left(-\sum\limits_{k=1}^{M}|\tilde\sigma_{ik}|^2\left(M+\frac{\beta\alpha^2\Delta\tau}{2U\left(a-\cos\left(2\pi\frac{k}{M}\right)\right)}\right)+\tilde\sigma_{iM}\frac{M\lambda cU\omega^2}{U\omega^2-\alpha^2}\right)}.$$
$$\cdot\det\left(E+\prod_{j=1}^{M}\left(e^{\lambda\sum\limits_{k=1}^{M}e^{-\frac{2\pi ijk}{M}}\tilde G^{(k)}}e^{t\Delta\tau h_{\text{kin}}}\right)\right)^2 d\sigma \qquad \blacksquare$$

5.5 Limit for zero Coulomb Energy

As a special case the limit case $U \to 0$ should be investigated.
Simply setting $U = 0$ in this determinant representation does not work, because already in the first step, the HS transformation (56) is only valid for finite U. Also taking the limit leads to some problems, because the condition (57), which has to be fulfilled in order to make the representation (59) valid, will be violated for very small positive values of U. The limiting process is therefore restricted to negative U.
The partition function $Z_{U=0} = \lim\limits_{U \to 0^-} (Z)$ in this limit is given by

$$\boxed{\begin{aligned} Z = \left(\frac{e^{-\frac{\beta\omega^2\mu^2}{2\alpha^2}}}{\pi^{\frac{M}{2}} \Delta\tau^M} \right)^N \int\limits_{\mathbb{R}^{N\times M}} & e^{\frac{1}{\Delta\tau^2} \sum\limits_{i=1}^{N} \vec{\sigma}_i^T \left(B - (\Delta\tau^2\omega^2+2)E\right)\vec{\sigma}_i - |\sigma| \frac{\sqrt{2\Delta\tau}\mu\omega^2}{\alpha}} \cdot \\ & \cdot \det\left(E + \prod_{j=1}^{M} \left(e^{\alpha\sqrt{2\Delta\tau}G^{(j)}} e^{t\Delta\tau h_{\text{kin}}} \right) \right)^2 d\sigma \,. \end{aligned}} \tag{64}$$

with $B = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 1 \\ 1 & 0 & 1 & \dots & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & 0 & \dots & 1 & 0 \end{pmatrix}$

The complicated matrix R from (59), which couples all the time slices j, reduces to a matrix B, which couples only to the neighboring timeslices.

Proof:

After a closer look at the partition function (59), one sees that in the limit $U \to 0^-$, the integral in the nominator as well as Ω^M in the denominator diverges. Because it is not allowed to exchange the order of integration and the limiting process in this '$\frac{\infty}{\infty}$' case, the substitution of the divergent $\frac{1}{\sqrt{-U}}$ part, by $\sigma \to \frac{\sqrt{-U}}{\alpha}\,\sigma$, has to be done first.

$$\begin{aligned} Z = \left(\frac{\alpha^{2M} e^{\frac{\beta U^2 c^2 \omega^2}{U\omega^2 - \alpha^2}}}{\pi^M (-U)^M (\Omega^M - 1)(1 - \Omega^{-M})} \right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times M}} & e^{\frac{\alpha^2}{U} \sum\limits_{i=1}^{N} \vec{\sigma}_i^T \left(E + \frac{\alpha^2 \Delta\tau^2}{2U(1-\Omega^{-M})\sqrt{a^2-1}} R \right) \vec{\sigma}_i + |\sigma| \frac{\alpha\sqrt{2\Delta\tau} c U \omega^2}{U\omega^2 - \alpha^2}} \cdot \\ & \cdot \det\left(E + \prod_{j=1}^{M} \left(e^{\alpha\sqrt{2\Delta\tau}G^{(j)}} e^{t\Delta\tau h_{\text{kin}}} \right) \right)^2 d\sigma \end{aligned}$$

The limit $U \to 0^-$ can now be performed by doing some expansions.

- $\underline{\Omega} = \frac{\Delta\tau^2}{2}(\omega^2 - \frac{\alpha^2}{U}) + 1 + \sqrt{\left(\frac{\Delta\tau^2}{2}(\omega^2 - \frac{\alpha^2}{U}) + 1\right)^2 - 1} =$
  $= -\frac{\Delta\tau^2\alpha^2}{2U} - \frac{\Delta\tau^2\alpha^2}{2U} + \mathcal{O}(1) =$
  $= \underline{-\frac{\Delta\tau^2\alpha^2}{U} + \mathcal{O}(1)}$
- $\underline{1 - \Omega^{-M}} = 1 - \left(-\frac{\Delta\tau^2\alpha^2}{U} + \mathcal{O}(1) \right)^{-M} =$
  $= 1 - \left(-\frac{U}{\Delta\tau^2\alpha^2} + \mathcal{O}(U^2) \right)^M = \underline{1 + \mathcal{O}(U^M)}$
- $\underline{(-U)^M(\Omega^M - 1)} = (-U)^M \left(\left(-\frac{\Delta\tau^2\alpha^2}{U} + \mathcal{O}(1) \right)^M - 1 \right) =$
  $= (-U)^M \left(\left(-\frac{\Delta\tau^2\alpha^2}{U} \right)^M + \mathcal{O}(\frac{1}{U^{M-1}}) - 1 \right) =$
  $= \underline{(\Delta\tau^2\alpha^2)^M + \mathcal{O}(U)}$
- $\underline{cU} = \left(\frac{\mu}{U} - \frac{1}{2} \right) U = \underline{\mu + \mathcal{O}(U)}$

- $\sqrt{a^2-1} = \sqrt{\left(\frac{\Delta\tau^2}{2}(\omega^2 - \frac{\alpha^2}{U}) + 1\right)^2 - 1} =$
  $= \sqrt{\Delta\tau^2\omega^2\left(\frac{\Delta\tau^2\omega^2}{4} + 1\right) - \frac{\Delta\tau^2\alpha^2}{U}\left(\frac{\Delta\tau^2\omega^2}{2} + 1\right) + \frac{\Delta\tau^4\alpha^4}{4U^2}} =$
  $= -\frac{\Delta\tau^2\alpha^2}{2U} + \frac{\Delta\tau^2\alpha^2(\frac{\Delta\tau^2\omega^2}{2}+1)}{2\frac{\Delta\tau^2\alpha^2}{2}} + \mathcal{O}(U) =$
  $= \underline{-\frac{\Delta\tau^2\alpha^2}{2U} + \frac{\Delta\tau^2\omega^2}{2} + 1 + \mathcal{O}(U)}$

- $R = E + \Omega^{-1}B + \mathcal{O}(\Omega^{-2})$

  $\Rightarrow \underline{R} = E + \frac{1}{-\frac{\Delta\tau^2\alpha^2}{U} + \mathcal{O}(1)}B + \mathcal{O}(U^2) =$
  $= E + \left(-\frac{U}{\Delta\tau^2\alpha^2} + \mathcal{O}(U^2)\right)B + \mathcal{O}(U^2) =$
  $= \underline{E - \frac{U}{\Delta\tau^2\alpha^2}B + \mathcal{O}(U^2)}$

- $\underline{\frac{1}{(1-\Omega^{-M})\sqrt{a^2-1}}}R = \frac{1}{(1+\mathcal{O}(U^M))\left(-\frac{\Delta\tau^2\alpha^2}{2U} + \frac{\Delta\tau^2\omega^2}{2} + 1 + \mathcal{O}(U)\right)}\left(E - \frac{U}{\Delta\tau^2\alpha^2}B + \mathcal{O}(U^2)\right) =$
  $= \left(-\frac{2U}{\Delta\tau^2\alpha^2} - \frac{\frac{\Delta\tau^2\omega^2}{2}+1}{\frac{\Delta\tau^4\alpha^4}{4}}U^2 + \mathcal{O}(U^3)\right)\left(E - \frac{U}{\Delta\tau^2\alpha^2}B + \mathcal{O}(U^2)\right) =$
  $= \underline{-\frac{2U}{\Delta\tau^2\alpha^2}E + \frac{2U^2}{\Delta\tau^4\alpha^4}\left(B - (\Delta\tau^2\omega^2 + 2)E\right) + \mathcal{O}(U^3)}$

Thus, the partition function in the limit $U \to 0^-$ becomes:

$$\underline{\underline{Z}} = \left(\frac{e^{-\frac{\beta\omega^2\mu^2}{2\alpha^2}}}{\pi^{\frac{M}{2}}\Delta\tau^M}\right)^N \int_{\mathbb{R}^{N\times M}} e^{\frac{1}{\Delta\tau^2}\sum_{i=1}^{N}\vec{\sigma}_i^T\left(B-(\Delta\tau^2\omega^2+2)E\right)\vec{\sigma}_i - |\sigma|\frac{\sqrt{2\Delta\tau}\mu\omega^2}{\alpha}} \cdot$$
$$\underline{\underline{\cdot\det\left(E + \prod_{j=1}^{M}\left(e^{\alpha\sqrt{2\Delta\tau}G^{(j)}}e^{t\Delta\tau h_{\text{kin}}}\right)\right)^2 d\sigma}} \qquad \blacksquare$$

In order to prove the correctness of this formula, the special case '1 site' is calculated in the Appendix (88) and compared with the direct result of the definition of the partition function $Z = \text{tr}(e^{-\beta H(U=0)})$ of a Hamiltonian without Coulomb term.
Also in the Appendix (87), the phonon trace is calculated out directly without applying the Continuous HS transformation in the first place.

6 Conclusions

In order to solve the sign problem in the repulsive Hubbard model away from half filling, new Hubbard-Stratonovich transformations were introduced in the sections 2.2 - 2.4. All the transformations achieved, that the main part of the formulas, the determinant, became positive, but the sign was shifted into the prefactor instead and the overall behaviour of the sign did not change at all. In particular the sign as a function of the inverse temperature β was investigated, which turned out to decay exponentially with increasing β (see figures 5, 7 and 8).
In chapter 3 all the transformations of chapter 2 were combined with a complexification of the magnetic field (41), which leads to a form (42) of a discrete Fourier series, where the Fourier coefficients are given by the canonical partition functions for a fixed value of the magnetisation. The representation of the partition function in the different HS transformations (48), (51) and (52) are the main results of this chapter. They gave hope for a solution of the sign problem, because in an approximation for $\beta|U| \gg 1$, the addends of the New HS transformation (48) seemed to converge to something positive. Unfortunately these approximations were too rough to make the Trotter error converge. Instead, the sign still decays exponentially with growing β for every magnetisation (except of $m = 0$) and every considered HS transformation. This can be seen in the figures 12 and 14.
Nevertheless this representation with canonical partition functions has the advantage, that one is no longer faced with the partition function over the whole grandcanonical ensemble, but only has to calculate the partition functions with respect to the smaller space of constant magnetisation. Another advantage appears in the Approximated New HS transformation (49), namely the sum only consists of two elements $\sigma \in \{\pm 1\}$ and the determinant is h-independent. This keeps the computational effort small and allows to consider different values of the magnetic field with only a small amount of additional computational time.

The HS transformations (especially the Continuous HS transformation) from the first part of the thesis are also applicable to the more general Hubbard Holstein model. There, the coupling between electrons and phonons lead to an effective shift in the chemical potential and in the end to a coupling between different Trotter timeslices, which shows up in the appearance of the nondiagonal matrix R in eq.(59). The phonon trace of the partition function can be integrated out analytically and leads to a form of the partition function in the most general case with finite Trotter timeslices $\Delta\tau$. It contains no approximations except of the Trotter decomposition, but has the disadvantage of the $(N \times M)$-dimensional σ-integral. It turns out, that in the Continuous HS transformation the phonon parameters do not appear inside the determinant, but only in the quiet simple exponential prefactor. Two nice practical advantages which follow out of this are, that one can calculate the partition function for different phonon parameters simultaniously with only a small additional amount of computational effort and one can also rather easy differentiate with respect to these parameters.
Future investigations can try to apply the promising Approximated New HS transformation onto the Hubbard Holstein model. This transformation has mainly the same advantages as the Continuous HS transformation, but a simple two element sum, instead of the high-dimensional integral.

A Appendix

A.1 Fermionic trace as a determinant

In a lattice with N sites, the corresponding grandcanonical phase space has dimension $2^N \times 2^N$, because of the two possible occupations on every site. So the trace of an operator in this space is the sum over the diagonal of the respective $2^N \times 2^N$-dimensional matrix. If in addition Trotter timeslices are introduced, this sum has to be calculated for every imaginary time slice $j \in \{1, \dots, M\}$. Because of the large computational effort, alternative ways of calculating the trace are beneficial.
For a *fermionic* trace, one of which is to hide it inside the determinant of a $N \times N$ matrix. This is possible, because the definition of the determinant is also a sum over 2^N elements. But because there are much more effective ways to calculate the determinant, this form will be very beneficial. Also in numerical calculations this determinant can be calculated recursively by updating the determinant of the previous step, either exact or by an approximation.
The goal of this section is, to transform the fermionic trace of an arbitrary operator, acting in a 2^N-dimensional phase space, into the determinant of a corresponding $N \times N$-matrix. The proof will mainly follow [18] and is splitted into three parts. The first two parts are the statements (65) and (68), followed by the main equivalence statement (69).

<u>**Statement 1**</u>:

Let $(T_n)_{n=1}^L \in \mathbb{C}^{N\times N}$ diagonalizable, $P \in \mathbb{C}^{N\times M}$, then the following identity holds

$$\boxed{\left(\prod_{n=1}^{L} e^{\vec{c}^{\,\dagger} T_n \vec{c}}\right) \prod_{m=1}^{M} (\vec{c}^{\,\dagger} P)_m \left|0\right\rangle = \prod_{m=1}^{M} \left(\vec{c}^{\,\dagger} \left(\prod_{n=1}^{L} e^{T_n}\right) P\right)_m \left|0\right\rangle} \tag{65}$$

<u>Proof:</u>

The proof will be made by induction with respect to L.

<u>Induction basis</u>: <u>$L = 1$</u>:

Because T is diagonalizable it can decomposed in the form

$$\exists U, D \in \mathbb{C}^{N\times N} : U \text{ unitary},\ D \text{ diagonal},\ T = UDU^\dagger$$

Define $\underline{\vec{\gamma}^{\,\dagger} = \vec{c}^{\,\dagger} U} \wedge \underline{\vec{\gamma} = U^\dagger \vec{c}}$, then $\vec{\gamma}$ satisfies the fermionic anticommutator relations.

- $\underline{\{\gamma_i, \gamma_j\}} = \sum\limits_{k=1}^{N} \sum\limits_{l=1}^{N} U^\dagger_{i,k} U^\dagger_{j,l} \{c_k, c_l\} = \underline{0}$
- $\underline{\{\gamma_i^\dagger, \gamma_j^\dagger\}} = \sum\limits_{k=1}^{N} \sum\limits_{l=1}^{N} U_{k,i} U_{l,j} \{c_k^\dagger, c_l^\dagger\} = \underline{0}$
- $\underline{\{\gamma_i, \gamma_j^\dagger\}} = \sum\limits_{k=1}^{N} \sum\limits_{l=1}^{N} U^\dagger_{i,k} U_{l,j} \{c_k, c_l^\dagger\} = \{c_k, c_l^\dagger\} = \sum\limits_{k=1}^{N} U^\dagger_{i,k} U_{k,j} = (U^\dagger U)_{i,j} = \underline{\delta_{i,j}}$

Where the anticommutator relations $\{c_k, c_l\} = 0$, $\{c_k^\dagger, c_l^\dagger\} = 0$ and $\{c_k, c_l^\dagger\} = \delta_{kl}$ were used.

This new fermionic operators $\gamma_i^\dagger$ can now be used to some kind of diagonalize the right hand side of (65) with respect to $\vec{c}^\dagger$.

$$\begin{aligned}
\underline{e^{\vec{c}^{\,\dagger} T \vec{c}} \prod_{m=1}^{M} (\vec{c}^{\,\dagger} P)_m \left|0\right\rangle} &= e^{\vec{\gamma}^{\,\dagger} D \vec{\gamma}} \prod_{m=1}^{M} (\vec{\gamma}^{\,\dagger} U^\dagger P)_m \left|0\right\rangle = \\
&= e^{\sum_{i=1}^{N} D_i \gamma_i^\dagger \gamma_i} \prod_{m=1}^{M} \sum_{k=1}^{N} \gamma_k^\dagger (U^\dagger P)_{k,m} \left|0\right\rangle = \\
&= \underline{\sum_{k_1,\dots,k_M=1}^{N} e^{\sum_{i=1}^{N} D_i \gamma_i^\dagger \gamma_i} \prod_{m=1}^{M} \gamma_{k_m}^\dagger (U^\dagger P)_{k_m,m} \left|0\right\rangle}
\end{aligned}$$

Because of the anticummutator relations, $\gamma_k^\dagger \gamma_k^\dagger |0\rangle = 0$ is true and every product $\prod_{m=1}^{M} \gamma_{k_m}^\dagger$ has to consist out of pairwise different creation operators.

$$e^{\vec{c}^{\,\dagger} T \vec{c}} \prod_{m=1}^{M} (\vec{c}^{\,\dagger} P)_m |0\rangle = \sum_{k_1 \neq \cdots \neq k_M = 1}^{N} e^{\sum_{i=1}^{N} D_i \gamma_i^\dagger \gamma_i} \prod_{m=1}^{M} \gamma_{k_m}^\dagger (U^\dagger P)_{k_m, m} |0\rangle \tag{66}$$

The exponential shall now be shifted to the right side of the product, or at least as far as possible. For this, the following three properties are needed.

a) For $\underline{i \neq k}$ it is: $\underline{e^{D_i \gamma_i^\dagger \gamma_i}\ \gamma_k^\dagger = \gamma_k^\dagger\ e^{D_i \gamma_i^\dagger \gamma_i}}$ because $[\gamma_i^\dagger \gamma_i, \gamma_k^\dagger] = 0$

b) For $\underline{i = k}$ it is: $\underline{e^{D_i \gamma_i^\dagger \gamma_i}\ \gamma_i^\dagger} = \sum_{n=0}^{\infty} \frac{1}{n!} (D_i \gamma_i^\dagger \gamma_i)^n \gamma_i^\dagger = \sum_{n=0}^{\infty} \frac{1}{n!} D_i^n \gamma_i^\dagger = \underline{e^{D_i}\ \gamma_i^\dagger}$

Where $\gamma_i^\dagger \gamma_i \gamma_i^\dagger = \gamma_i^\dagger (1 - \gamma_i^\dagger \gamma_i) = \gamma_i^\dagger$ was used.

c) $\underline{e^{D_i \gamma_i^\dagger \gamma_i} |0\rangle} = \sum_{n=0}^{\infty} \frac{1}{n!} (D_i \gamma_i^\dagger \gamma_i)^n |0\rangle = \frac{1}{0!} |0\rangle = \underline{|0\rangle}$ because $\gamma_i |0\rangle = 0$

Property a) says, that the exponential can be shifted through the product, as long as $i \neq k_m$. If a factor $i = k_m$ is met, property b) comes into play and the exponential operator becomes a simple factor e^{D_i} at this point. This can happen only once, because the $(\gamma_{k_m})_{m=1}^{M}$ are pairwise different. If there is no $i = k_m$ in the product the exponential can be shifted to the very right and makes the whole term vanish because of c).

Not every exponential has a corresponding γ_{k_m} in the product, but because every $i \in \{1, \ldots, N\}$ appears in the exponential, every γ_{k_m} of the product has exactly one correponding γ_{k_m} in the exponential. All the others vanish.

So the left hand side can be written as

$$e^{\vec{c}^{\,\dagger} T \vec{c}} \prod_{m=1}^{M} (\vec{c}^{\,\dagger} P)_m |0\rangle = \sum_{k_1 \neq \cdots \neq k_M = 1}^{N} \prod_{m=1}^{M} e^{D_{k_m}} \gamma_{k_m}^\dagger (U^\dagger P)_{k_m, m} |0\rangle \tag{67}$$

To make this argument work, all duplicate k_m were removed in (66), but with the same argument they can be added again in (67). Afterwards the transformation $\vec{\gamma} = U^\dagger \vec{c}$ is reversed again and leads to the stated formula.

$$\begin{aligned}
\underline{\underline{e^{\vec{c}^{\,\dagger} T \vec{c}} \prod_{m=1}^{M} (\vec{c}^{\,\dagger} P)_m |0\rangle}} &= \sum_{k_1, \ldots, k_M = 1}^{N} \prod_{m=1}^{M} e^{D_{k_m}} \gamma_{k_m}^\dagger (U^\dagger P)_{k_m, m} |0\rangle = \\
&= \prod_{m=1}^{M} \sum_{k=1}^{M} e^{D_k} \gamma_k^\dagger (U^\dagger P)_{k, m} |0\rangle = \\
&= \prod_{m=1}^{M} \left(\vec{\gamma}^{\,\dagger} e^{D} U^\dagger P\right)_m |0\rangle = \\
&= \underline{\underline{\prod_{m=1}^{M} \left(\vec{c}^{\,\dagger} e^{T} P\right)_m |0\rangle}}
\end{aligned}$$

The easier part of the proof of this first statement is the induction step.

Induction step: $L \to L + 1$

At first the induction basis can be applied to the matrix T_{L+1}, in order to shift into the right product.

$$\left(\prod_{n=1}^{L+1} e^{\vec{c}^{\,\dagger} T_n \vec{c}}\right) \prod_{m=1}^{M} (\vec{c}^{\,\dagger} P)_m |0\rangle = \left(\prod_{n=1}^{L} e^{\vec{c}^{\,\dagger} T_n \vec{c}}\right) \prod_{m=1}^{M} (\vec{c}^{\,\dagger} e^{T_{L+1}} P)_m |0\rangle$$

This right hand side looks like the induction assumption, but with a different matrix $P \to e^{T_{L+1}} P$. But because the matrix P was arbitrary, the induction assumption holds also for this matrix $e^{T_{L+1}} P$.

$$\underline{\underline{\left(\prod_{n=1}^{L+1} e^{\vec{c}^{\,\dagger} T_n \vec{c}}\right) \prod_{m=1}^{M} (\vec{c}^{\,\dagger} P)_m |0\rangle}} = \prod_{m=1}^{M} \left(\vec{c}^{\,\dagger} \left(\prod_{n=1}^{L} e^{T_n}\right) e^{T_{L+1}} P\right)_m |0\rangle =$$

$$= \underline{\underline{\prod_{m=1}^{M} \left(\vec{c}^{\,\dagger} \left(\prod_{n=1}^{L+1} e^{T_n}\right) P\right)_m |0\rangle}} \quad \blacksquare$$

The second statment gives the link between a matrix element and the determinant.

Statement 2 :

Let $P, Q \in \mathbb{C}^{N\times M}$ two arbitrary matrices, then the following identity holds

$$\boxed{\langle 0| \left(\prod_{m=M}^{1} (P^\dagger \vec{c})_m \cdot \prod_{l=1}^{M} (\vec{c}^{\,\dagger} Q)_l\right) |0\rangle = \det(P^\dagger Q)} \tag{68}$$

Proof:

The matrix-vector multiplication $(P^\dagger \vec{c})$ can be written as a sum, and the sum carried out in front of the product.

$$\prod_{m=M}^{1} (P^\dagger \vec{c})_m = \sum_{i_1,\ldots,i_M=1}^{N} \prod_{m=M}^{1} P^\dagger_{m,i_m} c_{i_m}$$

The same can be done for the second product $\prod_{l=1}^{M} (\vec{c}^\dagger Q)_l$ on the left hand side of (68).

$$\prod_{l=1}^{M} (\vec{c}^\dagger Q)_l = \sum_{k_1,\ldots,k_M=1}^{N} \prod_{l=1}^{M} c^\dagger_{k_l} Q_{k_l,l}$$

So, the main elements to investigate are $\langle 0| \left(\prod_{m=M}^{1} P^\dagger_{m,i_m} c_{i_m}\right) \left(\prod_{l=1}^{M} c^\dagger_{k_l} Q_{k_l,l}\right) |0\rangle$.

This expression starts and ends in the vacuumstate. Thus, all the particles created by the $c^\dagger_{k_l}$ have to be annihilated by any of the c_{i_m}.

For this, the elements $(k_l)_{l=1}^{M}$ have to be a permutation of $(i_m)_{m=1}^{M}$ and the sum $\sum_{k_1,\ldots,k_M=1}^{N}$ reduces to the sum over all permutations $\sum_{\pi\in S_M}$.

$$\langle 0| \left(\prod_{m=M}^{1} (P^\dagger \vec{c})_m \cdot \prod_{l=1}^{M} (\vec{c}^{\,\dagger} Q)_l\right) |0\rangle = \sum_{i_1,\ldots,i_M=1}^{N} \sum_{\pi\in S_M} \langle 0| \left(\prod_{m=M}^{1} P^\dagger_{m,i_m} c_{i_m}\right) \left(\prod_{l=1}^{M} c^\dagger_{i_{\pi(l)}} Q_{i_{\pi(l)},l}\right) |0\rangle$$

The product of all the prefactors $P^\dagger_{m,i_m}$ and $Q_{i_{\pi(l)},l}$ can be written in front of the inner product and it remains $\langle 0| \left(\prod_{m=M}^{1} c_{i_m}\right) \left(\prod_{l=1}^{M} c^\dagger_{i_{\pi(l)}}\right) |0\rangle$, which would equal 1 if the creation operators were in the correct order. But because of the permutation π this equals $(-1)^{|\pi|}$.

$$\langle 0| \left(\prod_{m=M}^{1} (P^\dagger \vec{c})_m \cdot \prod_{l=1}^{M} (\vec{c}^{\,\dagger} Q)_l\right) |0\rangle = \sum_{i_1,\ldots,i_M=1}^{N} \sum_{\pi\in S_M} \left(\prod_{m=1}^{M} P^\dagger_{m,i_m} Q_{i_m,\pi(m)}\right) (-1)^{|\pi|}$$

Where for coefficients, which are complex numbers, the order in the product plays no role any more and $\prod_{l=1}^{M} Q_{i_{\pi(l)},l} = \prod_{l=1}^{M} Q_{i_l,\pi(l)}$ can be used.

The sum $\sum_{i_1,\ldots,i_M=1}^{M}$ can be written insight the product again and leads to final result of this statement.

$$\langle 0| \left(\prod_{m=M}^{1} (P^\dagger \vec{c})_m \cdot \prod_{l=1}^{M} (\vec{c}^{\,\dagger} Q)_l \right) |0\rangle = \sum_{\pi \in S_M} (-1)^{|\pi|} \prod_{m=1}^{M} \sum_{i=1}^{N} P^\dagger_{m,i} Q_{i,\pi(m)} =$$
$$= \sum_{\pi \in S_M} (-1)^{|\pi|} \prod_{m=1}^{M} (P^\dagger Q)_{m,\pi(m)} =$$
$$= \det(P^\dagger Q) \quad \blacksquare$$

With the two statements (65) and (68), a fermionic trace (which is a sum over 2^N elements) can be written as a determinant of a $N \times N$ matrix.

Equivalence of trace and determinant

Let $(H_n)_{n=1}^L \in \mathbb{C}^{N\times N}$ be diagonalizable matrices, then the following statement holds.

$$\boxed{\mathrm{tr}\left(\prod_{n=1}^{L} e^{\vec{c}^{\,\dagger} H_n \vec{c}} \right) = \det\left(E + \prod_{n=1}^{L} e^{H_n} \right)} \tag{69}$$

The trace is ment to be the sum over all possible states with every possible number of particles in the system (grandcanonical ensemble).

Proof:

For a simpler notation define

$$B = \prod_{n=1}^{L} e^{H_n} \ . \tag{70}$$

then the determinant on the right hand side has the form.

$$\det(E+B) = \sum_{\pi \in S_N} (-1)^{|\pi|} \prod_{i=1}^{N} (\delta_{\pi(i),i} + B_{\pi(i),i})$$

This product can now be extended and sorted after powers of B.

$$\det(E+B) = \sum_{\pi \in S_N} (-1)^{|\pi|} \sum_{M=0}^{N} \sum_{i_1 > \dots > i_M = 1}^{N} \prod_{m=1}^{M} B_{\pi(i_m),i_m} \prod_{\substack{l=1 \\ l \notin \{i_1,\dots,i_M\}}}^{N} \delta_{\pi(l),l} \tag{71}$$

A closer look at one part of the sum

$$S_{i_1,\dots,i_M} := \sum_{\pi \in S_N} (-1)^{|\pi|} \prod_{m=1}^{M} B_{\pi(i_m),i_m} \prod_{\substack{l=1 \\ l \notin \{i_1,\dots,i_M\}}}^{N} \delta_{\pi(l),l} \tag{72}$$

gives some further simplifications.

Because of the δ-functions, the sum over all permutations in S_N is restricted to all permutations in S_M. To make sure that the new permutations $\pi \in S_M$ access the right elements of the matrix B, B has to be restricted to its rows and columns $\{i_1, \dots, i_M\}$. This can be done by multiplying B from left and right with a matrix $P \in \mathbb{C}^{N\times M}$ of the form

$$P_{i_1,1} = \dots = P_{i_M,M} = 1 \text{ and } P_{i,j} = 0 \text{ everywhere else.} \tag{73}$$

$$S_{i_1,\dots,i_M} = \sum_{\sigma \in S_M} (-1)^{|\sigma|} \prod_{m=1}^{M} (P^T B P)_{\sigma(m),m} \tag{74}$$

The sign $(-1)^{|\pi|} = (-1)^{|\sigma|}$ stays the same, because all elements l from π that vanished, had the property $\pi(l) = l$ (because of the δ-functions), and therefore, these elements had no contribution to $|\pi|$.

The righthand side of (74) is now exactly the definition of the determinant of the of the M-dimensional matrix $P^T BP$.

$$S_{i_1,\ldots,i_M} = \det(P^T BP)$$

With the help of statement 2 (68) this determinant can be written in terms of creation and annihilation operators.

$$S_{i_1,\ldots,i_M} = \langle 0| \left(\prod_{m=M}^{1} (P^T \vec{c})_m \right) \left(\prod_{l=1}^{M} (\vec{c}^{\,\dagger} BP)_l \right) |0\rangle$$

Putting in the definition (70) and using statement 1 (65), leads to the equation

$$S_{i_1,\ldots,i_M} = \langle 0| \left(\prod_{m=M}^{1} (P^T \vec{c})_m \right) \left(\prod_{n=1}^{L} e^{\vec{c}^{\,\dagger} H_n \vec{c}} \right) \left(\prod_{l=1}^{M} \left(\vec{c}^{\,\dagger} P\right)_l \right) |0\rangle \ .$$

Because the explicit form of P is known, also the expressions $P^T \vec{c}$ and $\vec{c}^{\,\dagger} P$ can be calculated

- $\underline{(P^T \vec{c})_m} = \sum\limits_{i=1}^{N} P_{i,m} c_i = \sum\limits_{k=1}^{M} \delta_{i_k,m} c_{i_k} = \underline{c_{i_m}}$
- $\underline{(\vec{c}^{\,\dagger} P)_m} = (P^T \vec{c})^\dagger_m = \underline{c^\dagger_{i_m}}$

and so the addends $S_{i_1,\ldots,i_M}$ reduces to

$$S_{i_1,\ldots,i_M} = \langle 0| \left(\prod_{m=M}^{1} c_{i_m} \right) \left(\prod_{n=1}^{L} e^{\vec{c}^{\,\dagger} H_n \vec{c}} \right) \left(\prod_{l=1}^{M} c^\dagger_{i_l} \right) |0\rangle \ .$$

Now putting this addend back into (71), the determinant finally becomes

$$\begin{aligned}
\underline{\underline{\det(E+B)}} &= \sum_{M=0}^{N} \sum_{i_1 > \cdots > i_M = 1}^{N} \langle 0| \left(\prod_{m=M}^{1} c_{i_m} \right) \left(\prod_{n=1}^{L} e^{\vec{c}^{\,\dagger} H_n \vec{c}} \right) \left(\prod_{l=1}^{M} c^\dagger_{i_l} \right) |0\rangle = \\
&= \sum_{M=0}^{N} \sum_{i_1 > \cdots > i_M = 1}^{N} \langle i_1, \ldots, i_M | \prod_{n=1}^{L} e^{\vec{c}^{\,\dagger} H_n \vec{c}} |i_1, \ldots, i_M\rangle = \\
&= \underline{\underline{\mathrm{tr} \left(\prod_{n=1}^{L} e^{\vec{c}^{\,\dagger} H_n \vec{c}} \right)}} \ . \qquad \blacksquare
\end{aligned}$$

A.2 Calculating the integral I

The task of this section is the calculation of the following multi-dimensional Gaussian integral, with a periodic nearest neighbor coupling $x_i x_{i+1}$ in the quadratic term. Additionally, the coupling is constant in every dimension j. These two restrictions lead to a closed expression of the Gaussian integral.

$$\boxed{\int\limits_{\mathbb{R}^M} e^{\sum\limits_{j=1}^{M} (b_j x_j - a x_j^2 + x_j x_{j+1})} d\vec{x} = \sqrt{\frac{(2\pi)^M}{(\omega^M - 1)(1 - \omega^{-M})}} \exp\left(\frac{1}{4(1-\omega^{-M})\sqrt{a^2-1}} \sum_{j,k=1}^{M} b_k R_{|k-j|} b_j \right)} \quad (75)$$

with $\underline{\underline{R_n = \omega^{-n} + \omega^{-M+n}}}$ and $\underline{\underline{\omega = a + \sqrt{a^2-1}}}$

and arbitrary coefficients $\underline{a > 1}$ and $\underline{(b_j)_{j=1}^M \in \mathbb{R}}$.

<u>Proof</u>:

The exponent of the integrand can be written in the following matrix form.

$$\underline{I = \int\limits_{\mathbb{R}^M} e^{\langle \vec{b}, \vec{x}\rangle - \langle \vec{x}, A\vec{x}\rangle} d\vec{x}} \qquad \text{with } A = \begin{pmatrix} a & -1 & \dots & 0 & 0 \\ 0 & a & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & a & -1 \\ -1 & 0 & \dots & 0 & a \end{pmatrix}$$

Define $\underline{\vec{d} = (A + A^T)^{-1}\vec{b}}$ and $\underline{f = \frac{1}{2}\vec{b}^T(A + A^T)^{-1}\vec{b}}$, then the linear term $\langle \vec{b}, \vec{x}\rangle$ of the integrand vanishes, because of

$$f - (\vec{x} - \vec{d})^T A(\vec{x} - \vec{d}) = \langle \vec{b}, \vec{x}\rangle - \langle \vec{x}, A\vec{x}\rangle \ .$$

The prefactor e^f can be written in front of the integral and by a transformation $\vec{x} \to \vec{x} + \vec{d}$ the vector $\vec{d}$ vanishes. The remaining integral has the form of a standard multi-dimensional Gaussian integral.

$$I = e^{\frac{1}{2}\vec{b}^T(A+A^T)^{-1}\vec{b}} \sqrt{\frac{(2\pi)^M}{\det(A + A^T)}} \tag{76}$$

But because of the special shape of the matrix A, the terms in this analytic expression can be further simplified.

So the two remaining tasks are:
- calculating the determinant $\det(A + A^T)$
- and the exponent $\vec{b}^T(A + A^T)^{-1}\vec{b}$.

To make notation easier, define the symmetric matrix

$$\underline{B = A + A^T = \begin{pmatrix} 2a & -1 & \dots & 0 & -1 \\ -1 & 2a & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 2a & -1 \\ -1 & 0 & \dots & -1 & 2a \end{pmatrix}} \tag{77}$$

Before any calculations in the exponent are done, some determinantes will be calculated, which will be the main ingredients to the solution of the integral.

The first statement is about the determinant of the B-matrix without periodic boundary conditions. This determinant will be needed for $\det(B)$ and also for the inverse matrix B^{-1}.

$$\underline{\underline{\text{Statement}}} : \underline{\underline{d_M = \det \begin{pmatrix} 2a & -1 & \dots & 0 & 0 \\ -1 & 2a & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 2a & -1 \\ 0 & 0 & \dots & -1 & 2a \end{pmatrix} = \frac{1}{2(\omega - a)}\left(\omega^{M+1} - \frac{1}{\omega^{M+1}}\right)}} \tag{78}$$

This statement will be proven by first calculating a recursion formula and then solving this recursion.

By applying the Laplace expansion onto the determinant, one reduces the dimension of the matrix and gets from d_M to d_{M-1} and d_{M-2}.

$$\underline{d_M} = \det\nolimits_M \left(\begin{array}{c|ccccc} 2a & -1 & 0 & \dots & 0 & 0 \\ \hline -1 & 2a & -1 & \dots & 0 & 0 \\ \hline 0 & -1 & 2a & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2a & -1 \\ 0 & 0 & 0 & \dots & -1 & 2a \end{array}\right) =$$

$$= 2ad_{M-1} + \det_{M-1}\begin{pmatrix} -1 & 0 & \dots & 0 & 0 \\ \hline -1 & 2a & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 2a & -1 \\ 0 & 0 & \dots & -1 & 2a \end{pmatrix} =$$

$$= \underline{2ad_{M-1} - d_{M-2}}$$

This recursion is true for $M \geq 2$ and for $M = 0$ and 1, one gets the starting values $\underline{d_0 = 1}$ and $\underline{d_1 = 2a}$.

This is a recursion formula for the determinant and the remaining task is just to prove this recursion.

First it is obtained that all the powers of $\underline{\omega = a + \sqrt{a^2 - 1}}$, from (75), can be expressed by a linear function in ω. Up to the power ω^4 this representations are needed and calculated below.

$\underline{\omega^2} = 2a^2 + 2a\sqrt{a^2-1} - 1 = \underline{2a\omega - 1}$

$\underline{\omega^3} = \omega\,(2a\omega - 1) = 2a\,(2a\omega - 1) - \omega = \underline{\left(4a^2 - 1\right)\omega - 2a}$

$\underline{\omega^4} = (2a\omega - 1)^2 = 4a^2(2a\omega - 1) - 4a\omega + 1 = \underline{4a(2a^2 - 1)\omega - 4a^2 + 1}$

- $\underline{\underline{d_0}} = \frac{1}{2(\omega - a)}\left(\omega - \frac{1}{\omega}\right) = \frac{1}{2(\omega^2 - a\omega)}(\omega^2 - 1) = \frac{1}{2(a\omega - 1)}(2a\omega - 2) = \underline{\underline{1}}$
- $\underline{\underline{d_1}} = \frac{1}{2(\omega - a)}\left(w^2 - \frac{1}{w^2}\right) =$
  $= \frac{1}{2((4a^2-1)\omega - 2a - a(2a\omega - 1))}\left(4a\left(2a^2 - 1\right)\omega - 4a^2\right) =$
  $= \frac{4a}{2((2a^2-1)\omega - a)}((2a^2 - 1)\omega - a) = \underline{\underline{2a}}$
- $\underline{\underline{2ad_{M-1} - d_{M-2}}} = 2a\frac{1}{2(\omega - a)}\left(\omega^{M-1} - \omega^{-M+1}\right) - \frac{1}{2(\omega - a)}\left(\omega^{M-2} - \omega^{-M+2}\right) =$
  $= \frac{1}{2(\omega - a)}\left((2a\omega - 1)\omega^{M-2} - (2a\omega - \omega^2)\omega^{-M}\right) =$
  $= \frac{1}{2(\omega - a)}\left(\omega^2\omega^{M-2} - \omega^{-M}\right) = \underline{\underline{d_M}}$ $\quad\square_{\text{statement}}$

For the calculation of $\det(B)$, again the Laplace expansion is used to reduce the determinant to lower dimensions. At some points the determinants d_M from (78) will appear, which will then lead to an analytic expression.

$$\underline{\det(B)} = \det_M\begin{pmatrix} 2a & -1 & 0 & \dots & 0 & -1 \\ \hline -1 & 2a & -1 & \dots & 0 & 0 \\ \hline 0 & -1 & 2a & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2a & -1 \\ \hline -1 & 0 & 0 & \dots & -1 & 2a \end{pmatrix} =$$

$$= 2ad_{M-1} + \det_{M-1}\begin{pmatrix} -1 & 0 & \dots & 0 & -1 \\ \hline -1 & 2a & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 2a & -1 \\ 0 & 0 & \dots & -1 & 2a \end{pmatrix} -$$

$$-(-1)^{M+1}\det_{M-1}\begin{pmatrix} -1 & 0 & \dots & 0 & -1 \\ \hline 2a & -1 & \dots & 0 & 0 \\ -1 & 2a & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 2a & -1 \end{pmatrix} =$$

$$= 2ad_{M-1} + \left(-d_{M-2} - (-1)^M(-1)^{M-2}\right) + (-1)^M\left(-(-1)^{M-2} - (-1)^M d_{M-2}\right) =$$
$$= \underline{2ad_{M-1} - 2d_{M-2} - 2}$$

At this point, $\det(B)$ is reduced to the determinants of (78), which gives immediatly the analytic expression

$$\begin{aligned}
\underline{\underline{\det(B)}} &= 2a\tfrac{1}{2(\omega-a)}\left(\omega^M - \tfrac{1}{\omega^M}\right) - 2\tfrac{1}{2(\omega-a)}\left(\omega^{M-1} - \tfrac{1}{\omega^{M-1}}\right) - 2 = \\
&= \tfrac{1}{\omega-a}\left((a\omega-1)\omega^{M-1} - (a-\omega)\omega^{-M}\right) - 2 = \\
&= \left(\omega^M + \omega^{-M}\right) - 2 = \\
&= \underline{\underline{(\omega^M - 1)(1-\omega^{-M})}}\ ,
\end{aligned}$$

where at some point the identity $a\omega - 1 = \omega^2 - a\omega$ from above was used.

The last step is the calculation of the inverse matrix B^{-1}. This will be done by calculating the determinants of the matrices $B^{(i,j)}$ (which is the matrix B without the i-th row and the j-th column).

To make notation easier, every index should be understood modulo M from now on.

Because $\forall i \in \mathbb{N}, k \in \mathbb{N}_0 : B_{i+k,i} = B_{1+k,1}$ is true, this has to be true also for the inverse matrix.

$$\forall i \in \mathbb{N}, k \in \mathbb{N}_0 : B^{-1}_{i+k,i} = B^{-1}_{1+k,1} \tag{79}$$

So it is sufficient to calculate only the elements of the first column $B^{-1}_{k,1}$ of the inverse matrix.
This determinant can also be represented in terms of the determinants d_M and has according to (78) the following analytic expression.

$$\underline{\underline{\det(B^{(k,1)})}} = \det\nolimits_{M-1}\left(\begin{array}{c|cccc|c|cccc|cc}
-1 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 & -1 & {\scriptstyle 1} \\ \hline
2a & -1 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 & 0 & {\scriptstyle 2} \\
-1 & 2a & -1 & \dots & 0 & 0 & 0 & 0 & \dots & 0 & 0 & \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \\
0 & 0 & 0 & \dots & -1 & 0 & 0 & 0 & \dots & 0 & 0 & \\
0 & 0 & 0 & \dots & 2a & -1 & 0 & 0 & \dots & 0 & 0 & {\scriptstyle k-1} \\ \hline
0 & 0 & 0 & \dots & 0 & -1 & 2a & -1 & \dots & 0 & 0 & {\scriptstyle k} \\
0 & 0 & 0 & \dots & 0 & 0 & -1 & 2a & \dots & 0 & 0 & \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \\
0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 2a & -1 & \\
0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & -1 & 2a & {\scriptstyle M-1}
\end{array}\right) =$$

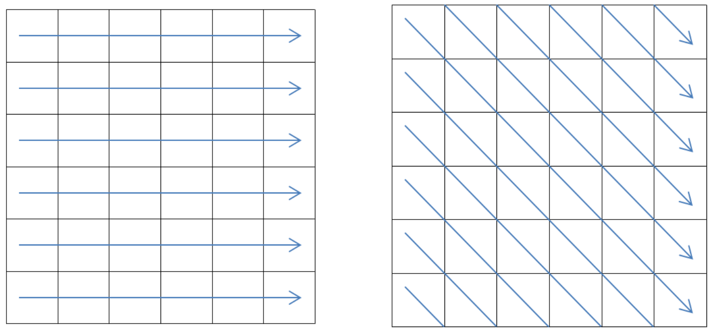
$$\begin{aligned}
&= -(-1)^{k-2}d_{M-k} - (-1)^M d_{k-2}(-1)^{M-k} = \\
&= \tfrac{(-1)^{k-1}}{2(\omega-a)}\left(\left(\omega^{M-k+1} - \omega^{-M+k-1}\right) + \left(\omega^{k-1} - \omega^{-k+1}\right)\right) = \\
&= \underline{\underline{\tfrac{(-1)^{k-1}(\omega^M - 1)}{2(\omega-a)} R_{k-1}}}
\end{aligned}$$

Where in the last line the definition $R_n = \omega^{-n} + \omega^{-M+n}$ of (75) was used.

Putting all parts together, gives tho following expression for the exponent.

$$\frac{1}{2}\vec{b}^T(A+A^T)^{-1}\vec{b} = \frac{1}{2}\sum_{i,k=1}^{M} b_i B^{-1}_{i,k} b_k$$

In this formula, for every fixed row i the sum over k is taken over every column. Instead of this, one also can sum over the diagonal elements $(i+k-1,k)$. This principle is shown in the following figure.



Rearranging the sum this way, leads to the result

$$\frac{1}{2}\vec{b}^T(A+A^T)^{-1}\vec{b} = \frac{1}{2}\sum_{i,k=1}^{M} b_{i+k-1}B^{-1}_{i+k-1,k}b_k \ ,$$

which is favourable, because the elements of B^{-1} on every diagonal are the same.

$$\frac{1}{2}\vec{b}^T(A+A^T)^{-1}\vec{b} = \frac{1}{2}\sum_{i=1}^{M} B^{-1}_{i,1}\sum_{k=1}^{M} b_{i+k-1}b_k$$

The elements of the inverse matrix were calculated above and are given by $B^{-1}_{i,1} = (-1)^{i+1}\frac{\det(B^{(i,1)})}{\det(B)}$.

$$\frac{1}{2}\vec{b}^T(A+A^T)^{-1}\vec{b} = \frac{1}{4\sqrt{a^2-1}(1-\omega^{-M})}\sum_{i=1}^{M} R_{i-1}\sum_{k=1}^{M} b_{i+k-1}b_k \tag{80}$$

Where also the definition $\omega = a+\sqrt{a^2-1}$ was used.

With the property $R_{M-n} = R_n$, the sum on the right hand side can be simplified even further.

$$\underline{\sum_{i=1}^{M} R_{i-1}\sum_{k=1}^{M} b_{i+k-1}b_k} = \sum_{k=1}^{M} b_k\left(\sum_{i=1}^{M-k+1} R_{i-1}b_{i+k-1} + \sum_{i=M-k+2}^{M} R_{i-1}b_{i+k-1}\right) =$$
$$= \sum_{k=1}^{M} b_k\left(\sum_{j=k}^{M} R_{j-k}b_j + \sum_{j=1}^{k-1} R_{j+M-k}b_{j+M}\right) =$$
$$= \underline{\sum_{k=1}^{M}\sum_{j=k}^{M} b_kR_{|k-j|}b_j}$$

This sum together with (80) and (76) gives the analytic expression of the integral.

$$I = \sqrt{\frac{(2\pi)^M}{(\omega^M-1)(1-\omega^{-M})}}\exp\left(\frac{1}{4(1-\omega^{-M})\sqrt{a^2-1}}\sum_{j,k=1}^{M} b_kR_{|k-j|}b_h\right) \qquad \blacksquare$$

This expression (75) was the main result of this section. Except of the matrix R, it consists out of simple objects. To do some calculations with the matrix R later on, some properties will be useful.

The sum over all columns is the same for every row.

$$\boxed{R\vec{1} = \sqrt{\frac{a+1}{a-1}}\left(1-\omega^{-M}\right)\vec{1}} \tag{81}$$

Proof:

Let $i \in \{1,\ldots,M\}$, then

$$(R\vec{1})_i = \sum_{j=1}^{M} \left(\omega^{-|i-j|} + \omega^{-M+|i-j|}\right) =$$
$$= \omega^{-i} \sum_{j=1}^{i-1} \omega^j + \omega^{-M+i} \sum_{j=1}^{i-1} \left(\tfrac{1}{\omega}\right)^j + \omega^i \sum_{j=i}^{M} \left(\tfrac{1}{\omega}\right)^j + \omega^{-M-i} \sum_{j=i}^{M} \omega^j$$

Applying the formula for the geometric sum $\sum_{k=a}^{b} q^k = \frac{q^a - q^{b+1}}{1-q}$ gives

$$\underline{(R\vec{1})_i} = \omega^{-i} \frac{\omega - \omega^i}{1-\omega} + \omega^{-M+i} \frac{\frac{1}{\omega} - \left(\frac{1}{\omega}\right)^i}{1 - \frac{1}{\omega}} + \omega^i \frac{\left(\frac{1}{\omega}\right)^i - \left(\frac{1}{\omega}\right)^{M+1}}{1 - \frac{1}{\omega}} + \omega^{-M-i} \frac{\omega^i - \omega^{M+1}}{1-\omega} =$$
$$= \frac{1}{1-\omega}(\omega^{-M} - 1) + \frac{\omega}{\omega - 1}(1 - \omega^{-M}) =$$
$$= \underline{\frac{\omega+1}{\omega-1}(1 - \omega^{-M})}$$

The prefactor $\frac{\omega+1}{\omega-1}$ can, due to the definition, be rewritten in terms of a, which will complete the proof.

$$\underline{\underline{\frac{w+1}{w-1}}} = \frac{a + \sqrt{a^2-1} + 1}{a + \sqrt{a^2-1} - 1} = \frac{\sqrt{a+1}(\sqrt{a+1} + \sqrt{a-1})}{\sqrt{a-1}(\sqrt{a-1} + \sqrt{a+1})} = \underline{\underline{\sqrt{\frac{a+1}{a-1}}}} \qquad \blacksquare$$

For applications in this work, the vector $\vec{b}$ in (75) will have the special form $\vec{b} = \vec{v} + \vec{1}$. With the help of (81) a simplified version of the product $\vec{b}^T R \vec{b}$ can be calculated.

$$\boxed{(\vec{v} + \vec{1})^T R (\vec{v} + \vec{1}) = \vec{v}^T R \vec{v} + \sqrt{\frac{a+1}{a-1}} (1 - \omega^{-M}) \left(2|\vec{v}| + M\right)} \tag{82}$$

Where $\underline{|\vec{v}| = \sum_{j=1}^{M} v_j}$ means the sum over all elements.

Proof:

$$\underline{\underline{(\vec{v} + \vec{1})^T R (\vec{v} + \vec{1})}} = \vec{v}^T R \vec{v} + \left(\vec{1}^T R \vec{v} + \vec{v}^T R \vec{1}\right) + \vec{1}^T R \vec{1} =$$
$$= \vec{v}^T R \vec{v} + \left(2\vec{v}^T + \vec{1}^T\right) \sqrt{\tfrac{a+1}{a-1}} (1 - \omega^{-M}) \vec{1}$$
$$= \underline{\underline{\vec{v}^T R \vec{v} + (2|\vec{v}| + M) \sqrt{\tfrac{a+1}{a-1}} (1 - \omega^{-M})}} \qquad \blacksquare$$

The formulas (82) and (75) combined now give an analytic expression of the integral with the special choice of the vector $\vec{b} = \vec{y} + y\vec{1}$.

$$\boxed{\int_{\mathbb{R}^M} e^{\sum_{j=1}^{M} ((v_j + y) x_j - a x_j^2 + x_j x_{j+1})} d\vec{x} = \sqrt{\frac{(2\pi)^M}{(1 - \omega^{-M})(\omega^M - 1)}} \exp\left(\frac{\vec{v}^T R \vec{v}}{4(1 - \omega^{-M})\sqrt{a^2-1}} + \frac{y(2|\vec{v}| + My)}{4(a-1)}\right)} \tag{83}$$

A.3 Calculating the integral II

In section A.2 the Gaussian integral is done by inverting matrices. Because of the constant coefficients a and 1 in front of the quadratic terms and the coupling of only nearest neighbors (including periodic boundaries), the exponent should be diagonal in Fourier space. So with the help of Fourier transformation another representation of the integral (75) is found.

$$\boxed{\int_{\mathbb{R}^M} e^{\sum_{j=1}^{M} \left(b_j x_j - a x_j^2 + x_j x_{j+1}\right)} d\vec{x} = \sqrt{\frac{(2\pi)^M}{(\omega^M - 1)(1 - \omega^{-M})}} \exp\left(\frac{M}{4} \sum_{k=1}^{M} \frac{|\tilde{b}_k|^2}{1 - \cos\left(2\pi \frac{k}{M}\right)}\right)} \tag{84}$$

with arbitrary coefficients
- $a > 1, (b_j)_{j=1}^{M} \in \mathbb{R}$
- $\omega = a + \sqrt{a^2 - 1}$
- $\tilde{b}_k = \frac{1}{M} \sum_{j=1}^{M} e^{2\pi i \frac{jk}{M}} b_j$

Proof:

Applying the Fourier transformation means, doing an integral transformation with the Fourier transformed variables $(\tilde{x}_k)_{k=1}^M$, defined as follows.

$$\forall k \in \{1,\ldots,M\} : \underline{\tilde{x}_k = \frac{1}{M}\sum_{j=1}^{M} e^{-2\pi i \frac{jk}{M}} x_j} \Rightarrow \forall j \in \{1,\ldots,M\} : \underline{x_j = \sum_{k=1}^{M} e^{2\pi i \frac{jk}{M}} \tilde{x}_k}$$

These variables have the properties:

- $$\underline{\forall k \in \{1,\ldots,M-1\}} : \underline{\tilde{x}_{M-k}} = \frac{1}{M}\sum_{j=1}^{M} e^{-2\pi i \frac{j(M-k)}{M}} x_j = \frac{1}{M}\sum_{j=1}^{M} e^{2\pi i \frac{jk}{M}} x_j = \underline{\tilde{x}_k^*} \qquad (85)$$
- $\underline{\tilde{x}_M} = \frac{1}{M}\sum_{j=1}^{M} x_j \in \underline{\mathbb{R}}$

The exponent can now be written in terms of the new variables and one sees that it becomes diagonal.

- $$\underline{\sum_{j=1}^{M} b_j x_j} = \sum_{j=1}^{M} b_j \sum_{k=1}^{M} e^{2\pi i \frac{jk}{M}} \tilde{x}_k = \underline{M \sum_{k=1}^{M} \tilde{x}_k \tilde{b}_k}$$
- $$\begin{aligned} \underline{\sum_{j=1}^{M} x_j^2} &= \sum_{k=1}^{M}\sum_{l=1}^{M} \tilde{x}_k \tilde{x}_l \sum_{j=1}^{M} e^{2\pi i \frac{j(k+l)}{M}} = \\ &= \sum_{k=1}^{M}\sum_{l=1}^{M} \tilde{x}_k \tilde{x}_l M \left(\delta_{k+l,M} + \delta_{k+l,2M}\right) = \\ &= \underline{M \sum_{k=1}^{M} |\tilde{x}_k|^2} \end{aligned}$$
- $$\begin{aligned} \underline{\sum_{j=1}^{M} x_j x_{j+1}} &= \sum_{j=1}^{M-1} \left(\sum_{k=1}^{M} e^{2\pi i \frac{jk}{M}} \tilde{x}_k\right)\left(\sum_{l=1}^{M} e^{2\pi i \frac{(j+1)l}{M}} \tilde{x}_l\right) + \left(\sum_{k=1}^{M} e^{2\pi i \frac{Mk}{M}} \tilde{x}_k\right)\left(\sum_{l=1}^{M} e^{2\pi i \frac{l}{M}} \tilde{x}_l\right) = \\ &= \sum_{k=1}^{M}\sum_{l=1}^{M} \tilde{x}_k \tilde{x}_l e^{2\pi i \frac{l}{M}} M \left(\delta_{l+k,M} + \delta_{l+k,2M}\right) = \\ &= \underline{M \sum_{k=1}^{M} |\tilde{x}_k|^2 e^{-2\pi i \frac{k}{M}}} \end{aligned}$$

Because the initial integral had M independent realvalued variables $(x_j)_{j=1}^M$, the complex variables $(\tilde{x}_k)_{k=1}^M$ have to reduce to M independent real variables as well.
To get the M independent variables of $(\tilde{x}_k)_{k=1}^M$ one has to distinguish between M odd or even. Because the calculations in these two cases are the same, only the odd case is presented here.

Because of the properties (85), the variables $(\tilde{x}_k)_{k=1}^M$ can be expressed in terms of the following M realvalued variables $(u_k)_{k=0}^{\frac{M-1}{2}}$ and $(v_k)_{k=1}^{\frac{M-1}{2}}$.

$$\begin{aligned} \Rightarrow\ & \tilde{x}_1 = u_1 + i v_1 \\ & \vdots \\ & \tilde{x}_{\frac{M-1}{2}} = u_{\frac{M-1}{2}} + i v_{\frac{M-1}{2}} \\ & \tilde{x}_{\frac{M+1}{2}} = u_{\frac{M-1}{2}} - i v_{\frac{M-1}{2}} \\ & \vdots \\ & \tilde{x}_{M-1} = u_1 - i v_1 \\ & \underline{\tilde{x}_M = u_0} \end{aligned}$$

The transformation in this variables looks like

$$\underline{\forall j \in \{1,\dots,M\}} : \underline{x_j} = \sum_{k=1}^{\frac{M-1}{2}} e^{2\pi i \frac{jk}{M}}(u_k + iv_k) + \sum_{k=\frac{M+1}{2}}^{M-1} e^{2\pi i \frac{jk}{M}}(u_{M-k} - iv_{M-k}) + u_0 =$$
$$= \sum_{k=1}^{\frac{M-1}{2}} e^{2\pi i \frac{jk}{M}}(u_k + iv_k) + \sum_{k=1}^{\frac{M-1}{2}} e^{-2\pi i \frac{jk}{M}}(u_k - iv_k) + u_0 =$$
$$= \underline{u_0 + 2\sum_{k=1}^{\frac{M-1}{2}} \left(u_k \cos\left(2\pi \frac{jk}{M}\right) - v_k \sin\left(2\pi \frac{jk}{M}\right)\right)}\ .$$

To apply the integral substitution, the integrand has to be written in terms of the new variables $(u_k)_{k=0}^{\frac{M-1}{2}}$, $(v_k)_{k=1}^{\frac{M-1}{2}}$ and the determinant of the jacobian $\frac{d\vec{x}}{d(\vec{u},\vec{v})}$ has to be calculated.

- $$\underline{\sum_{j=1}^{M} b_j x_j} = M\left(\sum_{k=1}^{\frac{M-1}{2}} (u_k + iv_k)\tilde{b}_k + \sum_{k=\frac{M+1}{2}}^{M-1} (u_{M-k} - iv_{M-k})\tilde{b}_k + u_0\tilde{b}_M\right) =$$
$$= M\left(\sum_{k=1}^{\frac{M-1}{2}} (u_k + iv_k)\tilde{b}_k + \sum_{k=1}^{\frac{M-1}{2}} (u_k - iv_k)\tilde{b}_k^* + u_0\tilde{b}_M\right) =$$
$$= \underline{M\left(u_0\tilde{b}_M + 2\sum_{k=1}^{\frac{M-1}{2}} \left(u_k \mathrm{Re}(\tilde{b}_k) - v_k \mathrm{Im}(\tilde{b}_k)\right)\right)}$$

- $$\underline{\sum_{j=1}^{M} x_j^2} = M\sum_{k=1}^{M} |\tilde{x}_k|^2 = \underline{M\left(u_0^2 + 2\sum_{k=1}^{\frac{M-1}{2}} (u_k^2 + v_k^2)\right)}$$

- $$\underline{\sum_{j=1}^{M} x_j x_{j+1}} = M\left(\sum_{k=1}^{\frac{M-1}{2}} (u_k^2 + v_k^2)e^{-2\pi i \frac{k}{M}} + \sum_{k=\frac{M+1}{2}}^{M-1} (u_{M-k}^2 + v_{M-k}^2)e^{-2\pi i \frac{k}{M}} + u_0^2\right) =$$
$$= M\left(\sum_{k=1}^{\frac{M-1}{2}} (u_k^2 + v_k^2)e^{-2\pi i \frac{k}{M}} + \sum_{k=1}^{\frac{M-1}{2}} (u_k^2 + v_k^2)e^{2\pi i \frac{k}{M}} + u_0^2\right) =$$
$$= \underline{M\left(u_0^2 + 2\sum_{k=1}^{\frac{M-1}{2}} (u_k^2 + v_k^2)\cos\left(2\pi \frac{k}{M}\right)\right)}$$

- $$\underline{\left|\det\left(\frac{d\vec{x}}{d(\vec{u},\vec{v})}\right)\right| = 2^{\frac{M-1}{2}} M^{\frac{M}{2}}}$$

The integral in the new variables $(u_k)_{k=0}^{\frac{M-1}{2}}, (v_k)_{k=1}^{\frac{M-1}{2}}$ has then the form stated in (84.

$$\underline{\underline{I}} = 2^{\frac{M-1}{2}} M^{\frac{M}{2}} \int_{\mathbb{R}} e^{M\tilde{b}_M u_0 - M(a-1)u_0^2} du_0 \cdot$$
$$\cdot \prod_{k=1}^{\frac{M-1}{2}} \left(\int_{\mathbb{R}} e^{2M\mathrm{Re}(\tilde{b}_k)u_k - 2M\left(a-\cos\left(2\pi \frac{k}{M}\right)\right)u_k^2} du_k \int_{\mathbb{R}} e^{-2M\mathrm{Im}(\tilde{b}_k)v_k - 2M\left(a-\cos\left(2\pi \frac{k}{M}\right)\right)v_k^2} dv_k\right) =$$
$$= 2^{\frac{M-1}{2}} M^{\frac{M}{2}} \sqrt{\frac{\pi}{M(a-1)}} e^{\frac{M^2\tilde{b}_M^2}{4M(a-1)}} \cdot$$
$$\cdot \prod_{k=1}^{\frac{M-1}{2}} \left(\sqrt{\frac{\pi}{2M\left(a-\cos\left(2\pi\frac{k}{M}\right)\right)}} e^{\frac{4M^2\mathrm{Re}(\tilde{b}_k)^2}{8M\left(a-\cos\left(2\pi\frac{k}{M}\right)\right)}} \sqrt{\frac{\pi}{2M\left(a-\cos\left(2\pi\frac{k}{M}\right)\right)}} e^{\frac{4M^2\mathrm{Im}(\tilde{b}_k)^2}{8M\left(a-\cos\left(2\pi\frac{k}{M}\right)\right)}}\right) =$$
$$= \frac{\pi^{\frac{M}{2}}}{\sqrt{a-1}} e^{\frac{M\tilde{b}_M^2}{4(a-1)}} \prod_{k=1}^{\frac{M-1}{2}} \left(\frac{1}{a-\cos(2\pi\frac{k}{M})} e^{\frac{M|\tilde{b}_k|^2}{2\left(a-\cos\left(2\pi\frac{k}{M}\right)\right)}}\right) =$$
$$= \frac{\pi^{\frac{M}{2}}}{\sqrt{a-1}} e^{\frac{M\tilde{b}_M^2}{4(a-1)}} \prod_{k=1}^{M-1} \left(\frac{1}{\sqrt{a-\cos\left(2\pi\frac{k}{M}\right)}} e^{\frac{M|\tilde{b}_k|^2}{4\left(a-\cos(2\pi\frac{k}{M})\right)}}\right) =$$
$$= \underline{\underline{\pi^{\frac{M}{2}} \prod_{k=1}^{M} \left(\frac{1}{\sqrt{a-\cos(2\pi\frac{k}{M})}} e^{\frac{M|\tilde{b}_k|^2}{4\left(a-\cos\left(2\pi\frac{k}{M}\right)\right)}}\right)}}$$

The last step is to simplify the prefactor.
Comparing this result with (75) for $\vec{b} = \vec{0}$, one can identify the two prefactors and get the solution (84).

$\frac{2^M}{(\omega^M-1)(1-\omega^{-M})} = \prod_{k=1}^{M} \frac{1}{a-\cos\left(2\pi\frac{k}{M}\right)}$ ■

Similar to (82), also in this representation of the Fourier integral, the special case $\vec{b} = \vec{v} + y\vec{1}$ is considered.

$$\int_{\mathbb{R}^M} e^{\sum_{j=1}^{M}\left((y+v_j)x_j - ax_j^2 + x_j x_{j+1}\right)} d\vec{x} = \sqrt{\frac{(2\pi)^M}{(\omega^M-1)(1-\omega^{-M})}}\, e^{\frac{My^2}{4(a-1)} + \frac{My\tilde{v}_M}{2(a-1)} + \frac{M}{4}\sum_{k=1}^{M}\frac{|\tilde{v}_k|^2}{a-\cos\left(2\pi\frac{k}{M}\right)}} \tag{86}$$

with $\tilde{v}_k = \frac{1}{M}\sum_{j=1}^{M} e^{2\pi i \frac{jk}{M}} v_j$

Proof:

The only thing to do is calculating the Fourier transformed $\tilde{b}_k$.

$$\tilde{b}_k = \frac{1}{M}\sum_{j=1}^{M} e^{2\pi i\frac{jk}{M}}(y+v_j) = y\delta_{k,M} + \tilde{v}_k$$

Using this in (84) gives the expression for the integral.

$$\underline{\underline{I}} = \sqrt{\frac{(2\pi)^M}{(\omega^M-1)(1-\omega^{-M})}}\, e^{\frac{M}{4}\sum_{k=1}^{M}\frac{|y\delta_{k,M}+\tilde{v}_k|^2}{a-\cos\left(2\pi\frac{k}{M}\right)}} =$$
$$= \sqrt{\frac{(2\pi)^M}{(\omega^M-1)(1-\omega^{-M})}}\, e^{\frac{My^2}{4(a-1)} + \frac{My\tilde{v}_M}{2(a-1)} + \frac{M}{4}\sum_{k=1}^{M}\frac{|\tilde{v}_k|^2}{a-\cos\left(2\pi\frac{k}{M}\right)}} \quad ■$$

A.4 Integrating out the phonons without HS transformation

In chapter 5, the Continuous HS transformation was applied in order to rewrite the electron trace as a determinant. After that, the phonon trace was integrated analytically. Now, with the in principle same calculation, one can solve the phonon trace also without HS transformation.
Like in chapter 5, also here, the partition function will be calculated in the more general form with finitely many timeslices $\Delta\tau$. However, in A.4.2 the limit $\Delta\tau \to 0$ is done, to make sure that this form is indeed a generalisation of the commonly used continuum limit [16, 17].

A.4.1 Partition function for arbitrary timeslices

In the proof of (58), the HS transformation led to an additional $\frac{\Delta\tau\alpha^2}{2U}x_i^2$ term in the partition function. This term was carried through the whole calculation, until in the end the term appeared in the parameter a of (59).
By integrating out the phonon trace without HS transformation, this factor never appears and also the parameter $\tilde{a}$ does not contain this additional factor $\frac{\Delta\tau\alpha^2}{2U}$.
The disadvantage is, that after the phonon trace is integrated, the number operators $n_i^{(j)}$ of different timeslices are coupled to each other and it is no longer possible to apply a HS transformation and write the electron trace as a determinant.

$$Z = \left(\frac{1}{(\tilde{\Omega}^M-1)(1-\tilde{\Omega}^{-M})}\right)^{\frac{N}{2}} \sum_{\vec{n}^{(1)},\ldots,\vec{n}^{(M)}} \prod_{j=1}^{M} \left\langle \vec{n}^{(j)}\right| e^{-\Delta\tau H_e} \left|\vec{n}^{(j+1)}\right\rangle \cdot$$
$$\cdot e^{\frac{\alpha^2\Delta\tau^2}{4\omega(1-\tilde{\Omega}^{-M})\sqrt{\frac{\Delta\tau^2\omega^2}{4}+1}}\sum_{i=1}^{N}\sum_{j,k=1}^{M} n_i^{(k)}\tilde{R}_{|k-j|}n_i^{(j)}} \tag{87}$$

with $\tilde{a} = \frac{\Delta\tau^2\omega^2}{2} + 1$
$\tilde{\Omega} = \tilde{a} + \sqrt{\tilde{a}^2 - 1}$
$\underline{\tilde{R}_n = \tilde{\Omega}^{-n} + \tilde{\Omega}^{-M+n}}$

Proof:

The Hamiltonian of the Hubbard-Holstein model is given by (55)

$$\underline{H = H_e + \sum_{i=1}^{N} \left(-\alpha x_i(n_{i\uparrow} + n_{i\downarrow}) + \frac{p_i^2}{2} + \frac{\omega^2}{2}x_i^2\right)}$$

with $H_e = H_{\text{kin}} + H_{\text{cou}} + H_\mu$ acting only on the electronic part of the state and will be not of great interest in this proof.

The electron, as well as the phonon trace of the partition function, can now be written as a sum or integral, and the Trotter decomposition can be applied in order to split up the momentum part of the Hamiltonian.

$$Z = \sum_{\vec{n}^{(1)}} \int_{\mathbb{R}^N} \left\langle \vec{n}^{(1)}, \vec{x}^{(1)} \right| \left(e^{-\Delta\tau H_e} e^{-\Delta\tau\left(\frac{\omega^2}{2}\vec{x}^2 - \alpha\langle\vec{x},\vec{n}\rangle\right)} e^{-\Delta\tau\frac{\vec{p}^2}{2}} \right)^M \left| \vec{n}^{(1)}, \vec{x}^{(1)} \right\rangle d\vec{x}^{(1)}$$

Between every of the M timeslices the identity operator $\sum_{\vec{n}} \int_{\mathbb{R}^N} |\vec{n}, \vec{x}\rangle \langle\vec{n}, \vec{x}| \, d\vec{x}$ can be inserted, to get to the form.

$$Z = \sum_{\vec{n}^{(1)},\ldots,\vec{n}^{(M)}} \int_{\mathbb{R}^{N\times M}} \prod_{j=1}^{M} \left(\left\langle \vec{n}^{(j)} \right| e^{-\Delta\tau H_e} \left| \vec{n}^{(j+1)} \right\rangle e^{-\Delta\tau\left(\frac{\omega^2}{2}\vec{x}^{(j)2} - \alpha\langle\vec{x}^{(j)},\vec{n}^{(j+1)}\rangle\right)} \left\langle \vec{x}^{(j)} \right| e^{-\Delta\tau\frac{\vec{p}^2}{2}} \left| \vec{x}^{(j+1)} \right\rangle \right) d\vec{x}$$

In (61) the matrix elements $\langle\vec{x}| \, e^{-\Delta\tau\frac{\vec{p}}{2}} \, |\vec{y}\rangle = \left(\frac{1}{2\pi\Delta\tau}\right)^{\frac{N}{2}} e^{-\frac{(\vec{x}-\vec{y})^2}{2\Delta\tau}}$ were calculated and can be used here as well.

$$\begin{aligned} Z = \left(\tfrac{1}{2\pi\Delta\tau}\right)^{\frac{NM}{2}} & \sum_{\vec{n}^{(1)},\ldots,\vec{n}^{(M)}} \prod_{j=1}^{M} \left\langle \vec{n}^{(j)} \right| e^{-\Delta\tau H_e} \left| \vec{n}^{(j+1)} \right\rangle \cdot \\ & \cdot \int_{\mathbb{R}^{N\times M}} \prod_{j=1}^{M} \left(e^{-\Delta\tau\left(\frac{\omega^2}{2}\vec{x}^{(j)2} - \alpha\langle\vec{x}^{(j)},\vec{n}^{(j+1)}\rangle\right)} e^{-\frac{\left(\vec{x}^{(j)}-\vec{x}^{(j+1)}\right)^2}{2\Delta\tau}} \right) d\vec{x} = \\ = \left(\tfrac{1}{2\pi}\right)^{\frac{NM}{2}} & \sum_{\vec{n}^{(1)},\ldots,\vec{n}^{(M)}} \prod_{j=1}^{M} \left\langle \vec{n}^{(j)} \right| e^{-\Delta\tau H_e} \left| \vec{n}^{(j+1)} \right\rangle \cdot \\ & \cdot \prod_{i=1}^{N} \int_{\mathbb{R}^M} e^{\sum_{j=1}^{M} \left(\alpha\Delta\tau^{\frac{3}{2}} x^{(j)} n_i^{(j+1)} - \left(\frac{\Delta\tau^2\omega^2}{2}+1\right) x^{(j)2} + x^{(j)} x^{(j+1)}\right)} d\vec{x} \end{aligned}$$

Where in the last equation the substitution $\vec{x} \to \sqrt{\Delta\tau}\vec{x}$ was applied.

The partition function is now in a form to apply the analytic expression of the multi-dimensional Gaussian integral (75), which leads to the final form.

$$\begin{aligned} \underline{\underline{Z}} = \left(\frac{1}{(\tilde{\Omega}^M - 1)(1 - \tilde{\Omega}^{-M})}\right)^{\frac{N}{2}} & \sum_{\vec{n}^{(1)},\ldots,\vec{n}^{(M)}} \prod_{j=1}^{M} \left\langle \vec{n}^{(j)} \right| e^{-\Delta\tau H_e} \left| \vec{n}^{(j+1)} \right\rangle \cdot \\ & \underline{\underline{\cdot \prod_{i=1}^{N} e^{\frac{\alpha^2\Delta\tau^3}{4(1-\tilde{\Omega}^{-M})\sqrt{\tilde{a}^2-1}} \sum_{j,k=1}^{M} n_i^{(k)} \tilde{R}_{|k-j|} n_i^{(j)}}}} \qquad \blacksquare \end{aligned}$$

A.4.2 Partition function in the continuum limit

In (87) the partition function is given for an arbitrary number of timeslices M. The only error in this transformation is the Trotter error, which vanishes in the limit $\Delta\tau \to 0$. For this reason and to compare the formula with given results, this continuum limit is done in this section.

To do so, the main part is to expand all the main $\Delta\tau$-depending paramters of (87).

- $\underline{\sqrt{\tilde{a}^2-1}} = \sqrt{\left(\frac{\Delta\tau^2\omega^2}{2}+1\right)^2-1} =$
  $= \Delta\tau\omega\sqrt{\frac{\Delta\tau^2\omega^2}{4}+1} =$
  $= \underline{\Delta\tau\omega + \mathcal{O}(\Delta\tau^3)}$

- $\underline{\tilde{\Omega}} = \tilde{a} + \sqrt{\tilde{a}^2-1} =$
  $= \frac{\Delta\tau^2\omega^2}{2} + 1 + \Delta\tau\omega + \mathcal{O}(\Delta\tau^3) =$
  $= \underline{e^{\Delta\tau\omega} + \mathcal{O}(\Delta\tau^3)}$

- $\underline{\tilde{R}_n} = \tilde{\Omega}^{-n} + \tilde{\Omega}^{-M+n} = \underline{e^{-n\Delta\tau\omega} + e^{-\beta\omega}e^{n\Delta\tau\omega}}$

Thus, the continuum limit of the partition function (87) is given by

$$\underline{\underline{Z}} = \left(\frac{1}{2(\cosh(\beta\omega)-1)}\right)^{\frac{N}{2}} \sum_{\vec{n}^{(1)},\ldots,\vec{n}^{(M)}} \prod_{j=1}^{M} \left\langle \vec{n}^{(j)} \right| e^{-\Delta\tau H_e} \left| \vec{n}^{(j+1)} \right\rangle e^{\frac{\alpha^2}{4\omega(1-e^{-\beta\omega})} \sum_{i=1}^{N} \sum_{j,k=1}^{M} n_i^{(k)} R(|k-j|)\, n_i^{(j)} \Delta\tau^2} =$$

$$= \underline{\underline{\left(\frac{1}{2(\cosh(\beta\omega)-1)}\right)^{\frac{N}{2}} \sum_{\vec{n}^{(1)},\ldots,\vec{n}^{(M)}} \prod_{j=1}^{M} \left\langle \vec{n}^{(j)} \right| e^{-\Delta\tau H_e} \left| \vec{n}^{(j+1)} \right\rangle e^{\frac{\alpha^2}{4\omega(1-e^{-\beta\omega})} \sum_{i=1}^{N} \int_0^\beta \int_0^\beta n_i(\kappa) R(|\kappa-\tau|) n_i(\tau) d\kappa d\tau}}}$$

with $\underline{\underline{R(\tau) = e^{-\omega\tau} + e^{-\beta\omega}e^{\omega\tau}}}$

This formula can be compared with the solutions in [16, 17] for the same problem.
(87) is the generalisation for an arbitrary number of timeslices M, and the main formula applicable for numerical calculations.

A.5 Rewrite as Standard HS transformation

The Hubbard-Holstein model in the Continuous HS transformation (59) is a form, from witch the partition function can be theoretically calculated. But due to the fact that M has to be large to make the Trotter error small, the calculation of the $(N \times M)$-dimensional integral becomes very time consuming. The origin of this integral is the Continuous HS transformation (56).
The try is now, to undo the HS transformation again (i.e. integrating out the σ-integral) and get back to a form of a generalised Hubbard model with site-dependent parameters. The Standard HS transformation (23) could then be applied to this Hamiltonian and one had reduced the continuous integration over $\mathbb{R}^{N\times M}$ to a simple sum over $\{\pm 1\}^{N\times M}$.

For a shorter notation define $A = E + \frac{\alpha^2\Delta\tau^2}{2U(1-\Omega^{-M})\sqrt{a^2-1}} R$

$$\vec{b} = \frac{cU\omega^2}{U\omega^2-\alpha^2}\vec{1}$$

$$\underline{C = \left(\frac{e^{\frac{\beta U^2 c^2 \omega^2}{U\omega^2-\alpha^2}}}{\pi^M(\Omega^M-1)(1-\Omega^{-M})}\right)^{\frac{N}{2}}}$$ for this chapter

To undo the Continuous HS transformation, the determinant has to be rewritten as the electronic trace, see (69).

$$\underline{Z} = C \int_{\mathbb{R}^{N\times M}} e^{\sum_{i=1}^{N}\left(-\vec{\sigma}_i^T A\vec{\sigma}_i + \lambda\vec{b}^T\vec{\sigma}_i\right)} \mathrm{det}\left(E + \prod_{j=1}^{M}\left(e^{\lambda G^{(j)}} e^{t\Delta\tau h_{\text{kin}}}\right)\right)^2 d\sigma =$$

$$= \underline{C \int_{\mathbb{R}^{N\times M}} e^{\sum_{i=1}^{N}\left(-\vec{\sigma}_i^T A\vec{\sigma}_i + \lambda\vec{b}^T\vec{\sigma}_i\right)} \mathrm{tr}\left(\prod_{j=1}^{M}\left(\prod_{i=1}^{N} e^{\lambda\sigma_{ij}n_i}\right) e^{-\Delta\tau H_{\text{kin}}}\right) d\sigma}$$

The trace is still σ-dependent, this means, that it has to be pushed over the integral, to add the σ_{ij} to the exponent.

$$\underline{Z} = C \int_{\mathbb{R}^{N\times M}} e^{\sum_{i=1}^{N}\left(-\vec{\sigma}_i^T A\vec{\sigma}_i+\lambda\vec{b}^T\vec{\sigma}_i\right)} \sum_{\vec{n}^{(1)}} \left\langle \vec{n}^{(1)}\right| \prod_{j=1}^{M}\left(\prod_{i=1}^{N} e^{\lambda\sigma_{ij}n_i}\right) e^{-\Delta\tau H_{\text{kin}}} \left|\vec{n}^{(1)}\right\rangle d\sigma =$$

$$= C \int_{\mathbb{R}^{N\times M}} e^{\sum_{i=1}^{N}\left(-\vec{\sigma}_i^T A\vec{\sigma}_i+\lambda\vec{b}^T\vec{\sigma}_i\right)} \sum_{\vec{n}^{(1)},\ldots,\vec{n}^{(M)}} \prod_{j=1}^{M} \left\langle \vec{n}^{(j)}\right| \left(\prod_{i=1}^{N} e^{\lambda\sigma_{ij}n_i}\right) e^{-\Delta\tau H_{\text{kin}}} \left|\vec{n}^{(j+1)}\right\rangle d\sigma =$$

$$= \underline{C \sum_{\vec{n}^{(1)},\ldots,\vec{n}^{(M)}} \left(\prod_{i=1}^{N}\int_{\mathbb{R}^M} e^{-\vec{\sigma}^T A\vec{\sigma}+\lambda(\vec{b}+\vec{n}_i)^T\vec{\sigma}} d\sigma\right) \prod_{j=1}^{M} \left\langle \vec{n}^{(j)}\right| e^{-\Delta\tau H_{\text{kin}}} \left|\vec{n}^{(j+1)}\right\rangle}$$

Now the σ-integral can be done analytically, using the identity $\int_{\mathbb{R}^M} e^{-\vec{x}^T A\vec{x}+\vec{b}^T\vec{x}} d\vec{x} = \sqrt{\frac{\pi^M}{\det(A)}}\, e^{\frac{1}{4}\vec{b}^T A^{-1}\vec{b}}$.

$$\underline{Z} = C \sum_{\vec{n}^{(1)},\ldots,\vec{n}^{(M)}} \left(\prod_{i=1}^{N} e^{\frac{\lambda^2}{4}(\vec{b}+\vec{n}_i)^T A^{-1}(\vec{b}+\vec{n}_i)} \sqrt{\frac{\pi^M}{\det(A)}}\right) \prod_{j=1}^{M} \left\langle \vec{n}^{(j)}\right| e^{-\Delta\tau H_{\text{kin}}} \left|\vec{n}^{(j+1)}\right\rangle =$$

$$= C\left(\frac{\pi^M}{\det(A)}\right)^{\frac{N}{2}} \sum_{\vec{n}^{(1)},\ldots,\vec{n}^{(M)}} e^{\frac{\lambda^2}{4}\sum_{i=1}^{N}\left(\vec{b}^T A^{-1}\vec{b}+2\vec{b}^T A^{-1}\vec{n}_i+\vec{n}_i^T A^{-1}\vec{n}_i\right)} \prod_{j=1}^{M} \left\langle \vec{n}^{(j)}\right| e^{-\Delta\tau H_{\text{kin}}} \left|\vec{n}^{(j+1)}\right\rangle =$$

$$= \underline{C\left(\frac{\pi^M e^{\frac{\lambda^2}{2}\vec{b}^T A^{-1}\vec{b}}}{\det(A)}\right)^{\frac{N}{2}} \sum_{\vec{n}^{(1)},\ldots,\vec{n}^{(M)}} \prod_{j=1}^{M} \left(e^{\frac{\lambda^2}{4}\sum_{i=1}^{N}\left(2(\vec{b}^T A^{-1})_j n_i^{(j)} + \sum_{k=1}^{M} n_i^{(k)} A^{-1}_{kj} n_i^{(j)}\right)} \left\langle \vec{n}^{(j)}\right| e^{-\Delta\tau H_{\text{kin}}} \left|\vec{n}^{(j+1)}\right\rangle\right)}$$

To make further progress, $\left\langle \vec{n}^{(j)}\right|$ has to be carried over to the left of the exponential. But because there are the number operators of all timeslices $k \in \{1,\ldots,M\}$ in the way, and not only the one from timeslice j, this is not possible.
So the calculation stops at this point and it is not possible to end up with an effective Hubbard Hamiltonian for the Hubbard-Holstein model.

A.6 Special case: 1 site, U=0

For the $U = 0$ case of the partition function (64), the special case $N = 1$ is calculated exactly. This is possible, because there is only one site and the kinetic term vanishes. This makes the matrix inside determinant diagonal and so the determinant calculable.

$$\boxed{Z = \frac{1}{\sqrt{(\tilde{\Omega}^M - 1)(1-\tilde{\Omega}^{-M})}}\left(1+2e^{\beta\left(\frac{\alpha^2}{2\omega^2}-\mu\right)} + e^{2\beta\left(\frac{\alpha^2}{\omega^2}-\mu\right)}\right)} \qquad (88)$$

with $\tilde{a} = \frac{\Delta\tau^2\omega^2}{2} + 1$
$\underline{\tilde{\Omega} = \tilde{a} + \sqrt{\tilde{a}^2 - 1}}$

or in the limit $\Delta\tau \to 0$:

$$\boxed{Z = \frac{1}{\sqrt{2(\cosh(\beta\omega)-1)}}\left(1+2e^{\beta\left(\frac{\alpha^2}{2\omega^2}-\mu\right)} + e^{2\beta\left(\frac{\alpha^2}{\omega^2}-\mu\right)}\right)} \qquad (89)$$

Proof:

From (64) with $N = 1$ the partition function has the form.

$$Z = \frac{e^{-\frac{\beta\omega^2\mu^2}{2\alpha^2}}}{\pi^{\frac{M}{2}}\Delta\tau^M} \int_{\mathbb{R}^M} e^{\frac{1}{\Delta\tau^2}\vec{\sigma}^T\left(B-(\Delta\tau^2\omega^2+2)E\right)\vec{\sigma} - |\sigma|\frac{\sqrt{2\Delta\tau}\mu\omega^2}{\alpha}} \left(1+e^{\alpha\sqrt{2\Delta\tau}|\sigma|}\right)^2 d\sigma$$

With the transformation $\vec{\sigma} \to \frac{\Delta\tau}{\sqrt{2}}\vec{\sigma}$ and the definition of the matrix B, the partition function becomes

$$Z = \frac{e^{-\frac{\beta\omega^2\mu^2}{2\alpha^2}}}{(2\pi)^{\frac{M}{2}}} \int_{\mathbb{R}^M} e^{\sum_{j=1}^{M}\left(\sigma_j\sigma_{j+1} - (\frac{\Delta\tau^2\omega^2}{2}+1)\sigma_j^2 - \sigma_j\frac{\Delta\tau^{\frac{3}{2}}\mu\omega^2}{\alpha}\right)} \left(1+e^{\alpha\Delta\tau^{\frac{3}{2}}|\sigma|}\right)^2 d\sigma =$$

$$= \frac{e^{-\frac{\beta\omega^2\mu^2}{2\alpha^2}}}{(2\pi)^{\frac{M}{2}}} \left(\int_{\mathbb{R}^M} e^{\sum_{j=1}^{M}\left(\sigma_j\sigma_{j+1} - (\frac{\Delta\tau^2\omega^2}{2}+1)\sigma_j^2 - \sigma_j\frac{\Delta\tau^{\frac{3}{2}}\mu\omega^2}{\alpha}\right)} d\sigma + \right.$$

$$+2\int_{\mathbb{R}^M} e^{\sum_{j=1}^{M}\left(\sigma_j\sigma_{j+1}-(\frac{\Delta\tau^2\omega^2}{2}+1)\sigma_j^2+\sigma_j\Delta\tau^{\frac{3}{2}}\left(\alpha-\frac{\mu\omega^2}{\alpha}\right)\right)} d\sigma+ \int_{\mathbb{R}^M} e^{\sum_{j=1}^{M}\left(\sigma_j\sigma_{j+1}-(\frac{\Delta\tau^2\omega^2}{2}+1)\sigma_j^2+\sigma_j\Delta\tau^{\frac{3}{2}}(2\alpha-\frac{\mu\omega^2}{\alpha})\right)} d\sigma\Bigg) .$$

Now the integral is in a form to apply (83)
with $\vec{v}=\vec{0}$ and $y=-\Delta\tau^{\frac{3}{2}}\frac{\mu\omega^2}{\alpha}$ or $y=\Delta\tau^{\frac{3}{2}}\left(\alpha-\frac{\mu\omega^2}{\alpha}\right)$ or $y=\Delta\tau^{\frac{3}{2}}\left(2\alpha-\frac{\mu\omega^2}{\alpha}\right)$.

This gives the solution for an arbitrary number of time slices M.

$$\underline{\underline{Z}} = \frac{e^{-\frac{\beta\omega^2\mu^2}{2\alpha^2}}}{(2\pi)^{\frac{M}{2}}}\sqrt{\frac{(2\pi)^M}{(\tilde{\Omega}^M-1)(1-\tilde{\Omega}^{-M})}}\left(e^{\frac{M\Delta\tau^3\frac{\mu^2\omega^4}{\alpha^2}}{4(\tilde{a}-1)}}+2e^{\frac{M\Delta\tau^3\left(\alpha-\frac{\mu\omega^2}{\alpha}\right)^2}{4(\tilde{a}-1)}}+e^{\frac{M\Delta\tau^3\left(2\alpha-\frac{\mu\omega^2}{\alpha}\right)^2}{4(\tilde{a}-1)}}\right)=$$
$$=\frac{e^{-\frac{\beta\omega^2\mu^2}{2\alpha^2}}}{\sqrt{(\tilde{\Omega}^M-1)(1-\tilde{\Omega}^{-M})}}\left(e^{\frac{\beta\frac{\mu^2\omega^4}{\alpha^2}}{2\omega^2}}+2e^{\frac{\beta\left(\alpha-\frac{\mu\omega^2}{\alpha}\right)^2}{2\omega^2}}+e^{\frac{\beta\left(2\alpha-\frac{\mu\omega^2}{\alpha}\right)^2}{2\omega^2}}\right)=$$
$$=\underline{\underline{\frac{1}{\sqrt{(\tilde{\Omega}^M-1)(1-\tilde{\Omega}^{-M})}}\left(1+2e^{\beta\left(\frac{\alpha^2}{2\omega}-\mu\right)}+e^{2\beta\left(\frac{\alpha^2}{\omega^2}-\mu\right)}\right)}}$$

The only part that remains being $\Delta\tau$-dependent, is Ω. So, for the limit $\Delta\tau\to 0$, Ω has to be expanded.

$$\underline{\tilde{\Omega}} = \tilde{a}+\sqrt{\tilde{a}^2-1}$$
$$=\frac{\Delta\tau^2\omega^2}{2}+1+\Delta\tau\omega\sqrt{\frac{\Delta\tau^2\omega^2}{4}+1}= \qquad / \sqrt{1+x}=1+\mathcal{O}(x)$$
$$=\frac{\Delta\tau^2\omega^2}{2}+1+\Delta\tau\omega+\mathcal{O}(\Delta\tau^3)=$$
$$=\underline{e^{\Delta\tau\omega}+\mathcal{O}(\Delta\tau^3)}$$

Thus, the partition function it the limit $\Delta\tau\to 0$ becomes

$$\underline{\underline{Z}} = \frac{1}{\sqrt{(e^{\beta\omega}-1)(1-e^{-\beta\omega})}}\left(1+2e^{\beta\left(\frac{\alpha^2}{2\omega}-\mu\right)}+e^{2\beta\left(\frac{\alpha^2}{\omega^2}-\mu\right)}\right)=$$
$$=\underline{\underline{\frac{1}{\sqrt{2(\cosh(\beta\omega)-1)}}\left(1+2e^{\beta\left(\frac{\alpha^2}{2\omega}-\mu\right)}+e^{2\beta\left(\frac{\alpha^2}{\omega^2}-\mu\right)}\right)}} . \qquad \blacksquare$$

To compare this result with the exact result of the partition function, the trace is calculated directly from the definition $Z=\text{tr}\left(e^{-\beta H}\right)$, in the special case $U=0$, $N=1$. Because of $U=0$, the Coulomb term H_{cou} vanishes, and because of $N=1$, no hopping can take place and the kinetic term H_{kin} vanishes.

$$\underline{\underline{Z}} = \text{tr}\left(e^{-\beta\left((\mu-\alpha x)n+\frac{p^2}{2}+\frac{\omega^2x^2}{2}\right)}\right)=$$
$$=\sum_n\int_{\mathbb{R}}\langle n,x|\, e^{-\beta\left((\mu-\alpha x)n+\frac{p^2}{2}+\frac{\omega^2x^2}{2}\right)}\,|n,x\rangle=$$
$$=\sum_n e^{-\beta\mu n}\int_{\mathbb{R}}\langle x|\, e^{-\beta\left(-\alpha xn+\frac{p^2}{2}+\frac{\omega^2x^2}{2}\right)}\,|x\rangle=$$
$$=\underline{\sum_n e^{-\beta\left(\mu n-\frac{\alpha^2n^2}{2\omega^2}\right)}\int_{\mathbb{R}}\langle x|\, e^{-\beta\left(\frac{p^2}{2}+\frac{\omega^2x^2}{2}\right)}\,|x\rangle}$$

The integral now ist the standard partition function of a harmonic oscillator. It can be replaced by the sum over all eigenvalues $E_k=\omega(k+\frac{1}{2})$.

$$\underline{\underline{Z}} = \sum_n e^{-\beta\left(\mu n-\frac{\alpha^2n^2}{2\omega^2}\right)}\sum_{k=0}^{\infty}e^{-\beta\omega(k+\frac{1}{2})}=$$
$$=\sum_n e^{-\beta\left(\mu n-\frac{\alpha^2n^2}{2\omega^2}\right)}\frac{e^{-\beta\frac{\omega}{2}}}{1-e^{-\beta\omega}}=$$
$$=\underline{\underline{\left(1+2e^{\beta\left(\frac{\alpha^2}{2\omega^2}-\mu\right)}+e^{2\beta\left(\frac{\alpha^2}{\omega^2}-\mu\right)}\right)\frac{1}{\sqrt{2(\cosh(\beta\omega)-1)}}}}$$

This is the same result as in (89), and it is proven that the formula (at least in the case $N=1$) is correct.

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