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Benchmarking Hubbard-Stratonovich transformations for a determinant quantum Monte Carlo study of the Hubbard and the Hubbard-Holstein model

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Abstract

This thesis will illustrate the determinant quantum Monte Carlo method and apply it to strongly correlated many-body problems. At the same time two models will be studied using three different Hubbard-Stratonovich transformations. The organization of this work is as follows:

The first part will provide all the fundamental concepts that lay behind the determinant quantum Monte Carlo algorithm and apply it to the Hubbard model.

In the second part we will modify the Hubbard model and the determinant quantum Monte Carlo algorithm that we will have introduced in the previous part by using the real continuous Hubbard-Stratonovich transformation instead of the real discrete one.

In the third and last part we will for the first time introduce the Hubbard-Holstein model, a simple model capturing the physics of itinerant electrons with both electron-electron and electron-phonon interactions. In this model the motion of the lattice sites is described by a set of independent harmonic oscillators, one at each site i. The electron-electron interaction is treated as usual and the electron-phonon interaction arises from a linear coupling of the local density n_i to the atomic displacement x_i.
At the same time we will present a totally new approach where we will be using the complex continuous Hubbard-Stratonovich transformation to derive an expression for the grand canonical partition function of the Hubbard-Holstein model with the phonon degrees of freedom being explicitly integrated out in order not to have to sample the phonon fields.

Kurzfassung

Diese Diplomarbeit erklärt die Determinanten-Quanten-Monte-Carlo-Methode und wendet sie auf stark wechselwirkende Vielteilchenprobleme an. Dabei werden zwei Modelle mittels dreier verschiedener Hubbard-Stratonovich-Transformationen untersucht. Die Gliederung dieser Arbeit lautet wie folgt:

Der erste Teil liefert alle grundlegenden Konzepte, die sich hinter dem Determinanten-Quanten-Monte-Carlo-Algorithmus verbergen und wendet diesen auf das Hubbard-Modell an.

Im zweiten Teil modifizieren wir das Hubbard-Modell und den Determinanten-Quanten-Monte-Carlo-Algorithmus, die wir im vorigen Teil eingeführt haben, indem wir die reelle kontinuierliche Hubbard-Stratonovich-Transformation statt der reellen diskreten verwenden.

Im dritten und letzten Teil führen wir zum ersten Mal das Hubbard-Holstein-Modell ein, ein einfaches Modell, das die Physik von umherziehenden Elektronen mit beiden, Elektron-Elektron- und Elektron-Phonon-, Wechselwirkungen erfasst. In diesem Modell wird die Bewegung der Gitterplätze durch eine Menge unabhängiger harmonischer Oszillatoren beschrieben, einer auf jedem Platz i. Die Elektron-Elektron-Wechselwirkung wird wie gewöhnlich behandelt und die Elektron-Phonon-Wechselwirkung entsteht aus einer linearen Kopplung der lokalen Dichte n_i an die atomare Verschiebung x_i.
Dabei präsentieren wir einen völlig neuen Ansatz wo wir die komplexe kontinuierliche Hubbard-Stratonovich-Transformation verwenden, um einen Ausdruck für die großkanonische Zustandssumme für das Hubbard-Holstein-Modell herzuleiten, bei dem die Phononen-Freiheitsgrade explizit aufintegriert sind um keine Stichproben von Phononen-Feldern nehmen zu müssen.

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Contents

I The Hubbard model using the real discrete Hubbard-Stratonovich transformation

1 Introduction

Markov Chain Monte Carlo (MCMC) is an efficient approach to perform importance sampling in many dimensions, where configurations x are created iteratively in such a way that their distribution corresponds to a desired distribution $p(x)$ [1]. Because of this iterative construction, consecutive configurations are usually highly correlated and thus one needs to make sure to skip enough configurations such that two consecutive samples in average values are uncorrelated in order to get useful and reliable results. With these samples one can then evaluate the high-dimensional integrals/sums that arise in the formulation of the many-body problem. But it is assumed that the reader of this work is familiar with the basics of MCMC and thus they will not be treated here.
Instead, we will directly dive into the realm of strongly correlated many-body problems, where the number of basis states for a reasonably sized lattice is extremely large, and concern ourselves in detail with the determinant quantum Monte Carlo (DQMC) method. With this highly efficient technique one can carry out simulations within the grand canonical ensemble. In addition, we will make use of matrix decomposition methods to allow ourselves to study systems at low temperatures.
This first part of the thesis will provide all the fundamental concepts that lay behind the DQMC algorithm and apply it to the Hubbard model.

2 The Hubbard model

The Hubbard model is a simple model for interacting electrons in narrow bands [2]. Assuming localized orbitals and a strong screening of the Coulomb interaction, only the local density-density repulsion is allowed. The mere on-site interaction is certainly a crude approximation to the Coulomb interaction, but, for certain phenomena, it bears already the essential features of strongly correlated electrons.

The model is defined by

$$\begin{aligned}\mathcal{H} &= H - \mu N = H_{\text{kin}} + H_{\text{C}} - \mu N = \\ &= -t \sum_{\sigma=\uparrow,\downarrow} \sum_{<i,j>} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + U \sum_{i=1}^{N} \left(n_{i\uparrow} - \tfrac{1}{2} \right) \left(n_{i\downarrow} - \tfrac{1}{2} \right) - \mu \sum_{i=1}^{N} \left(n_{i\uparrow} + n_{i\downarrow} \right), \end{aligned} \tag{1}$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) create (annihilate) fermions of spin $\sigma = \uparrow, \downarrow$ in a Wannier orbital centered at site i. $n_{i\sigma}$ denotes the occupation number operator $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$. The electrons move in tight-binding bands, with a transfer integral t between nearest-neighbor sites, as indicated by $< i, j >$. The strength of the Coulomb interaction is U and μ is the chemical potential.

3 The determinant quantum Monte Carlo approach

For the following discussion we will write the Hamilton operator of the Hubbard model (1) as

$$\begin{aligned}\mathcal{H} &= H - \mu N = \\ &= \underbrace{U \sum_i \left(n_{i\uparrow} - \tfrac{1}{2}\right)\left(n_{i\downarrow} - \tfrac{1}{2}\right)}_{=:V} + \underbrace{\sum_{\sigma=\uparrow,\downarrow} \underbrace{\left(-t \sum_{<i,j>} \left(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}\right) - \mu \sum_i n_{i\sigma}\right)}_{=:K_\sigma}}_{=:K} = \\ &= V + K, \end{aligned} \tag{2}$$

where K is the kinetic energy operator plus the chemical potential term and V the operator of the Coulomb repulsion.

3.1 The Suzuki-Trotter decomposition

A quantity of central interest is the thermodynamic expectation value of an operator O in a grand canonical ensemble

$$\langle O \rangle = \frac{1}{Z} \operatorname{tr}\left(O e^{-\beta(H-\mu N)}\right) \tag{3}$$

with $\beta = \frac{1}{k_B T}$ the inverse temperature and $Z = \operatorname{tr}\left(e^{-\beta(H-\mu N)}\right)$ the grand canonical partition function [2].

Rewriting the grand canonical partition function by dividing the imaginary-time interval $0 < \tau < \beta$ into L intervals of width $\Delta\tau = \frac{\beta}{L}$ yields

$$Z = \operatorname{tr}\left(e^{-\beta(H-\mu N)}\right) = \operatorname{tr}\left(e^{-L\Delta\tau(V+K)}\right).$$

Furthermore, taking into account the identity

$$e^{x(A+B)} = e^{xA} e^{xB} + O(x^2),$$

which holds for any two non-commuting operators A and B, and applying it to each factor in $e^{-L\Delta\tau(V+K)} = \left(e^{-\Delta\tau(V+K)}\right)^L$,

$$\left(e^{-\Delta\tau(V+K)}\right)^L = \left(e^{-\Delta\tau V} e^{-\Delta\tau K} + O(\Delta\tau^2)\right)^L,$$

the grand canonical partition function becomes

$$Z = \operatorname{tr}\left(\left(e^{-\Delta\tau V} e^{-\Delta\tau K} + O(\Delta\tau^2)\right)^L\right) \approx \operatorname{tr}\left(\left(e^{-\Delta\tau V} e^{-\Delta\tau K}\right)^L\right). \tag{4}$$

This is the only approximation in DQMC. Apart from that, it is exact.

3.2 The Hubbard-Stratonovich transformation

The key element of the DQMC algorithm, to determine thermodynamic expectation values, is the elimination of the electronic degrees of freedom to obtain an effective action for (auxiliary) boson fields to which standard Monte Carlo techniques can be applied [2]. This approach yields immediately the exact result for independent electron theories.

To eliminate the electronic interaction we perform the Hubbard-Stratonovich transformation, which is in general based on either one of the integrals

$$e^{\frac{a}{2}x^2} = \frac{1}{\sqrt{2\pi a}} \int_{-\infty}^{\infty} e^{-\frac{1}{2a}y^2 - xy} \, \mathrm{d}y \tag{5}$$

$$e^{-\frac{a}{2}x^2} = \frac{1}{\sqrt{2\pi a}} \int_{-\infty}^{\infty} e^{-\frac{1}{2a}y^2 - \mathrm{i}xy} \, \mathrm{d}y, \tag{6}$$

depending on the sign of the argument of the exponential function to be transformed (a has to be real and positive). We will use it to linearize the density operator in the Coulomb repulsion term and introduce an auxiliary scalar field. By this, our particle theory will be converted into its respective field theory.
Here, for our endeavor to eliminate the electronic interaction, we will choose to perform the so-called real discrete Hubbard-Stratonovich transformation by claiming

$$e^{-\Delta\tau U(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})} = e^{-\Delta\tau\frac{U}{4}} \frac{1}{2} \left(e^{-\Delta\tau\lambda(n_{i\uparrow}-n_{i\downarrow})} + e^{\Delta\tau\lambda(n_{i\uparrow}-n_{i\downarrow})} \right) \tag{7}$$

for an arbitrary $i \in \{1, \ldots, N\}$.

Proof.
Because $n_{i\uparrow}$ and $n_{i\downarrow}$ can just be either 0 or 1, we get:

$n_{i\uparrow}$	$n_{i\downarrow}$	$n_{i\uparrow} - n_{i\downarrow}$	$e^{-\Delta\tau U(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})}$	$e^{-\Delta\tau\frac{U}{4}} \frac{1}{2} \left(e^{-\Delta\tau\lambda(n_{i\uparrow}-n_{i\downarrow})} + e^{\Delta\tau\lambda(n_{i\uparrow}-n_{i\downarrow})} \right)$
0	0	0	$e^{-\Delta\tau\frac{U}{4}}$	$e^{-\Delta\tau\frac{U}{4}}$
1	0	1	$e^{\Delta\tau\frac{U}{4}}$	$e^{-\Delta\tau\frac{U}{4}} \cosh(\Delta\tau\lambda)$
0	1	-1	$e^{\Delta\tau\frac{U}{4}}$	$e^{-\Delta\tau\frac{U}{4}} \cosh(\Delta\tau\lambda)$
1	1	0	$e^{-\Delta\tau\frac{U}{4}}$	$e^{-\Delta\tau\frac{U}{4}}$

This means that we have to choose λ in such a way that

$$\cosh(\Delta\tau\lambda) = e^{\Delta\tau\frac{U}{2}},$$

i.e. $\lambda = \frac{1}{\Delta\tau}\operatorname{arcosh}(e^{\Delta\tau\frac{U}{2}})$. □

The transformation reduces the quartic self-interaction of the electrons to a quadratic interaction with the auxiliary Hubbard-Stratonovich field variables $\pm\lambda$, which represent bosonic degrees of freedom, but have no true physical interpretation [3]. However, this representation is amenable to numerical treatment as the summation of the fields can be performed by simulation (e.g. Monte Carlo) methods.

3.3 Transformation of the grand canonical partition function

Next, we introduce (7) at each lattice point i and each imaginary-time slice $l \in \{1, \ldots, L\}$ in (4) yielding

$$\begin{aligned}
Z &\approx \operatorname{tr}\left(\left(e^{-\Delta\tau V}e^{-\Delta\tau K}\right)^L\right) = \operatorname{tr}\left(\left(e^{-\Delta\tau U\sum_i(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})}e^{-\Delta\tau K}\right)^L\right) = \\
&= \operatorname{tr}\left(\left(\prod_i\left(e^{-\Delta\tau U(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})}\right)e^{-\Delta\tau K}\right)^L\right) = \operatorname{tr}\left(\left(\prod_i\left(e^{-\Delta\tau\frac{U}{4}}\frac{1}{2}\sum_{S\in\{\pm1\}}e^{-\Delta\tau\lambda S(n_{i\uparrow}-n_{i\downarrow})}\right)e^{-\Delta\tau K}\right)^L\right) = \\
&= \left(\frac{e^{-\beta\frac{U}{4}}}{2^L}\right)^N\sum_{S\in\{\pm1\}^{N\times L}}\operatorname{tr}\left(\prod_{l=L}^{1}\underbrace{e^{-\Delta\tau\lambda\sum_i S_{il}(n_{i\uparrow}-n_{i\downarrow})}e^{-\Delta\tau K}}_{=:e^{-\Delta\tau\mathscr{H}^{(l)}}}\right) = \\
&= \left(\frac{e^{-\beta\frac{U}{4}}}{2^L}\right)^N\sum_{S\in\{\pm1\}^{N\times L}}\operatorname{tr}\left(\prod_{l=L}^{1}e^{-\Delta\tau\mathscr{H}^{(l)}}\right),
\end{aligned} \tag{8}$$

where we have chosen the time ordering, which is arbitrary, in decreasing order. We have also used the fact that the arguments of the exponentials are single-particle operators and have introduced effective single-particle Hamilton operators (in second quantization) $\mathscr{H}^{(l)} = \sum_{\sigma=\uparrow,\downarrow}\sum_{ij}h^{(l)}_{ij,\sigma}c^\dagger_{i\sigma}c_{j\sigma} =: \sum_{\sigma=\uparrow,\downarrow}\mathscr{H}^{(l)}_\sigma$ [2]. It is clear-cut that the two spin contributions decouple and (8) becomes

$$Z = \left(\frac{e^{-\beta\frac{U}{4}}}{2^L}\right)^N\sum_{S\in\{\pm1\}^{N\times L}}\operatorname{tr}_\uparrow\left(\prod_{l=L}^{1}e^{-\Delta\tau\mathscr{H}^{(l)}_\uparrow}\right)\operatorname{tr}_\downarrow\left(\prod_{l=L}^{1}e^{-\Delta\tau\mathscr{H}^{(l)}_\downarrow}\right). \tag{9}$$

Now we want to prove that the product of exponentials of (effective) one-particle Hamilton operators, $\mathscr{H}^{(l)}_\sigma = \sum_{ij}h^{(l)}_{ij,\sigma}c^\dagger_{i\sigma}c_{j\sigma}$, is again an exponential of an effective one-particle operator $\widetilde{\mathscr{H}_\sigma} = \sum_{ij}\widetilde{h}_{ij,\sigma}c^\dagger_{i\sigma}c_{j\sigma}$ [2], i.e.

$$\mathcal{U}_\sigma := \prod_{l=L}^{1}e^{-\Delta\tau\mathscr{H}^{(l)}_\sigma} = e^{-\Delta\tau\widetilde{\mathscr{H}_\sigma}}.$$

Proof.
We start out with the time evolution of an arbitrary electron creation operator $c^\dagger_{k\sigma}$ in an effective one-particle system described by $\mathscr{H}^{(l)}_\sigma = \sum_{ij} h^{(l)}_{ij,\sigma} c^\dagger_{i\sigma} c_{j\sigma}$,

$$c^\dagger_{k\sigma}(\tau) = e^{-\tau\mathscr{H}^{(l)}_\sigma} c^\dagger_{k\sigma} e^{\tau\mathscr{H}^{(l)}_\sigma}. \qquad \left|\frac{\mathrm{d}}{\mathrm{d}\tau} \right. \implies$$

$$\begin{aligned}
\implies \frac{\mathrm{d}}{\mathrm{d}\tau} c^\dagger_{k\sigma}(\tau) &= e^{-\tau\mathscr{H}^{(l)}_\sigma}\left(-\mathscr{H}^{(l)}_\sigma\right) c^\dagger_{k\sigma} e^{\tau\mathscr{H}^{(l)}_\sigma} + e^{-\tau\mathscr{H}^{(l)}_\sigma} c^\dagger_{k\sigma} \mathscr{H}^{(l)}_\sigma e^{\tau\mathscr{H}^{(l)}_\sigma} = \\
&= -e^{-\tau\mathscr{H}^{(l)}_\sigma}\left[\mathscr{H}^{(l)}_\sigma, c^\dagger_{k\sigma}\right] e^{\tau\mathscr{H}^{(l)}_\sigma} = \Big| \left[\mathscr{H}^{(l)}_\sigma, c^\dagger_{k\sigma}\right] = \sum_{ij} h^{(l)}_{ij,\sigma}\left[c^\dagger_{i\sigma} c_{j\sigma}, c^\dagger_{k\sigma}\right] = \\
&= \Big| \left[c^\dagger_{i\sigma} c_{j\sigma}, c^\dagger_{k\sigma}\right] = c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{k\sigma} - c^\dagger_{k\sigma} c^\dagger_{i\sigma} c_{j\sigma} = c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{k\sigma} + c^\dagger_{i\sigma} c^\dagger_{k\sigma} c_{j\sigma} = \\
&= c^\dagger_{i\sigma}\left\{c_{j\sigma}, c^\dagger_{k\sigma}\right\} = c^\dagger_{i\sigma}\delta_{jk} \Big| = \\
&= \sum_{ij} h^{(l)}_{ij,\sigma} c^\dagger_{i\sigma}\delta_{jk} = \sum_i c^\dagger_{i\sigma} h^{(l)}_{ik,\sigma} \Big| = -e^{-\tau\mathscr{H}^{(l)}_\sigma}\left(\sum_i c^\dagger_{i\sigma} h^{(l)}_{ik,\sigma}\right) e^{\tau\mathscr{H}^{(l)}_\sigma} = \\
&= -\sum_i c^\dagger_{i\sigma}(\tau)\, h^{(l)}_{ik,\sigma} \quad \Longleftrightarrow \quad \frac{\mathrm{d}}{\mathrm{d}\tau}\vec{c^\dagger_\sigma}(\tau) = -\vec{c^\dagger_\sigma}(\tau)\, h^{(l)}_\sigma \quad \Longrightarrow
\end{aligned}$$

$$\implies \vec{c^\dagger_\sigma}(\tau) = \vec{c^\dagger_\sigma} e^{-\tau h^{(l)}_\sigma} \tag{10}$$

$h^{(l)}_\sigma$ is the matrix defining the operator $\mathscr{H}^{(l)}_\sigma$. We learn from (10) how an arbitrary one-particle orbital $a^\dagger_{\mu\sigma} \coloneqq \sum_i c^\dagger_{i\sigma} A_{i\mu}$ evolves:

$$\begin{aligned}
a^\dagger_{\mu\sigma}(\tau) &= \sum_i c^\dagger_{i\sigma}(\tau)\, A_{i\mu} = \sum_i \sum_j c^\dagger_{j\sigma}\left(e^{-\tau h^{(l)}_\sigma}\right)_{ji} A_{i\mu} = \sum_j c^\dagger_{j\sigma} \sum_i \left(e^{-\tau h^{(l)}_\sigma}\right)_{ji} A_{i\mu} \overset{!}{=} \\
&\overset{!}{=} e^{-\tau\mathscr{H}^{(l)}_\sigma} a^\dagger_{\mu\sigma} e^{\tau\mathscr{H}^{(l)}_\sigma} \quad \Longleftrightarrow \\
\Longleftrightarrow \quad e^{-\Delta\tau\mathscr{H}^{(l)}_\sigma} a^\dagger_{\mu\sigma} &= \sum_j c^\dagger_{j\sigma} \sum_i \left(e^{-\Delta\tau h^{(l)}_\sigma}\right)_{ji} A_{i\mu} e^{-\Delta\tau\mathscr{H}^{(l)}_\sigma} \quad \Longrightarrow \\
\Longrightarrow \quad \mathcal{U}_\sigma a^\dagger_{\mu\sigma} &= \prod_{l=L}^{1} e^{-\Delta\tau\mathscr{H}^{(l)}_\sigma} a^\dagger_{\mu\sigma} = \sum_j c^\dagger_{j\sigma} \sum_i \underbrace{\left(\prod_{l=L}^{1} e^{-\Delta\tau h^{(l)}_\sigma}\right)_{ji}}_{=:\left(e^{-\Delta\tau\widetilde{h}_\sigma}\right)_{ji}} A_{i\mu}\mathcal{U}_\sigma = \\
&= \sum_j c^\dagger_{j\sigma} \sum_i \left(e^{-\Delta\tau\widetilde{h}_\sigma}\right)_{ji} A_{i\mu}\mathcal{U}_\sigma \quad \Longleftrightarrow \\
\Longleftrightarrow \quad \mathcal{U}_\sigma a^\dagger_{\mu\sigma}(\mathcal{U}_\sigma)^{-1} &= \sum_j c^\dagger_{j\sigma} \sum_i \left(e^{-\Delta\tau\widetilde{h}_\sigma}\right)_{ji} A_{i\mu} = e^{-\Delta\tau\widetilde{\mathscr{H}_\sigma}} a^\dagger_{\mu\sigma} e^{\Delta\tau\widetilde{\mathscr{H}_\sigma}}
\end{aligned}$$

So, $\mathcal{U}_\sigma$ can be viewed as a single exponential of an effective one-particle operator $\widetilde{\mathscr{H}_\sigma}$. □

Next, we want to prove that for the traces in (9) one can obtain

$$\mathrm{tr}_\sigma\left(\prod_{l=L}^{1} e^{-\Delta\tau\mathscr{H}_\sigma^{(l)}}\right) = \mathrm{tr}_\sigma\left(\prod_{l=L}^{1} e^{-\Delta\tau\sum\limits_{ij} h_{ij,\sigma}^{(l)} c_{i\sigma}^\dagger c_{j\sigma}}\right) = \mathrm{tr}_\sigma\left(\prod_{l=L}^{1} e^{-\Delta\tau\vec{c_\sigma}^\dagger h_\sigma^{(l)}\vec{c_\sigma}}\right) = \det\left(\mathbb{1} + \prod_{l=L}^{1} e^{-\Delta\tau h_\sigma^{(l)}}\right).$$

Proof.
To this end we first diagonalize the effective one-particle Hamilton operator $\widetilde{\mathscr{H}_\sigma} = \sum\limits_{ij}\widetilde{h}_{ij,\sigma}c_{i\sigma}^\dagger c_{j\sigma} = \vec{c_\sigma}^\dagger\widetilde{h}_\sigma\vec{c_\sigma}$ being introduced in the paragraph preceding the last proof by defining a matrix B, whose columns are the orthonormal eigenvectors of $\widetilde{h}_\sigma$ [2]. This means that B is a unitary matrix, $B^\dagger = B^{-1}$ and $BB^\dagger = B^\dagger B = \mathbb{1}$, i.e. the rows and columns are orthonormal to each other. So, B is the transformation matrix that diagonalizes $\widetilde{h}_\sigma$:

$$\begin{aligned}
\widetilde{\mathscr{H}_\sigma} = \vec{c_\sigma}^\dagger\widetilde{h}_\sigma\vec{c_\sigma} &= \underbrace{\vec{c_\sigma}^\dagger B}_{=:\vec{b_\sigma}^\dagger}\underbrace{B^\dagger\widetilde{h}_\sigma B}_{=:\widetilde{\varepsilon}_\sigma}\underbrace{B^\dagger\vec{c_\sigma}}_{=:\vec{b_\sigma}} = \vec{b_\sigma}^\dagger\widetilde{\varepsilon}_\sigma\vec{b_\sigma} = \\
&= \sum_i \widetilde{\varepsilon}_{i,\sigma} b_{i\sigma}^\dagger b_{i\sigma} \implies \qquad (11)\\
\implies -\Delta\tau\widetilde{\mathscr{H}_\sigma} &= \sum_i \underbrace{(-\Delta\tau)\widetilde{\varepsilon}_{i,\sigma}}_{=:\varepsilon_{i,\sigma}} b_{i\sigma}^\dagger b_{i\sigma} = \sum_i \varepsilon_{i,\sigma} b_{i\sigma}^\dagger b_{i\sigma} \implies \\
\implies \mathrm{tr}_\sigma\left(\prod_{l=L}^{1} e^{-\Delta\tau\mathscr{H}_\sigma^{(l)}}\right) &= \mathrm{tr}_\sigma\left(e^{-\Delta\tau\widetilde{\mathscr{H}_\sigma}}\right) = \mathrm{tr}_\sigma\left(e^{\sum\limits_i \varepsilon_{i,\sigma} b_{i\sigma}^\dagger b_{i\sigma}}\right) = \sum_{\substack{\vec{n_\sigma}\in\{0,1\}^N \\ \sum\limits_i n_{i\sigma}=1}} \langle\vec{n_\sigma}|\, e^{\sum\limits_i \varepsilon_{i,\sigma} n_{i\sigma}}\,|\vec{n_\sigma}\rangle \qquad (12)
\end{aligned}$$

$|\vec{n_\sigma}\rangle$ are the eigenstates of $\widetilde{\mathscr{H}_\sigma}$ in the occupation number representation. The summation over all possible particle number configurations, for one particle with spin σ, can immediately be performed yielding

$$\begin{aligned}
\mathrm{tr}_\sigma\left(\prod_{l=L}^{1} e^{-\Delta\tau\mathscr{H}_\sigma^{(l)}}\right) &= \prod_i \sum_{n_{i\sigma}=0}^{1} e^{\varepsilon_{i,\sigma} n_{i\sigma}} = \prod_i (1 + e^{\varepsilon_{i,\sigma}}) = \prod_i \left(1 + e^{-\Delta\tau\widetilde{\varepsilon}_{i,\sigma}}\right) = \\
&= \begin{vmatrix} 1 + e^{-\Delta\tau\widetilde{\varepsilon}_{1,\sigma}} & & 0 \\ & \ddots & \\ 0 & & 1 + e^{-\Delta\tau\widetilde{\varepsilon}_{N,\sigma}} \end{vmatrix} = \det\left(\mathbb{1} + e^{-\Delta\tau\widetilde{\varepsilon}_\sigma}\right). \qquad (13)
\end{aligned}$$

Rotating the result back to the original basis gives us what we wanted to prove,

$$\begin{aligned}
\mathrm{tr}_\sigma\left(\prod_{l=L}^{1} e^{-\Delta\tau \mathscr{H}_\sigma^{(l)}}\right) &= \mathrm{tr}_\sigma\left(e^{-\Delta\tau \widetilde{\mathscr{H}_\sigma}}\right) = \det\left(\mathbb{1} + e^{-\Delta\tau \widetilde{\varepsilon}_\sigma}\right) = \det\left(\mathbb{1} + e^{-\Delta\tau B^\dagger \widetilde{h}_\sigma B}\right) = \\
&= \det\left(\mathbb{1} + B^\dagger e^{-\Delta\tau \widetilde{h}_\sigma} B\right) = \det\left(B^\dagger \left(BB^\dagger + e^{-\Delta\tau \widetilde{h}_\sigma}\right) B\right) = \\
&= \underbrace{\det\left(B^\dagger\right)}_{=\pm 1} \det\left(\mathbb{1} + e^{-\Delta\tau \widetilde{h}_\sigma}\right) \underbrace{\det(B)}_{=\pm 1} = \det\left(\mathbb{1} + e^{-\Delta\tau \widetilde{h}_\sigma}\right) = \\
&= \det\left(\mathbb{1} + \prod_{l=L}^{1} e^{-\Delta\tau h_\sigma^{(l)}}\right).
\end{aligned}$$

□

We finally obtain for the grand canonical partition function of the Hubbard model (9)

$$Z = \left(\frac{e^{-\beta\frac{U}{4}}}{2^L}\right)^N \sum_{S\in\{\pm 1\}^{N\times L}} \underbrace{\det\left(\mathbb{1} + \prod_{l=L}^{1} e^{-\Delta\tau h_\uparrow^{(l)}}\right) \det\left(\mathbb{1} + \prod_{l=L}^{1} e^{-\Delta\tau h_\downarrow^{(l)}}\right)}_{=:\rho(S)} = \left(\frac{e^{-\beta\frac{U}{4}}}{2^L}\right)^N \sum_{S\in\{\pm 1\}^{N\times L}} \rho(S)\,.$$

The grand canonical partition function has now been expressed to a classical Monte Carlo problem and, through our discussion, we have also shown that every d-dimensional quantum system can be mapped onto a $(d+1)$-dimensional classical system. The required matrices are the respective operators' matrix representations for one particle and the information content of the many-body problem has been cast into the summation over all field values [2]. The number of auxiliary fields is extremely large and statistical methods have to be invoked to obtain estimates for the relevant quantities. The importance sampling idea is well suited for this task.

3.4 Thermodynamic expectation values

Next, we want to outline how to evaluate thermodynamic expectation values [2]. For an equal-time correlation function of operators A and B, $\langle AB\rangle$, we have, using (3) and (8),

$$\langle AB\rangle = \frac{1}{Z}\left(\frac{e^{-\beta\frac{U}{4}}}{2^L}\right)^N \sum_{S\in\{\pm 1\}^{N\times L}} \mathrm{tr}\left(AB\prod_{l=L}^{1} e^{-\Delta\tau \mathscr{H}^{(l)}}\right) =: \frac{1}{Z}\left(\frac{e^{-\beta\frac{U}{4}}}{2^L}\right)^N \sum_{S\in\{\pm 1\}^{N\times L}} g^S(AB)\;\rho(S)\,, \tag{14}$$

so the Green's function for a given Hubbard-Stratonovich configuration S is defined as

$$g^S(AB) := \frac{1}{\rho(S)}\,\mathrm{tr}\left(AB\prod_{l=L}^{1} e^{-\Delta\tau \mathscr{H}^{(l)}}\right). \tag{15}$$

Equation (14) is in a form amenable to importance sampling with the probability density

$$P(S) = \frac{\rho(S)}{Z} = \frac{1}{Z} \det\left(\mathbb{1} + \prod_{l=L}^{1} e^{-\Delta\tau h_{\uparrow}^{(l)}}\right) \det\left(\mathbb{1} + \prod_{l=L}^{1} e^{-\Delta\tau h_{\downarrow}^{(l)}}\right). \tag{16}$$

Given a single Hubbard-Stratonovich field value S we are dealing with a one-particle problem. Therefore Wick's theorem applies and it suffices to consider the one-particle Green's function $g^S(c_{i\sigma}c_{j\sigma}^{\dagger})$. The correlation effects come into play through the sum over all Hubbard-Stratonovich fields.

We will now prove that for $g^S(c_{i\sigma}c_{j\sigma}^{\dagger})$ one can derive the expression

$$g^S(c_{i\sigma}c_{j\sigma}^{\dagger}) = \left(\left(\mathbb{1} + \prod_{l=L}^{1} e^{-\Delta\tau h_{\sigma}^{(l)}}\right)^{-1}\right)_{ij}. \tag{17}$$

Proof.
We consider the equal-time Green's function for a single Hubbard-Stratonovich configuration S [2]. According to its definition (15), the Green's function reads

$$g^S(c_{i\sigma}c_{j\sigma}^{\dagger}) = \frac{\mathrm{tr}_{\sigma}\left(c_{i\sigma}c_{j\sigma}^{\dagger} \prod_{l=L}^{1} e^{-\Delta\tau \mathscr{H}_{\sigma}^{(l)}}\right)}{\mathrm{tr}_{\sigma}\left(\prod_{l=L}^{1} e^{-\Delta\tau \mathscr{H}_{\sigma}^{(l)}}\right)}. \tag{18}$$

Just like in the previous proof, we will first rotate the problem to diagonal form and then rotate the result back to the original basis. To this end we again define a unitary matrix B, whose columns are the orthonormal eigenvectors of $\widetilde{h}_{\sigma}$. We use the equations (12) and (13) in the previous proof to rewrite (18):

$$g^S(c_{i\sigma}c_{j\sigma}^{\dagger}) = \frac{\mathrm{tr}_{\sigma}\left(c_{i\sigma}c_{j\sigma}^{\dagger} e^{\sum_{\mu} \varepsilon_{\mu,\sigma} b_{\mu\sigma}^{\dagger} b_{\mu\sigma}}\right)}{\prod_{\mu}(1 + e^{\varepsilon_{\mu,\sigma}})} \tag{19}$$

Now we want to expand the electron operators in the eigenstates of $\widetilde{\mathscr{H}_{\sigma}}$. In (11) in the previous proof we introduced $\overrightarrow{b_{\sigma}} = B^{\dagger}\overrightarrow{c_{\sigma}}$, with which we immediately get $\overrightarrow{c_{\sigma}} = B\overrightarrow{b_{\sigma}}$ and further:

$$\begin{aligned} c_{i\sigma} &= \sum_{\nu} B_{i\nu} b_{\nu\sigma} = \sum_{\nu} \langle i|\, B\, |\nu\rangle\, b_{\nu\sigma} = \sum_{\nu} \langle e_i|\nu\rangle\, b_{\nu\sigma} \quad \Longrightarrow \\ \Longrightarrow \quad c_{j\sigma}^{\dagger} &= \sum_{\nu'} \langle e_j|\nu'\rangle^{*}\, b_{\nu'\sigma}^{\dagger} = \sum_{\nu'} \langle \nu'|e_j\rangle\, b_{\nu'\sigma}^{\dagger} \\ \Longrightarrow \quad c_{i\sigma}c_{j\sigma}^{\dagger} &= \sum_{\nu\nu'} \langle e_i|\nu\rangle \langle \nu'|e_j\rangle\, b_{\nu\sigma} b_{\nu'\sigma}^{\dagger} \end{aligned} \tag{20}$$

$\langle e_i|$ and $|e_j\rangle$ are canonical basis vectors and $|\nu\rangle$ and $\langle\nu'|$ are, just like in the previous proof, the eigenstates of $\widetilde{\mathscr{H}_\sigma}$ in the occupation number representation (for one particle with spin σ). Inserting the expansion of the electron operators in the eigenstates of $\widetilde{\mathscr{H}_\sigma}$ (20) into (19) yields

$$
\begin{aligned}
g^S(c_{i\sigma}c^\dagger_{j\sigma}) &= \sum_{\nu\nu'} \langle e_i|\nu\rangle\langle\nu'|e_j\rangle \frac{\mathrm{tr}_\sigma\left(b_{\nu\sigma}b^\dagger_{\nu'\sigma}e^{\sum_\mu \varepsilon_{\mu,\sigma}b^\dagger_{\mu\sigma}b_{\mu\sigma}}\right)}{\prod_\mu(1+e^{\varepsilon_{\mu,\sigma}})} = \\
&= \frac{1}{\prod_\mu(1+e^{\varepsilon_{\mu,\sigma}})}\sum_{\nu\nu'}\langle e_i|\nu\rangle\langle\nu'|e_j\rangle \sum_{\substack{\vec{n_\sigma}\in\{0,1\}^N \\ \sum_i n_{i\sigma}=1}} \langle\vec{n_\sigma}|\, b_{\nu\sigma}b^\dagger_{\nu'\sigma}e^{\sum_\mu \varepsilon_{\mu,\sigma}n_{\mu\sigma}}\,|\vec{n_\sigma}\rangle = \\
&= \frac{1}{\prod_\mu(1+e^{\varepsilon_{\mu,\sigma}})}\sum_{\nu}\langle e_i|\nu\rangle\langle\nu|e_j\rangle \sum_{\substack{\vec{n_\sigma}\in\{0,1\}^N \\ \sum_i n_{i\sigma}=1}} \langle\vec{n_\sigma}|\,(1-n_{\nu\sigma})\,|\vec{n_\sigma}\rangle \prod_\mu e^{\varepsilon_{\mu,\sigma}n_{\mu\sigma}} = \\
&= \frac{1}{\prod_\mu(1+e^{\varepsilon_{\mu,\sigma}})}\sum_{\nu}\langle e_i|\nu\rangle\langle\nu|e_j\rangle \sum_{n_{\nu\sigma}=0}^{1}(1-n_{\nu\sigma})\,e^{\varepsilon_{\nu,\sigma}n_{\nu\sigma}}\prod_{\mu\neq\nu}\sum_{n_{\mu\sigma}=0}^{1}e^{\varepsilon_{\mu,\sigma}n_{\mu\sigma}} = \\
&= \frac{1}{\prod_\mu(1+e^{\varepsilon_{\mu,\sigma}})}\sum_{\nu}\langle e_i|\nu\rangle\langle\nu|e_j\rangle \quad 1\cdot\prod_{\mu\neq\nu}(1+e^{\varepsilon_{\mu,\sigma}}) = \\
&= \sum_\nu \langle e_i|\nu\rangle\langle\nu|e_j\rangle\frac{1}{1+e^{\varepsilon_{\nu,\sigma}}} = \langle e_i|\left(\sum_\nu \frac{1}{1+e^{-\Delta\tau\widetilde{\varepsilon}_{\nu,\sigma}}}|\nu\rangle\langle\nu|\right)|e_j\rangle = \\
&= \langle e_i|\left(\frac{\mathbb{1}}{\mathbb{1}+e^{-\Delta\tau\widetilde{\varepsilon}_\sigma}}\right)|e_j\rangle\,.
\end{aligned}
$$

Rotating the result back to the original basis gives us (17),

$$
\begin{aligned}
g^S(c_{i\sigma}c^\dagger_{j\sigma}) &= \langle e_i|\left(\frac{\mathbb{1}}{\mathbb{1}+e^{-\Delta\tau B^\dagger\widetilde{h}_\sigma B}}\right)|e_j\rangle = \langle e_i|\left(\frac{\mathbb{1}}{\mathbb{1}+B^\dagger e^{-\Delta\tau\widetilde{h}_\sigma}B}\right)|e_j\rangle = \\
&= \langle e_i|\left(\frac{\mathbb{1}}{B^\dagger\left(BB^\dagger+e^{-\Delta\tau\widetilde{h}_\sigma}\right)B}\right)|e_j\rangle = \langle e_i|\left(\frac{BB^\dagger}{\mathbb{1}+e^{-\Delta\tau\widetilde{h}_\sigma}}\right)|e_j\rangle = \langle e_i|\left(\frac{\mathbb{1}}{\mathbb{1}+\prod_{l=L}^{1}e^{-\Delta\tau h^{(l)}_\sigma}}\right)|e_j\rangle = \\
&= \left(\left(\mathbb{1}+\prod_{l=L}^{1}e^{-\Delta\tau h^{(l)}_\sigma}\right)^{-1}\right)_{ij}.
\end{aligned}
$$

□

By this we derived the expression for the one-particle Green's function, which is entirely determined by $N\times N$ matrices and is therefore well suited for numerical treatment [2].

3.5 An efficient update scheme

At first glance the algorithm looks far too inefficient to be of practical use [2]. There exists, however, an efficient scheme to update matrices and determinants if successive Hubbard-Stratonovich configurations S and S' in the Markov chain differ only in one spin (single spin-flips) and if the time slice l, where the spin-flip is to happen, stands at the very beginning of the product $\prod_{l=L}^{1} e^{-\Delta\tau h_\sigma^{(l)}}$, which means we need the cyclic permutation

$$e^{-\Delta\tau h_\sigma^{(l)}} \cdots e^{-\Delta\tau h_\sigma^{(1)}} e^{-\Delta\tau h_\sigma^{(L)}} \cdots e^{-\Delta\tau h_\sigma^{(l+1)}}.$$

We now say, on time slice l, the spin at site i is being flipped. In this case the matrix $e^{-\Delta\tau h_\sigma^{(l)}}$ is changed.

In order to get the matrix $e^{-\Delta\tau h_\sigma^{(l)}}$ defining the operator $e^{-\Delta\tau \mathscr{H}_\sigma^{(l)}} = e^{\mp\Delta\tau\lambda \sum_i S_{il} n_{i\sigma}} e^{-\Delta\tau K_\sigma}$, we need the matrix representations of the operators K_σ and $\sum_i S_{il} n_{i\sigma}$. From (2) we get for K_σ

$$K_\sigma = \overrightarrow{c_\sigma^\dagger}\,(-t)\,h_{\mathrm{kin}}\,\overrightarrow{c_\sigma} + \overrightarrow{c_\sigma^\dagger}\,(-\mu)\,\mathbb{1}\,\overrightarrow{c_\sigma} = \overrightarrow{c_\sigma^\dagger}\,\underbrace{(-t h_{\mathrm{kin}} - \mu\mathbb{1})}_{=:k}\,\overrightarrow{c_\sigma} = \overrightarrow{c_\sigma^\dagger}\,k\,\overrightarrow{c_\sigma}. \tag{21}$$

And for the interaction term we simply get

$$\sum_i S_{il}\, n_{i\sigma} = \overrightarrow{c_\sigma^\dagger}\, v(l)\, \overrightarrow{c_\sigma} \qquad , (v(l))_{ij} = \delta_{ij} S_{il}.$$

So, we finally get the matrix

$$e^{-\Delta\tau h_\sigma^{(l)}} = e^{\mp\Delta\tau\lambda v(l)} e^{-\Delta\tau k} =: B_l^{\uparrow/\downarrow} \qquad , (v(l))_{ij} = \delta_{ij} S_{il}, \tag{22}$$

with its own set of spin variables $S_{1l}, \ldots, S_{Nl} \in \{\pm 1\}$. From now on we will call the matrix $e^{-\Delta\tau h_\sigma^{(l)}}$ "single-particle propagator" $B_l^{\uparrow/\downarrow}$.

Next, we will introduce the so-called "fermion matrix" $M^{\uparrow/\downarrow}(l)$ and discuss its change with the spin at site i being flipped, $S_{il} \to -S_{il}$:

$$\begin{aligned}
& M^{\uparrow/\downarrow}(l) := \mathbb{1} + e^{\mp\Delta\tau\lambda v(l)} e^{-\Delta\tau k} \cdots B_1^{\uparrow/\downarrow} B_L^{\uparrow/\downarrow} \cdots B_{l+1}^{\uparrow/\downarrow} \implies \\
\implies\ & M^{\uparrow/\downarrow}(l)' = \mathbb{1} + e^{\mp\Delta\tau\lambda v(l)'} e^{-\Delta\tau k} \cdots B_1^{\uparrow/\downarrow} B_L^{\uparrow/\downarrow} \cdots B_{l+1}^{\uparrow/\downarrow} = \Big| e^x e^{\mp\Delta\tau\lambda S_{il}} = e^{\pm\Delta\tau\lambda S_{il}} \iff e^x = \\
& = e^{\pm 2\Delta\tau\lambda S_{il}} =: \left(\Delta^{\uparrow/\downarrow}(i,l)\right)_{ii} + 1 \Big| = \\
& = \mathbb{1} + \left(\mathbb{1} + \Delta^{\uparrow/\downarrow}(i,l)\right) \underbrace{e^{\mp\Delta\tau\lambda v(l)} e^{-\Delta\tau k} \cdots B_1^{\uparrow/\downarrow} B_L^{\uparrow/\downarrow} \cdots B_{l+1}^{\uparrow/\downarrow}}_{=:A^{\uparrow/\downarrow}(l)} = \mathbb{1} + \left(\mathbb{1} + \Delta^{\uparrow/\downarrow}(i,l)\right) A^{\uparrow/\downarrow}(l) = \\
& = M^{\uparrow/\downarrow}(l) + \Delta^{\uparrow/\downarrow}(i,l)\, A^{\uparrow/\downarrow}(l) \qquad , \left(\Delta^{\uparrow/\downarrow}(i,l)\right)_{jk} = \delta_{ji}\,\delta_{ki}\left(e^{\pm 2\Delta\tau\lambda S_{il}} - 1\right)
\end{aligned}$$

For the Metropolis-Hastings algorithm that we will be using throughout this whole thesis the ratio $R = \frac{R(S')}{R(S)}$ is needed. With (16) we get

$$R = \frac{\frac{1}{Z}\rho(S')}{\frac{1}{Z}\rho(S)} = \underbrace{\frac{\det\left(M^{\uparrow}(l)'\right)}{\det(M^{\uparrow}(l))}}_{=:R^{\uparrow}} \underbrace{\frac{\det\left(M^{\downarrow}(l)'\right)}{\det(M^{\downarrow}(l))}}_{=:R^{\downarrow}} = R^{\uparrow}R^{\downarrow}. \tag{23}$$

From now on we will also write our Green's functions for the successive Hubbard-Stratonovich configurations S and S' as $g^{\sigma}(l) = (M^{\sigma}(l))^{-1}$ and $g^{\sigma}(l)' = (M^{\sigma}(l)')^{-1}$.

So the ratio of the determinants after and before the spin-flip is

$$R^{\sigma} = 1 + \left(1 - (g^{\sigma}(l))_{ii}\right)(\Delta^{\sigma}(i,l))_{ii}\,.$$

Proof.

$$\begin{aligned} R^{\sigma} &= \frac{\det(M^{\sigma}(l)')}{\det(M^{\sigma}(l))} = \det(M^{\sigma}(l')\det\left((M^{\sigma}(l))^{-1}\right) = \det\left((M^{\sigma}(l) + \Delta^{\sigma}(i,l)\,A^{\sigma}(l))\,(M^{\sigma}(l))^{-1}\right) = \\ &= \det\left(\mathbb{1} + \Delta^{\sigma}(i,l)\,(M^{\sigma}(l) - \mathbb{1})\,(M^{\sigma}(l))^{-1}\right) = \det(\mathbb{1} + \Delta^{\sigma}(i,l)\,(\mathbb{1} - g^{\sigma}(l))) = \\ &= (\mathbb{1} + \Delta^{\sigma}(i,l)\,(\mathbb{1} - g^{\sigma}(l)))_{ii} = 1 + \left(1 - (g^{\sigma}(l))_{ii}\right)(\Delta^{\sigma}(i,l))_{ii} \end{aligned}$$

□

Next, we will apply the Sherman-Morrison formula to relate the new $g^{\sigma}(l)'$ to the old $g^{\sigma}(l)$. The Sherman-Morrison formula states that

$$\left(A + \vec{u}\,\vec{v}^{\,\mathrm{t}}\right)^{-1} = A^{-1} - \frac{A^{-1}\vec{u}\,\vec{v}^{\,\mathrm{t}}A^{-1}}{1 + \vec{v}^{\,\mathrm{t}}A^{-1}\vec{u}}, \tag{24}$$

where A is an invertible square matrix, $\vec{u}$, $\vec{v} \in \mathbb{C}^N$ and $1 + \vec{v}^{\,\mathrm{t}}A^{-1}\vec{u} \neq 0$.

Proof.
The right-hand side of (24), defined as the matrix Y, is the inverse of $A + \vec{u}\,\vec{v}^{\,\mathrm{t}}$, defined as the matrix X, if and only if $XY = YX = \mathbb{1}$.

$$\begin{aligned} XY &= \left(A + \vec{u}\,\vec{v}^{\,\mathrm{t}}\right)\left(A^{-1} - \frac{A^{-1}\vec{u}\,\vec{v}^{\,\mathrm{t}}A^{-1}}{1 + \vec{v}^{\,\mathrm{t}}A^{-1}\vec{u}}\right) = \\ &= AA^{-1} + \vec{u}\,\vec{v}^{\,\mathrm{t}}A^{-1} - \frac{AA^{-1}\vec{u}\,\vec{v}^{\,\mathrm{t}}A^{-1} + \vec{u}\,\vec{v}^{\,\mathrm{t}}A^{-1}\vec{u}\,\vec{v}^{\,\mathrm{t}}A^{-1}}{1 + \vec{v}^{\,\mathrm{t}}A^{-1}\vec{u}} = \\ &= \mathbb{1} + \vec{u}\,\vec{v}^{\,\mathrm{t}}A^{-1} - \frac{\vec{u}\left(1 + \vec{v}^{\,\mathrm{t}}A^{-1}\vec{u}\right)\vec{v}^{\,\mathrm{t}}A^{-1}}{1 + \vec{v}^{\,\mathrm{t}}A^{-1}\vec{u}} = \mathbb{1} \end{aligned}$$

Analogically, it is verified that $YX = \mathbb{1}$. □

So, if the inverse of A is already known, the formula provides a numerically cheap way to compute the inverse of A corrected by the matrix $\vec{u}\,\vec{v}^{\,\mathrm{t}}$, as it does not have to be computed

from scratch (which in general is expensive), but can be computed by correcting A^{-1}.
Now we apply the Sherman-Morrison formula to relate the new $g^\sigma(l)'$ to the old $g^\sigma(l)$, which leads to

$$g^\sigma(l)' = g^\sigma(l) - \frac{g^\sigma(l)\,\Delta^\sigma(i,l)\,(\mathbb{1} - g^\sigma(l))}{1 + (1 - (g^\sigma(l))_{ii})\,(\Delta^\sigma(i,l))_{ii}}. \tag{25}$$

Proof.

$$\begin{aligned}
g^\sigma(l)' &= (M^\sigma(l)')^{-1} = (M^\sigma(l) + \Delta^\sigma(i,l)\,A^\sigma(l))^{-1} = (M^\sigma(l) + (\Delta^\sigma(i,l))_{ii}\,\vec{e_i}\,(A^\sigma(l))_{i*})^{-1} = \\
&= (M^\sigma(l))^{-1} - \frac{(M^\sigma(l))^{-1}\,\Delta^\sigma(i,l)\,A^\sigma(l)\,(M^\sigma(l))^{-1}}{1 + (A^\sigma(l))_{i*}\,(M^\sigma(l))^{-1}\,\vec{e_i}\,(\Delta^\sigma(i,l))_{ii}} = \\
&= g^\sigma(l) - \frac{g^\sigma(l)\,\Delta^\sigma(i,l)\,(\mathbb{1} - g^\sigma(l))}{1 + (A^\sigma(l))_{i*}\,(g^\sigma(l))_{*i}\,(\Delta^\sigma(i,l))_{ii}} = g^\sigma(l) - \frac{g^\sigma(l)\,\Delta^\sigma(i,l)\,(\mathbb{1} - g^\sigma(l))}{1 + (A^\sigma(l)\,g^\sigma(l))_{ii}\,(\Delta^\sigma(i,l))_{ii}} = \\
&= g^\sigma(l) - \frac{g^\sigma(l)\,\Delta^\sigma(i,l)\,(\mathbb{1} - g^\sigma(l))}{1 + (\mathbb{1} - g^\sigma(l))_{ii}\,(\Delta^\sigma(i,l))_{ii}} = g^\sigma(l) - \frac{g^\sigma(l)\,\Delta^\sigma(i,l)\,(\mathbb{1} - g^\sigma(l))}{1 + (1 - (g^\sigma(l))_{ii})\,(\Delta^\sigma(i,l))_{ii}}
\end{aligned}$$

($(A^\sigma(l))_{i*}$ denotes the i-th row of $A^\sigma(l)$ and $(g^\sigma(l))_{*i}$ denotes the i-th column of $g^\sigma(l)$.) □

So, if the equal-time Green's function $g^\sigma(l)$ for an electron propagating through the field produced by the S_{il} is known, and the spin S_{il} is flipped, then its new value, $g^\sigma(l)'$, can be evaluated through this relation [3].

After all the spins on time slice l have been updated, we can obtain the equal-time Green's function on the next time slice $l + 1$ through the relation

$$g^\sigma(l+1) = B^\sigma_{l+1}\,g^\sigma(l)\,(B^\sigma_{l+1})^{-1}. \tag{26}$$

Proof.

$$\begin{aligned}
g^\sigma(l+1) &= (M^\sigma(l+1))^{-1} = (\mathbb{1} + B^\sigma_{l+1}B^\sigma_l \cdots B^\sigma_1 B^\sigma_L \cdots B^\sigma_{l+2})^{-1} = \\
&= \left(B^\sigma_{l+1}\,(\mathbb{1} + B^\sigma_l \cdots B^\sigma_1 B^\sigma_L \cdots B^\sigma_{l+2}B^\sigma_{l+1})\,(B^\sigma_{l+1})^{-1}\right)^{-1} = \left(B^\sigma_{l+1}\,M^\sigma(l)\,(B^\sigma_{l+1})^{-1}\right)^{-1} = \\
&= B^\sigma_{l+1}\,(M^\sigma(l))^{-1}\,(B^\sigma_{l+1})^{-1} = B^\sigma_{l+1}\,g^\sigma(l)\,(B^\sigma_{l+1})^{-1}
\end{aligned}$$

□

Next, we update all spins on time slice $l + 1$ following the same procedure that we described before. After all the spins on time slice $l + 1$ have been updated, we need to "wrap" the equal-time Green's function again and continue this process until all spins on all time slices have been updated.

3.6 The UDR decomposition

As we have seen, the Green's function, and not the grand canonical partition function, is the central object of the simulations [4]. It is needed to perform importance sampling and to make measurements. Unfortunately, numerical instabilities prevent the use of this algorithm [3]. In order to remove these instabilities, we must first understand their cause. They are not associated with the updating of the equal-time Green's function given in (25). On the other hand, the process of advancing the equal-time Green's function to a new time slice given in (26) does introduce numerical errors, as round-off errors will accumulate from the repeated adding-on of factors and the subsequent deletion by inverse multiplication. So one must periodically recompute the Green's function from scratch. The more serious difficulty is that at low temperatures, as β becomes large, the Green's function cannot be computed at all [4]. The reason is that as many B_l^σ matrices are multiplied together, the product becomes more and more ill-conditioned, with exponentially divergent numerical scales. And one simply cannot numerically compute the inverse (or the determinant) of an ill-conditioned matrix. This problem, however, can be dealt with in a relatively straightforward manner using matrix factorization methods such as the singular value decomposition (SVD) or the modified Gram-Schmidt (MGS) factorization, which happens to be even more efficient than SVD, and which we will just call "UDR decomposition."

Next, we will use the UDR decomposition to stabilize the numerical computation of inverses (and determinants) of ill-conditioned matrices [3]. Suppose that one can multiply m of the B_l^σ matrices without losing numerical accuracy. We then use the Gram-Schmidt orthogonalization procedure to write this product in the form

$$a_1^\sigma(l) \coloneqq B_{l+m}^\sigma B_{l+m-1}^\sigma \cdots B_{l+1}^\sigma = U_1^\sigma D_1^\sigma R_1^\sigma,$$

where U_1^σ is an orthogonal matrix, D_1^σ a diagonal matrix and R_1^σ a unit right triangular matrix. The orthogonal matrix U_1^σ is necessarily well-conditioned. R_1^σ need not be well-conditioned, but in practice it is. Only the diagonal matrix D_1^σ has large variations in the size of its elements. Next, we perform four operations in a very specific order, which is important.
We first multiply U_1^σ on the left by $B_{l+2m}^\sigma \cdots B_{l+m+1}^\sigma$. By assumption, m is small enough so that this matrix can be computed accurately.
We then multiply it on the right by D_1^σ. This only rescales the columns of the matrix and thus does no harm to the numerical stability of the next step, a UDR decomposition of this partial product,

$$\widetilde{a}_2^\sigma(l) = U_2^\sigma D_2^\sigma \widetilde{R}_2^\sigma.$$

For the last step we multiply the resulting unit right triangular matrix $\widetilde{R}_2^\sigma$ on the right by R_1^σ to obtain

$$a_2^\sigma(l) = U_2^\sigma D_2^\sigma \widetilde{R}_2^\sigma R_1^\sigma = U_2^\sigma D_2^\sigma R_2^\sigma.$$

This process is repeated $\frac{L}{m}$ times to obtain

$$A^\sigma(l) = a^\sigma_{\frac{L}{m}}(l) = U^\sigma_{\frac{L}{m}} D^\sigma_{\frac{L}{m}} R^\sigma_{\frac{L}{m}}.$$

To form $M^\sigma(l)$, we must add the unit matrix to $A^\sigma(l)$, but care must be taken to isolate the diagonal matrix $D^\sigma_{\frac{L}{m}}$, whose elements have large variations in size. We therefore write

$$M^\sigma(l) = \mathbb{1} + A^\sigma(l) = \mathbb{1} + U^\sigma_{\frac{L}{m}} D^\sigma_{\frac{L}{m}} R^\sigma_{\frac{L}{m}} = U^\sigma_{\frac{L}{m}} \left(\left(U^\sigma_{\frac{L}{m}} \right)^{-1} \left(R^\sigma_{\frac{L}{m}} \right)^{-1} + D^\sigma_{\frac{L}{m}} \right) R^\sigma_{\frac{L}{m}}$$

and make a final UDR decomposition of $\left(U^\sigma_{\frac{L}{m}} \right)^{-1} \left(R^\sigma_{\frac{L}{m}} \right)^{-1} + D^\sigma_{\frac{L}{m}}$ leading to

$$M^\sigma(l) = \underbrace{U^\sigma_{\frac{L}{m}} \widetilde{U}^\sigma}_{=:U^\sigma} D^\sigma \underbrace{\widetilde{R}^\sigma R^\sigma_{\frac{L}{m}}}_{=:R^\sigma} = U^\sigma D^\sigma R^\sigma.$$

Finally, we can form $g^\sigma(l)$ in a very trivial way,

$$g^\sigma(l) = (M^\sigma(l))^{-1} = (U^\sigma D^\sigma R^\sigma)^{-1} = (R^\sigma)^{-1} (D^\sigma)^{-1} (U^\sigma)^{-1}.$$

In all, we define numerical stability in an operational fashion.

Just as it is possible to multiply m of the B^σ_l matrices without losing numerical accuracy, it is also possible to advance the Green's function to a new time slice, using (26), m' times without introducing unacceptable errors [3]. Thus, one must completely recalculate the Green's function $\frac{L}{m'}$ times per lattice sweep.

3.7 The checkerboard breakup

For our numerical study of the Hubbard model we will first examine a 4×2 lattice, so $N = 8$. Hence we get for the matrix k in (21)

$$k = -t \begin{pmatrix} 0 & 1 & 0 & 1 & 2 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 2 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 2 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 2 \\ 2 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 2 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 2 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 2 & 1 & 0 & 1 & 0 \end{pmatrix} - \mu \mathbb{1}.$$

Next, we will choose to break the matrix $e^{-\Delta\tau k}$ in (22) further, because it is a dense matrix making the number of operations needed to perform a matrix multiplication scale as N^3 [4].

A sparse and extremely convenient approximate form for $e^{-\Delta\tau k}$ results from a further application of the Suzuki-Trotter decomposition to it,

$$e^{-\Delta\tau k} = e^{-\Delta\tau(-t h_{\text{kin}} - \mu\mathbb{1})} = e^{-\Delta\tau\left(\sum\limits_{<i,j>} k^{(ij)} - \mu\mathbb{1}\right)} \approx \prod_{<i,j>} e^{-\Delta\tau k^{(ij)}} \cdot e^{\Delta\tau\mu}, \tag{27}$$

where the $k^{(ij)}$ are sparse matrices with only $\left(k^{(ij)}\right)_{ij} = \left(k^{(ij)}\right)_{ji} =: k_{ij}$ nonzero. These sparse matrices are easily exponentiated giving

$$e^{-\Delta\tau k^{(ij)}} = e^{-\Delta\tau \begin{pmatrix} 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \cdots & 0 & \cdots & k_{ij} & \cdots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \cdots & k_{ij} & \cdots & 0 & \cdots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 \end{pmatrix}} =$$

$$= \begin{pmatrix} 1 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \cdots & \cosh(\Delta\tau k_{ij}) & \cdots & -\sinh(\Delta\tau k_{ij}) & \cdots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \cdots & -\sinh(\Delta\tau k_{ij}) & \cdots & \cosh(\Delta\tau k_{ij}) & \cdots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 1 \end{pmatrix},$$

with only the elements ii, ij, ji and jj differing from those of the unit matrix. If we replace the multiplication of the dense matrix by the series (27) of sparse-matrix multiplications, the number of operations for multiplication onto a $N \times N$ matrix is reduced from N^3 to N^2.
(27) is referred to as the "checkerboard breakup." Not only is the checkerboard breakup of $e^{-\Delta\tau k}$ reasonably fast, the evaluation of the inverse $e^{\Delta\tau k}$ requires no extra work: one only has to reverse the sign of the off-diagonal elements.
In the checkerboard breakup we use, we write $e^{-\Delta\tau k}$ as a product of four sparse matrices and the scalar factor $e^{\Delta\tau\mu}$. One of these matrices, a, allows hopping between sites (i_x, i_y) and sites $(i_x + 1, i_y)$ with i_x even, a second, b, with i_x odd. The third and fourth matrices, c and d, allow for hopping between sites (i_x, i_y) and $(i_x, i_y + 1)$ with i_y even and odd.

Explicitly, these matrices are:

$$a = -\begin{pmatrix} 0 & 0 & 0 & t & 0 & 0 & 0 & 0 \\ 0 & 0 & t & 0 & 0 & 0 & 0 & 0 \\ 0 & t & 0 & 0 & 0 & 0 & 0 & 0 \\ t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & t \\ 0 & 0 & 0 & 0 & 0 & 0 & t & 0 \\ 0 & 0 & 0 & 0 & 0 & t & 0 & 0 \\ 0 & 0 & 0 & 0 & t & 0 & 0 & 0 \end{pmatrix} \qquad b = -\begin{pmatrix} 0 & t & 0 & 0 & 0 & 0 & 0 & 0 \\ t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & t & 0 & 0 & 0 & 0 \\ 0 & 0 & t & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & t & 0 & 0 \\ 0 & 0 & 0 & 0 & t & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & t \\ 0 & 0 & 0 & 0 & 0 & 0 & t & 0 \end{pmatrix}$$

$$c = d = -\begin{pmatrix} 0 & 0 & 0 & 0 & t & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & t & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & t & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & t \\ t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & t & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & t & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & t & 0 & 0 & 0 & 0 \end{pmatrix}$$

With these we can write $e^{-\Delta\tau k}$ as

$$e^{-\Delta\tau k} \approx \underbrace{e^{-\Delta\tau a}}_{=:A}\underbrace{e^{-\Delta\tau b}}_{=:B}\underbrace{e^{-\Delta\tau c}}_{=:C}\underbrace{e^{-\Delta\tau d}}_{=:D} \cdot e^{\Delta\tau\mu} = ABCD \cdot e^{\Delta\tau\mu}$$

and $e^{\Delta\tau k}$ as

$$e^{\Delta\tau k} \approx \left(ABCD \cdot e^{\Delta\tau\mu}\right)^{-1} = e^{-\Delta\tau\mu} \cdot D^{-1}C^{-1}B^{-1}A^{-1}.$$

So we finally get for the single-particle propagator in (22)

$$B_l^{\uparrow/\downarrow} = e^{\mp\Delta\tau\lambda v(l)}e^{-\Delta\tau k} \approx e^{\mp\Delta\tau\lambda v(l)}ABCD \cdot e^{\Delta\tau\mu},$$

which means that the particles diffuse in real space for a small imaginary time $\Delta\tau$ according to $ABCD$, their propagators are amplified or attenuated through the scalar factor $e^{\Delta\tau\mu}$, and finally are scattered by the external fields described by $e^{\mp\Delta\tau\lambda v(l)}$, to which the up and down fermions couple differently [4].

3.8 The sign problem

The so-called "sign problem" is encountered when the functional integrals, which are to be evaluated, do not have a positive-semidefinite measure [2]. It is not related to any approximations or fundamental errors in our DQMC algorithm, it just describes the situation that the statistical error can become very large.

In general, the expectation value of any observable O can be written as

$$\langle O \rangle = \frac{\int O(x)\, p(x)\, \mathrm{d}x}{\int p(x)\, \mathrm{d}x},$$

where $O(x)$ and $p(x)$ are known real functions of the (continuous) field variable denoted by x. If $p(x)$ changes its sign, it cannot be considered as a probability distribution. The standard trick that is used to avoid this difficulty is to write $p(x)$ as $|p(x)|\,\mathrm{sgn}(p(x))$ and to absorb the sign of $p(x)$, $\mathrm{sgn}(p(x))$, in the quantity to be measured,

$$\langle O \rangle = \frac{\int O(x)\, |p(x)|\, \mathrm{sgn}(p(x))\, \mathrm{d}x}{\int |p(x)|\, \mathrm{sgn}(p(x))\, \mathrm{d}x} = \frac{\dfrac{\int O(x)\, \mathrm{sgn}(p(x))\, |p(x)|\, \mathrm{d}x}{\int |p(x)|\, \mathrm{d}x}}{\dfrac{\int \mathrm{sgn}(p(x))\, |p(x)|\, \mathrm{d}x}{\int |p(x)|\, \mathrm{d}x}} = \frac{\langle Os \rangle}{\langle s \rangle}. \tag{28}$$

However, if the average sign, $\langle s \rangle$, is close to zero, this estimator for $\langle O \rangle$ is very noisy [3].

We will illustrate this point guided by the average sign [2]. Denoting the probability for measuring a positive sign by p_+ and that for measuring a negative one by p_- ($p_+ + p_- = 1$), we get

$$\langle s \rangle = (+1)\, p_+ + (-1)\, p_- = p_+ - p_-.$$

Now, if $p_- \approx p_+$, we get $\langle s \rangle \approx 0$ and hence for the variance

$$\sigma^2 = \left\langle (\Delta s)^2 \right\rangle = (1 - \langle s \rangle)^2\, p_+ + (-1 - \langle s \rangle)^2\, p_- \approx p_+ + p_- = 1.$$

Furthermore, we get for the standard deviation $\sigma = \sqrt{\sigma^2} \approx 1$, which means that we finally get a relative statistical error

$$\mathrm{rel} = \frac{\sigma}{\langle s \rangle} \gg 1.$$

So in practice, one needs $\langle s \rangle > 0.1$ in order to obtain useful estimates for $\langle O \rangle$.

3.9 First measurements and comparison of the results with those obtained from exact diagonalization

In the half-filled Hubbard model, $\langle n \rangle = 1$, even though $\det(M^\sigma(l)) < 0$, particle-hole symmetry dictates $\mathrm{sgn}\Big(\det\Big(M^\uparrow(l)\Big)\Big) = \mathrm{sgn}\Big(\det\Big(M^\downarrow(l)\Big)\Big)$ and so the product $\det\Big(M^\uparrow(l)\Big)\det\Big(M^\downarrow(l)\Big)$ in (23) is never negative. Off half-filling, $\langle n \rangle \neq 1$, however, the product is negative for some configurations and one must use $\Big|\det\Big(M^\uparrow(l)\Big)\det\Big(M^\downarrow(l)\Big)\Big|$ as the probability distribution for the Monte Carlo simulation [3], and the expectation value of an observable O is calculated via (28).

Here we want to, for the first time, apply our DQMC algorithm to our 4×2 lattice at half-filling and compare the results with those obtained from exact diagonalization. To this end we first

need to figure out "good" values for the simulation parameters that we need. As mentioned in the very beginning, the expression (4) is only approximate since V and K do not commute. However, the approximation becomes better and better as $\Delta\tau$ decreases (L increases). The errors should be pretty small if

$$t\,U\,\Delta\tau^2 < \frac{1}{10}.$$

For typical parameters, $t = 1$ and $U = 4$, we choose $\Delta\tau = \frac{1}{30}$. And we have set m, the number of B_l^σ matrices one can multiply without losing numerical accuracy, as well as m', the number of times one can advance the Green's function to a new time slice, using (26), without introducing unacceptable errors, requiring that m and m' are roughly equal [3] and

$$t\,\Delta\tau\,m \leq 1.5,$$

both to 10. Furthermore, since we know $g^S(c_{i\sigma}c_{j\sigma}^\dagger) = (g^\sigma)_{ij}$, we immediately get the expression for $g^S(c_{i\sigma}^\dagger c_{j\sigma})$,

$$g^S(c_{i\sigma}^\dagger c_{j\sigma}) = g^S(\delta_{ij} - c_{j\sigma}c_{i\sigma}^\dagger) = g^S(\delta_{ij}) - g^S(c_{j\sigma}c_{i\sigma}^\dagger) = \delta_{ij} - (g^\sigma)_{ji}\,.$$

With this expression we can immediately write down the expression for the average electron density of spin σ on site i,

$$\langle n_{i\sigma}\rangle = \left\langle c_{i\sigma}^\dagger c_{i\sigma}\right\rangle = g^S(c_{i\sigma}^\dagger c_{i\sigma}) = 1 - (g^\sigma)_{ii}\,,$$

as well as that for the average double occupancy rate on site i,

$$\langle n_{i\uparrow}\,n_{i\downarrow}\rangle = \langle n_{i\uparrow}\rangle\,\langle n_{i\downarrow}\rangle = \left(1 - \left(g^\uparrow\right)_{ii}\right)\left(1 - \left(g^\downarrow\right)_{ii}\right).$$

With that and (1) in mind, we can now easily perform the evaluation of $\langle H\rangle$.

For the exact diagonalization method, one needs to find all eigenvalues $E^{(\nu)}_{N_\uparrow,N_\downarrow}$ for all possible particle number pairs for our 4×2 lattice, and then, using (3), calculate

$$Z = \sum_{N_\uparrow N_\downarrow}\sum_{\nu} e^{-\beta\left(E^{(\nu)}_{N_\uparrow,N_\downarrow} - \mu\left(N_\uparrow + N_\downarrow\right)\right)} \qquad \text{and}$$

$$\langle H\rangle = \frac{1}{Z}\sum_{N_\uparrow N_\downarrow}\sum_{\nu} E^{(\nu)}_{N_\uparrow,N_\downarrow} e^{-\beta\left(E^{(\nu)}_{N_\uparrow,N_\downarrow} - \mu\left(N_\uparrow + N_\downarrow\right)\right)}.$$

The results are shown in figure 1.

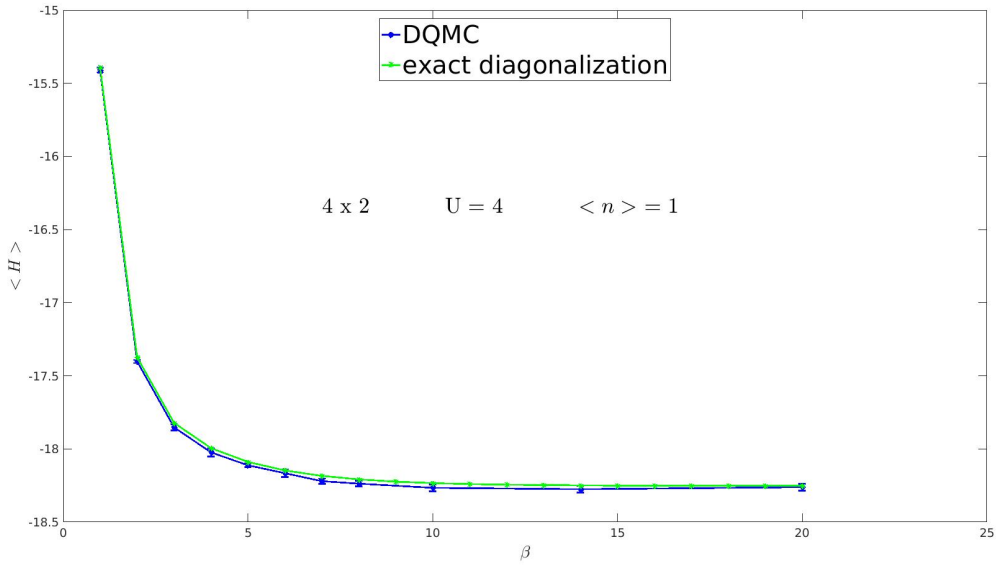

Figure 1: $\langle H \rangle$ vs β for a 4×2 lattice and comparison with the exact diagonalization method.

For a given inverse temperature β, the data point is obtained by doing 8000 full sweeps of the lattice for each of eight independent Markov chains, where unequal-time measurements are performed every second full sweep, yielding 32000 data points in total [5]. The statistical error bar is obtained from the sample variance over the eight independent chains.
In fact, for all simulations that are still to come throughout this work, we use exactly this set of simulation parameters, if not otherwise mentioned.

4 Numerical results

Here we just want to present a few results for a band off half-filling.

Figure 2 shows the average density $\langle n \rangle = \frac{\langle \hat{N} \rangle}{N} = \frac{1}{N} \sum_i (\langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle)$ as a function of the chemical potential μ for various lattice sizes and inverse temperatures.

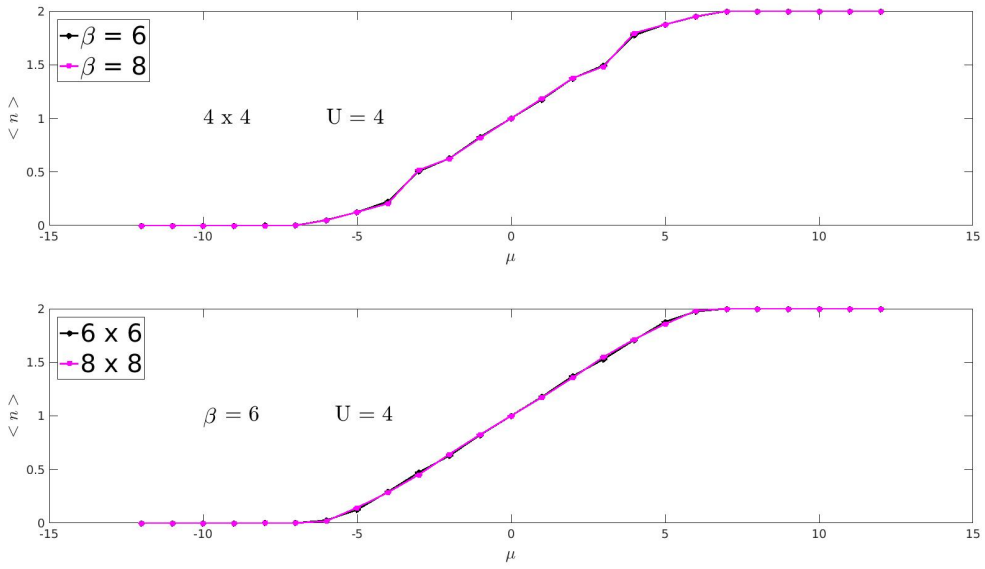

Figure 2: $\langle n \rangle$ vs μ for various lattice sizes and inverse temperatures.

As one can see, the curves are never less than zero, which corresponds to zero particles on the lattice, they are never greater than two, which means $N_\uparrow + N_\downarrow = 2N$, and they all represent half-filling, $\langle n \rangle = 1$, at $\mu = 0$.
Figure 3 shows the average sign as a function of band-filling for the same parameter set as in figure 2.

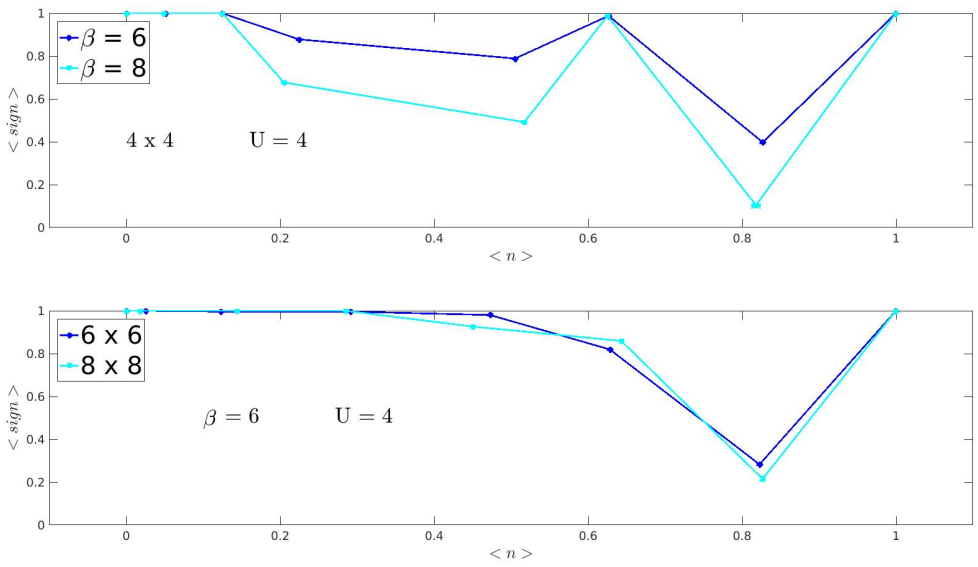

Figure 3: Average sign vs $\langle n \rangle$ for various lattice sizes and inverse temperatures.

As one can see, the sign problem is absent at half-filling, $\langle n \rangle = 1$, as well as at an empty band, $\langle n \rangle = 0$. In the region between zero and N particles on the lattice, the average sign decreases as the spatial and temporal sizes of the lattice increase [3]. The peak at a filling of 0.625 for the 4×4 lattice is striking. This filling corresponds to the presence of ten particles, which just fills the five lowest k-states, leaving a gap to the next empty k-state.

II The Hubbard model using the real continuous Hubbard-Stratonovich transformation

5 Introduction

In this second part of the thesis we will modify the Hubbard model and the DQMC algorithm that we have introduced in the previous part by using the real continuous Hubbard-Stratonovich transformation instead of the real discrete one. The reason for this is it lay the foundation to what we will be doing in the next part of the thesis, where we will be using the complex continuous Hubbard-Stratonovich transformation and apply it to the Hubbard-Holstein model. But, contrary to the previous part, we will not again explain the whole algorithm in detail, but instead only discuss what changes in our efficient update scheme.

6 A new transformation of the grand canonical partition function

We start out with the Hamilton operator of the Hubbard model (2)

$$\mathcal{H} = H - \mu N = U \sum_i \left(n_{i\uparrow} - \tfrac{1}{2}\right)\left(n_{i\downarrow} - \tfrac{1}{2}\right) + K.$$

Taking into account the useful relation

$$\left(n_{i\uparrow} \pm n_{i\downarrow}\right)^2 = {n_{i\uparrow}}^2 + {n_{i\downarrow}}^2 \pm 2 n_{i\uparrow} n_{i\downarrow} \quad \Longleftrightarrow \quad n_{i\uparrow} n_{i\downarrow} = \pm \frac{1}{2}\left(\left(n_{i\uparrow} \pm n_{i\downarrow}\right)^2 - \left(n_{i\uparrow} + n_{i\downarrow}\right)\right),$$

we get for the Coulomb repulsion on lattice point i

$$\begin{aligned} U\left(n_{i\uparrow} - \tfrac{1}{2}\right)\left(n_{i\downarrow} - \tfrac{1}{2}\right) &= U\left(n_{i\uparrow} n_{i\downarrow} + \frac{1}{4} - \frac{1}{2}\left(n_{i\uparrow} + n_{i\downarrow}\right)\right) = \\ &= U\left(-\frac{1}{2}\left(n_{i\uparrow} - n_{i\downarrow}\right)^2 + \frac{1}{2}\left(n_{i\uparrow} + n_{i\downarrow}\right) + \frac{1}{4} - \frac{1}{2}\left(n_{i\uparrow} + n_{i\downarrow}\right)\right) = \\ &= -\frac{U}{2}\left(n_{i\uparrow} - n_{i\downarrow}\right)^2 + \frac{U}{4}, \end{aligned} \tag{29}$$

where we have let it couple to the magnetization.
With that we can now, using (5), derive the expression for the real continuous Hubbard-Stratonovich transformation,

$$\begin{aligned} e^{-\Delta\tau U\left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right)} &= e^{-\Delta\tau \frac{U}{4}} e^{\Delta\tau \frac{U}{2}\left(n_{i\uparrow} - n_{i\downarrow}\right)^2} = e^{-\Delta\tau \frac{U}{4}} e^{\frac{2\Delta\tau U\left(n_{i\uparrow} - n_{i\downarrow}\right)^2}{4}} = \\ &= e^{-\Delta\tau \frac{U}{4}} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\sigma^2 - \sigma\sqrt{2\Delta\tau U}\left(n_{i\uparrow} - n_{i\downarrow}\right)} \, \mathrm{d}\sigma = \\ &= e^{-\Delta\tau \frac{U}{4}} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\sigma^2 - \sigma\lambda\left(n_{i\uparrow} - n_{i\downarrow}\right)} \, \mathrm{d}\sigma \qquad , \lambda = \sqrt{2\Delta\tau U}. \end{aligned}$$

We have now assembled all of the ingredients necessary to derive the new expression for the grand canonical partition function of the Hubbard model,

$$
\begin{aligned}
Z &= \operatorname{tr}\left(e^{-\beta(H-\mu N)}\right) = \operatorname{tr}\left(e^{-L\Delta\tau\left(U\sum_i\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)+K\right)}\right) = \operatorname{tr}\left(\left(e^{-\Delta\tau U\sum_i\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)}e^{-\Delta\tau K}+\mathcal{O}(\Delta\tau^2)\right)^L\right)\approx \\
&\approx \operatorname{tr}\left(\left(\prod_i\left(e^{-\Delta\tau U\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)}\right)e^{-\Delta\tau K}\right)^L\right) = \operatorname{tr}\left(\left(\prod_i\left(e^{-\Delta\tau\frac{U}{4}}\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}e^{-\sigma^2-\sigma\lambda\left(n_{i\uparrow}-n_{i\downarrow}\right)}\,\mathrm{d}\sigma\right)e^{-\Delta\tau K}\right)^L\right) = \\
&= \frac{e^{-\Delta\tau\frac{U}{4}NL}}{\pi^{\frac{NL}{2}}}\int_{\mathbb{R}^{N\times L}}\operatorname{tr}\left(\prod_{l=1}^{L}\prod_i\left(e^{-\sigma_{il}^2-\sigma_{il}\lambda\left(n_{i\uparrow}-n_{i\downarrow}\right)}\right)e^{-\Delta\tau K}\right)\mathrm{d}\sigma = \\
&= \left(\frac{e^{-\beta\frac{U}{2}}}{\pi^L}\right)^{\frac{N}{2}}\int_{\mathbb{R}^{N\times L}}e^{-|\sigma^2|}\operatorname{tr}\left(\prod_{l=1}^{L}e^{-\lambda\sum_i\sigma_{il}\left(n_{i\uparrow}-n_{i\downarrow}\right)}e^{-\Delta\tau\left(K_\uparrow+K_\downarrow\right)}\right)\mathrm{d}\sigma = \\
&= \left(\frac{e^{-\beta\frac{U}{2}}}{\pi^L}\right)^{\frac{N}{2}}\int_{\mathbb{R}^{N\times L}}e^{-|\sigma^2|}\prod_{s\in\{\pm1\}}\left(\operatorname{tr}_s\left(\prod_{l=1}^{L}e^{s(-\lambda)\sum_i\sigma_{il}n_{is}}e^{-\Delta\tau K_s}\right)\right)\mathrm{d}\sigma = \\
&= \left(\frac{e^{-\beta\frac{U}{2}}}{\pi^L}\right)^{\frac{N}{2}}\int_{\mathbb{R}^{N\times L}}e^{-|\sigma^2|}\prod_{s\in\{\pm1\}}\left(\operatorname{tr}_s\left(\prod_{l=1}^{L}e^{\vec{c_s}^\dagger s(-\lambda)G^{(l)}\vec{c_s}}e^{\vec{c_s}^\dagger(-\Delta\tau)k\vec{c_s}}\right)\right)\mathrm{d}\sigma = \\
&= \left(\frac{e^{-\beta\frac{U}{2}}}{\pi^L}\right)^{\frac{N}{2}}\int_{\mathbb{R}^{N\times L}}\underbrace{e^{-|\sigma^2|}\det\left(\mathbb{1}+\prod_{l=1}^{L}e^{-\lambda G^{(l)}}e^{-\Delta\tau k}\right)\det\left(\mathbb{1}+\prod_{l=1}^{L}e^{\lambda G^{(l)}}e^{-\Delta\tau k}\right)}_{=:\rho(\sigma)}\mathrm{d}\sigma = \\
&= \left(\frac{e^{-\beta\frac{U}{2}}}{\pi^L}\right)^{\frac{N}{2}}\int_{\mathbb{R}^{N\times L}}\rho(\sigma)\,\mathrm{d}\sigma,
\end{aligned}
$$

where $\left|\sigma^2\right| \coloneqq \sum_{l=1}^{L}\sum_i\sigma_{il}^2$ and $\left(G^{(l)}\right)_{ij} = \delta_{ij}\sigma_{il}$. This time we have chosen the time ordering in increasing order and, with $B_l^{\uparrow/\downarrow} \coloneqq e^{\mp\lambda G^{(l)}}e^{-\Delta\tau k}$, the fermion matrix $M^{\uparrow/\downarrow}(l)$ is now defined as

$$M^{\uparrow/\downarrow}(l) \coloneqq \mathbb{1} + B_l^{\uparrow/\downarrow}\cdots B_L^{\uparrow/\downarrow}B_1^{\uparrow/\downarrow}\cdots B_{l-1}^{\uparrow/\downarrow}.$$

7 Changes in the Monte Carlo simulation

So our grand canonical partition function has become continuous and we will from now on be using normally distributed random numbers for the Hubbard-Stratonovich fields in the Monte Carlo simulations instead of uniformly distributed ones.
In general, the probability density function (PDF) of the normal distribution with expectation value x_0 and variance v^2, $\mathcal{N}(x_0, v^2)$, is

$$f(x|x_0, v^2) = \frac{1}{\sqrt{2\pi v^2}}\, e^{-\frac{(x-x_0)^2}{2v^2}}.$$

We will sample our Hubbard-Stratonovich fields σ from $\mathcal{N}(0, \frac{1}{2})^{N\times L}$, hence we get for our PDF for the continuous field variable σ_{il} (for site i and imaginary-time slice l)

$$f(\sigma_{il}|0, \tfrac{1}{2}) = \frac{1}{\sqrt{\pi}}\, e^{-\sigma_{il}^2}. \tag{30}$$

In order to get the ratio $R = \frac{P(\sigma')}{P(\sigma)}$ for our Metropolis-Hastings algorithm we start out with the detailed balance condition,

$$P(\sigma'|\sigma)\, P(\sigma) = P(\sigma|\sigma')\, P(\sigma') \quad \Longleftrightarrow \quad \frac{P(\sigma'|\sigma)}{P(\sigma|\sigma')} = \frac{P(\sigma')}{P(\sigma)}.$$

Writing the transition probability $P(\sigma'|\sigma)$ as a product of the proposal distribution $g(\sigma'|\sigma)$ and the acceptance distribution $A(\sigma'|\sigma)$ leads to

$$\frac{g(\sigma'|\sigma)\, A(\sigma'|\sigma)}{g(\sigma|\sigma')\, A(\sigma|\sigma')} = \frac{P(\sigma')}{P(\sigma)} \quad \Longleftrightarrow \quad \frac{A(\sigma'|\sigma)}{A(\sigma|\sigma')} = \frac{P(\sigma')}{P(\sigma)}\, \frac{g(\sigma|\sigma')}{g(\sigma'|\sigma)} = \frac{\rho(\sigma')}{\rho(\sigma)}\, \frac{\frac{1}{Z}\, g(\sigma|\sigma')}{\frac{1}{Z}\, g(\sigma'|\sigma)}. \tag{31}$$

Now, in order to propose a $\sigma \in \mathcal{N}(0, \frac{1}{2})^{N\times L}$, we must introduce (30) for each site i and each time slice l in (31) yielding

$$\begin{aligned}\frac{A(\sigma'|\sigma)}{A(\sigma|\sigma')} = \frac{\rho(\sigma')}{\rho(\sigma)}\, \frac{\left(\frac{1}{\sqrt{\pi}}\right)^{NL} \prod_{l=1}^{L} \prod_{i} e^{-\sigma_{il}^2}}{\left(\frac{1}{\sqrt{\pi}}\right)^{NL} \prod_{l=1}^{L} \prod_{i} e^{-\sigma_{il}'^2}} = \frac{e^{-|\sigma'^2|}\, \det\!\left(M^{\uparrow}(l)'\right) \det\!\left(M^{\downarrow}(l)'\right)}{e^{-|\sigma^2|}\, \det(M^{\uparrow}(l)) \det(M^{\downarrow}(l))}\, \frac{e^{-|\sigma^2|}}{e^{-|\sigma'^2|}} = \\ = \frac{\det\!\left(M^{\uparrow}(l)'\right)}{\det(M^{\uparrow}(l))}\, \frac{\det\!\left(M^{\downarrow}(l)'\right)}{\det(M^{\downarrow}(l))}.\end{aligned} \tag{32}$$

So, we finally get for the acceptance probability $A(\sigma'|\sigma)$ that fulfills the condition above,

$$A(\sigma'|\sigma) = \min\left(1, \left|\frac{\det\!\left(M^{\uparrow}(l)'\right)}{\det(M^{\uparrow}(l))}\, \frac{\det\!\left(M^{\downarrow}(l)'\right)}{\det(M^{\downarrow}(l))}\right|\right).$$

The sign of the probability distribution for a given Hubbard-Stratonovich field value σ, $\rho(\sigma)$, simply is

$$\operatorname{sgn}(\rho(\sigma)) = \frac{\rho(\sigma)}{|\rho(\sigma)|} = \frac{e^{-|\sigma^2|}\det\left(M^{\uparrow}(l)\right)\det\left(M^{\downarrow}(l)\right)}{e^{-|\sigma^2|}\left|\det(M^{\uparrow}(l))\det(M^{\downarrow}(l))\right|} = \frac{\det\left(M^{\uparrow}(l)\right)\det\left(M^{\downarrow}(l)\right)}{\left|\det(M^{\uparrow}(l))\det(M^{\downarrow}(l))\right|}.$$

Furthermore, the matrix $\Delta^{\uparrow/\downarrow}(i,l)$ turns into

$$\left(\Delta^{\uparrow/\downarrow}(i,l)\right)_{jk} = \delta_{ji}\,\delta_{ki}\left(e^{\mp\lambda\left(\sigma'_{il}-\sigma_{il}\right)}-1\right).$$

Apart from everything that we have just discussed, the rest of the ingredients for our efficient update scheme stays the same, except for the wrapping of the Green's function, which now goes according to

$$g^{\uparrow/\downarrow}(l+1) = \left(B_l^{\uparrow/\downarrow}\right)^{-1} g^{\uparrow/\downarrow}(l)\,B_l^{\uparrow/\downarrow}.$$

8 Comparison of the new results with those obtained from exact diagonalization

Here we just want to apply the changes in the Monte Carlo simulation to our 4×2 lattice at half-filling and, just as we did before, compare the results with those obtained from exact diagonalization. The results are shown in figure 4.

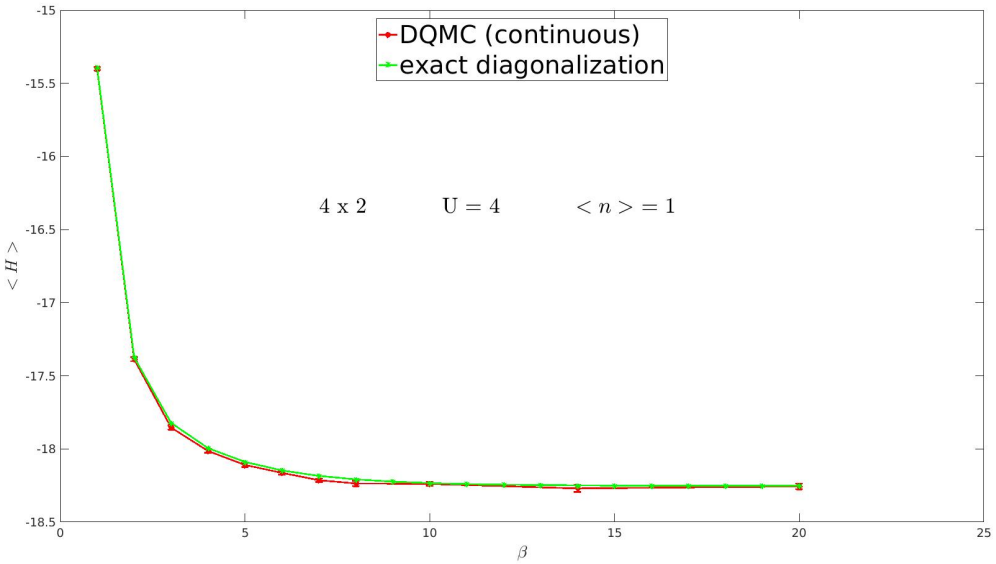

Figure 4: $\langle H \rangle$ vs β for a 4×2 lattice and comparison with the exact diagonalization method.

III The Hubbard-Holstein model using the complex continuous Hubbard-Stratonovich transformation

9 Introduction

In this third and last part of the thesis we will for the first time introduce the Hubbard-Holstein model, a simple model capturing the physics of itinerant electrons with both electron-electron and electron-phonon interactions [6]. In this model the motion of the lattice sites is described by a set of independent harmonic oscillators, one at each site i. The electron-electron interaction is treated as usual and the electron-phonon interaction arises from a linear coupling of the local density n_i to the atomic displacement x_i.
When carrying out simulations for the Hubbard-Holstein model, one usually needs to focus on the additional aspect associated with the treatment of the phonon degrees of freedom, meaning that one needs to sample the phonon fields separately. This will lead to a sign problem at half-filling for a nonzero electron-phonon coupling strength, because most phonon configurations $x \in \mathbb{R}^{N\times L}$ break the particle-hole symmetry.
But here, we will present a totally new approach where we will be using the complex continuous Hubbard-Stratonovich transformation to derive an expression for the grand canonical partition function of the Hubbard-Holstein model with the phonon degrees of freedom being explicitly integrated out in order not to have to sample the phonon fields. This will solve the sign problem at half-filling for any electron-phonon coupling strength, but only there.

10 The Hubbard-Holstein model

For the Hubbard-Holstein model the Hamilton operator is

$$H = H_{\text{el}} + H_{\text{ph}} + V_{\text{el-ph}},$$

where

$$\begin{aligned} H_{\text{el}} &= \mathcal{H} = H_{\text{kin}} + H_{\text{C}} - \mu N = \\ &= -t \sum_{\sigma=\uparrow,\downarrow} \sum_{<i,j>} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_i \left(n_{i\uparrow} - \tfrac{1}{2} \right) \left(n_{i\downarrow} - \tfrac{1}{2} \right) - \mu \sum_i \left(n_{i\uparrow} + n_{i\downarrow} \right), \\ H_{\text{ph}} &= \sum_i \left(\tfrac{p_i^2}{2m} + \tfrac{m\omega^2}{2} x_i^2 \right) \end{aligned}$$

describes longitudinal vibrations of the N sites, and

$$V_{\text{el-ph}} = -g \sum_i n_i \left(a_i^{\dagger} + a_i \right)$$

is the Holstein electron-phonon coupling.
Using the useful representation of x_i in terms of the ladder operators a_i and $a_i^{\dagger}$ for a N-dimensional harmonic oscillator,

$$x_i = \sqrt{\frac{\hbar}{2m\omega}} \left(a_i^{\dagger} + a_i \right),$$

we can rewrite $V_{\text{el-ph}}$ as

$$V_{\text{el-ph}} = -g \sqrt{\frac{2m\omega}{\hbar}} \sum_i \left(n_{i\uparrow} + n_{i\downarrow} \right) x_i.$$

For simplicity we set $m = \hbar = 1$, which finally leads to

$$\begin{aligned} H = &-t \sum_{\sigma=\uparrow,\downarrow} \sum_{<i,j>} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_i \left(n_{i\uparrow} - \tfrac{1}{2} \right) \left(n_{i\downarrow} - \tfrac{1}{2} \right) - \mu \sum_i \left(n_{i\uparrow} + n_{i\downarrow} \right) + \\ &+ \sum_i \left(\tfrac{p_i^2}{2} + \tfrac{\omega^2}{2} x_i^2 \right) - \alpha \sum_i \left(n_{i\uparrow} + n_{i\downarrow} \right) x_i, \end{aligned} \tag{33}$$

where $\alpha := g\sqrt{2\omega}$ is now our coupling constant.

Next, we will use the asymmetric particle-hole transformation

$$\begin{aligned} c_{i\uparrow}^\dagger &\to c_{i\uparrow}^\dagger & \qquad c_{i\downarrow}^\dagger &\to e^{\mathrm{i}\vec{Q}^\mathrm{t}\vec{x}_i}\, c_{i\downarrow} \\ c_{i\uparrow} &\to c_{i\uparrow} & \qquad c_{i\downarrow} &\to e^{-\mathrm{i}\vec{Q}^\mathrm{t}\vec{x}_i}\, c_{i\downarrow}^\dagger \end{aligned}, \tag{34}$$

which turns (33) into

$$\begin{aligned} \widetilde{H} &= -t\left(\sum_{<i,j>}\left(c_{i\uparrow}^\dagger c_{j\uparrow} + c_{j\uparrow}^\dagger c_{i\uparrow}\right) + \sum_{<i,j>}\left(e^{\mathrm{i}\vec{Q}^\mathrm{t}\vec{x}_i}\, c_{i\downarrow}\, e^{-\mathrm{i}\vec{Q}^\mathrm{t}\vec{x}_j}\, c_{j\downarrow}^\dagger + e^{\mathrm{i}\vec{Q}^\mathrm{t}\vec{x}_j}\, c_{j\downarrow}\, e^{-\mathrm{i}\vec{Q}^\mathrm{t}\vec{x}_i}\, c_{i\downarrow}^\dagger\right)\right) + \\ &+ U\sum_i\left(n_{i\uparrow} - \tfrac{1}{2}\right)\left(e^{\mathrm{i}\vec{Q}^\mathrm{t}\vec{x}_i}\, c_{i\downarrow}\, e^{-\mathrm{i}\vec{Q}^\mathrm{t}\vec{x}_i}\, c_{i\downarrow}^\dagger - \tfrac{1}{2}\right) - \mu\sum_i\left(n_{i\uparrow} + e^{\mathrm{i}\vec{Q}^\mathrm{t}\vec{x}_i}\, c_{i\downarrow}\, e^{-\mathrm{i}\vec{Q}^\mathrm{t}\vec{x}_i}\, c_{i\downarrow}^\dagger\right) + \\ &+ \sum_i\left(\tfrac{p_i^2}{2} + \tfrac{\omega^2}{2}x_i^2\right) - \alpha\sum_i\left(n_{i\uparrow} + e^{\mathrm{i}\vec{Q}^\mathrm{t}\vec{x}_i}\, c_{i\downarrow}\, e^{-\mathrm{i}\vec{Q}^\mathrm{t}\vec{x}_i}\, c_{i\downarrow}^\dagger\right)x_i = \\ &= -t\left(\sum_{<i,j>}\left(c_{i\uparrow}^\dagger c_{j\uparrow} + c_{j\uparrow}^\dagger c_{i\uparrow}\right) + \sum_{<i,j>}\left(e^{\mathrm{i}\vec{Q}^\mathrm{t}\left(\vec{x}_i - \vec{x}_j\right)}\left(-c_{j\downarrow}^\dagger c_{i\downarrow}\right) + e^{\mathrm{i}\vec{Q}^\mathrm{t}\left(\vec{x}_j - \vec{x}_i\right)}\left(-c_{i\downarrow}^\dagger c_{j\downarrow}\right)\right)\right) + \\ &+ U\sum_i\left(n_{i\uparrow} - \tfrac{1}{2}\right)\left(\tfrac{1}{2} - n_{i\downarrow}\right) - \mu\sum_i\left(n_{i\uparrow} + 1 - n_{i\downarrow}\right) + \sum_i\left(\tfrac{p_i^2}{2} + \tfrac{\omega^2}{2}x_i^2\right) - \alpha\sum_i\left(n_{i\uparrow} + 1 - n_{i\downarrow}\right)x_i. \end{aligned}$$

Because $\vec{x}_i$ and $\vec{x}_j$ are the position vectors of the two neighboring sites i and j we have

$$\vec{x}_i - \vec{x}_j = -\left(\vec{x}_j - \vec{x}_i\right) \in \left\{\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}, -\begin{pmatrix}1\\0\end{pmatrix}, -\begin{pmatrix}0\\1\end{pmatrix}\right\},$$

and with $\vec{Q} = \begin{pmatrix}\pi\\\pi\end{pmatrix}$ we get

$$\begin{aligned} e^{\mathrm{i}\vec{Q}^\mathrm{t}\left(\vec{x}_i - \vec{x}_j\right)} &= e^{\pm\mathrm{i}\pi} = -1 \qquad \text{and} \\ e^{\mathrm{i}\vec{Q}^\mathrm{t}\left(\vec{x}_j - \vec{x}_i\right)} &= e^{\mp\mathrm{i}\pi} = -1 \qquad \forall < i, j >, \end{aligned}$$

and hence

$$\begin{aligned} \widetilde{H} &= -t\sum_{\sigma=\uparrow,\downarrow}\sum_{<i,j>}\left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}\right) - U\sum_i\left(n_{i\uparrow} - \tfrac{1}{2}\right)\left(n_{i\downarrow} - \tfrac{1}{2}\right) - \mu\underbrace{\sum_i\left(n_{i\uparrow} - n_{i\downarrow}\right)}_{=\hat{M}} - \mu N + \\ &+ \sum_i\left(\tfrac{p_i^2}{2} + \tfrac{\omega^2}{2}x_i^2\right)\underbrace{-\alpha\sum_i\left(n_{i\uparrow} - n_{i\downarrow}\right)x_i - \alpha\sum_i x_i}_{=:H_\alpha} = \\ &= H_\mathrm{kin} - H_\mathrm{C} - \mu\hat{M} - \mu N + H_\mathrm{ph} + H_\alpha. \end{aligned} \tag{35}$$

So, the actual transformation was

$$\begin{aligned} n_{i\uparrow} &\to n_{i\uparrow} \\ n_{i\downarrow} &\to 1 - n_{i\downarrow} \end{aligned} \tag{36}$$

leaving the kinetic energy operator and the harmonic oscillator invariant, changing the sign of the Coulomb repulsion, which means that the interaction is now attractive instead, and introducing a homogeneous magnetic field.

11 Transformation of the grand canonical partition function

This time we will transform all parts of the Hamilton operator (35) that contain the occupation number operators $n_{i\uparrow}$ and $n_{i\downarrow}$, i.e.

$$f(\vec{n_\uparrow}, \vec{n_\downarrow}) \coloneqq -U \sum_i \left(n_{i\uparrow} - \tfrac{1}{2}\right)\left(n_{i\downarrow} - \tfrac{1}{2}\right) - \sum_i \left(n_{i\uparrow} - n_{i\downarrow}\right)(\mu + \alpha x_i)\,.$$

Using (29), we get for the i-th term of the function above

$$\begin{aligned} f(n_{i\uparrow}, n_{i\downarrow}) &= -U\left(n_{i\uparrow} - \tfrac{1}{2}\right)\left(n_{i\downarrow} - \tfrac{1}{2}\right) - (\mu + \alpha x_i)\left(n_{i\uparrow} - n_{i\downarrow}\right) = \\ &= \frac{U}{2}\left(n_{i\uparrow} - n_{i\downarrow}\right)^2 - \frac{U}{4} - (\mu + \alpha x_i)\left(n_{i\uparrow} - n_{i\downarrow}\right). \end{aligned}$$

With that we can now, using (6), derive the expression for the complex continuous Hubbard-Stratonovich transformation,

$$\begin{aligned} & e^{-\Delta\tau\left(-U\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)-(\mu+\alpha x_i)\left(n_{i\uparrow}-n_{i\downarrow}\right)\right)} = e^{\Delta\tau\frac{U}{4}} e^{-\Delta\tau\left(\frac{U}{2}\left(n_{i\uparrow}-n_{i\downarrow}\right)^2-(\mu+\alpha x_i)\left(n_{i\uparrow}-n_{i\downarrow}\right)\right)} = \\ & = e^{\Delta\tau\frac{U}{4}} e^{-\Delta\tau U\left(\frac{1}{2}\left(n_{i\uparrow}-n_{i\downarrow}\right)^2-\frac{\mu+\alpha x_i}{U}\left(n_{i\uparrow}-n_{i\downarrow}\right)\right)} = e^{\Delta\tau\frac{U}{4}} e^{-\frac{2\Delta\tau U\left(n_{i\uparrow}-n_{i\downarrow}\right)^2-4\Delta\tau U\frac{\mu+\alpha x_i}{U}\left(n_{i\uparrow}-n_{i\downarrow}\right)}{4}} = \\ & = e^{\Delta\tau\frac{U}{4}} e^{-\frac{\left(\sqrt{2\Delta\tau U}\left(n_{i\uparrow}-n_{i\downarrow}\right)-\sqrt{2\Delta\tau U}\frac{\mu+\alpha x_i}{U}\right)^2-2\Delta\tau U\frac{(\mu+\alpha x_i)^2}{U^2}}{4}} = \\ & = e^{\Delta\tau\frac{U}{4}} e^{\frac{\Delta\tau}{2U}(\mu+\alpha x_i)^2} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\sigma^2-\mathrm{i}\sigma\sqrt{2\Delta\tau U}\left(n_{i\uparrow}-n_{i\downarrow}-\frac{\mu+\alpha x_i}{U}\right)}\,\mathrm{d}\sigma = \\ & = e^{\Delta\tau\frac{U}{4}} e^{\frac{\Delta\tau}{2U}(\mu+\alpha x_i)^2} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\sigma^2-\mathrm{i}\sigma\lambda\left(n_{i\uparrow}-n_{i\downarrow}-\frac{\mu+\alpha x_i}{U}\right)}\,\mathrm{d}\sigma \qquad , \lambda = \sqrt{2\Delta\tau U}. \end{aligned}$$

By writing (35) as

$$\widetilde{H} = f(\vec{n_\uparrow}, \vec{n_\downarrow}) + H_{\text{kin}} + H_{\text{ph}} - \alpha \sum_i x_i - \mu N,$$

we have assembled all of the ingredients necessary to derive the expression for the grand canonical partition function of the Hubbard-Holstein model,

$$\begin{aligned}
Z &= \text{tr}\left(e^{-\beta\widetilde{H}}\right) = \text{tr}\left(e^{-L\Delta\tau\left(f(\vec{n_\uparrow},\vec{n_\downarrow})+H_{\text{kin}}+H_{\text{ph}}-\alpha\sum_i x_i-\mu N\right)}\right) = \\
&= \text{tr}\left(\left(e^{-\Delta\tau f(\vec{n_\uparrow},\vec{n_\downarrow})}e^{-\Delta\tau\left(H_{\text{kin}}+H_{\text{ph}}-\alpha\sum_i x_i-\mu N\right)} + O(\Delta\tau^2)\right)^L\right) \approx \\
&\approx \text{tr}\left(\left(e^{-\Delta\tau\sum_i\left(-U\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)-(\mu+\alpha x_i)\left(n_{i\uparrow}-n_{i\downarrow}\right)\right)}e^{-\Delta\tau\left(H_{\text{kin}}+H_{\text{ph}}-\alpha\sum_i x_i-\mu N\right)}\right)^L\right) \approx \\
&\approx \text{tr}\left(\left(\prod_i\left(e^{-\Delta\tau\left(-U\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)-(\mu+\alpha x_i)\left(n_{i\uparrow}-n_{i\downarrow}\right)\right)}\right)e^{-\Delta\tau\left(H_{\text{kin}}+H_{\text{ph}}-\alpha\sum_i x_i-\mu N\right)}\right)^L\right) = \\
&= \text{tr}\left(\left(\prod_i\left(e^{\Delta\tau\frac{U}{4}}e^{\frac{\Delta\tau}{2U}(\mu+\alpha x_i)^2}\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}e^{-\sigma^2-\text{i}\sigma\lambda\left(n_{i\uparrow}-n_{i\downarrow}-\frac{\mu+\alpha x_i}{U}\right)}\,\text{d}\sigma\right)e^{-\Delta\tau\left(H_{\text{kin}}+H_{\text{ph}}-\alpha\sum_i x_i-\mu N\right)}\right)^L\right) = \\
&= \left|\Delta\tau\frac{U}{4} + \frac{\Delta\tau}{2U}(\mu+\alpha x_i)^2 - \sigma^2 - \text{i}\sigma\lambda\left(n_{i\uparrow}-n_{i\downarrow}-\frac{\mu+\alpha x_i}{U}\right)\right. = \\
&= \frac{\Delta\tau U}{4} + \frac{\Delta\tau}{2U}\left(\mu^2+\alpha^2x_i^2+2\mu\alpha x_i\right) - \sigma^2 - \text{i}\sigma\lambda\left(n_{i\uparrow}-n_{i\downarrow}-\frac{\mu+\alpha x_i}{U}\right) = \\
&= \frac{\Delta\tau U}{4} + \frac{\Delta\tau}{2U}\mu^2 - \sigma^2 + \text{i}\sigma\lambda\frac{\mu}{U} - \text{i}\sigma\lambda\left(n_{i\uparrow}-n_{i\downarrow}\right) + \alpha x_i\left(\frac{\Delta\tau}{U}\mu + \frac{\text{i}\sigma\lambda}{U}\right) + \frac{\Delta\tau}{2U}\alpha^2x_i^2 = \\
&= \left|\frac{\mu}{U} =: c\right| = \\
&= \frac{\Delta\tau U}{4} + \frac{\Delta\tau U}{2}c^2 - \sigma^2 + \text{i}\sigma\lambda c - \text{i}\sigma\lambda\left(n_{i\uparrow}-n_{i\downarrow}\right) + \alpha x_i\left(\Delta\tau c + \frac{\text{i}\sigma\lambda}{U}\right) + \frac{\Delta\tau}{2U}\alpha^2x_i^2\right| = \\
&= \frac{e^{\frac{\Delta\tau U}{4}NL}e^{\frac{\Delta\tau U}{2}c^2NL}}{\pi^{\frac{NL}{2}}}\int_{\mathbb{R}^{N\times L}}\text{tr}\left(\prod_{l=1}^{L}\prod_i\left(e^{-\sigma_{il}^2+\text{i}\sigma_{il}\lambda c-\text{i}\sigma_{il}\lambda\left(n_{i\uparrow}-n_{i\downarrow}\right)+\alpha x_i\left(\Delta\tau c+\frac{\text{i}\sigma_{il}\lambda}{U}\right)+\frac{\Delta\tau}{2U}\alpha^2x_i^2}\right)\cdot\right. \\
&\qquad\left.\cdot\, e^{-\Delta\tau\left(H_{\text{kin}}+H_{\text{ph}}-\alpha\sum_i x_i\right)}e^{\Delta\tau\mu N}\right)\text{d}\sigma \approx
\end{aligned}$$

$$\approx e^{\beta\mu N}\left(\frac{e^{\beta U\left(c^2+\frac{1}{2}\right)}}{\pi^L}\right)^{\frac{N}{2}}\int\limits_{\mathbb{R}^{N\times L}} e^{-\left|\sigma^2\right|+\mathrm{i}|\sigma|\lambda c}\,\mathrm{tr}\Bigg(\prod_{l=1}^{L} e^{\sum\limits_i\left(-\mathrm{i}\sigma_{il}\,\lambda\left(n_{i\uparrow}-n_{i\downarrow}\right)+\alpha x_i\left(\Delta\tau c+\frac{\mathrm{i}\sigma_{il}\,\lambda}{U}\right)+\frac{\Delta\tau\alpha^2}{2U}x_i^2\right)}\cdot$$

$$\cdot\, e^{-\Delta\tau\left(H_{\mathrm{kin}}+H_{\mathrm{ph}}-\alpha\sum\limits_i x_i\right)}\Bigg)\mathrm{d}\sigma, \tag{37}$$

where $c=\frac{\mu}{U}$, $\left|\sigma^2\right|\coloneqq\sum\limits_{l=1}^{L}\sum\limits_i\sigma_{il}^2$ and $|\sigma|\coloneqq\sum\limits_{l=1}^{L}\sum\limits_i\sigma_{il}$. Again, it is clear-cut that the two spin contributions decouple, as well as $n_{i\uparrow}-n_{i\downarrow}$ and x_i.
By writing (37) as

$$Z=e^{\beta\mu N}\left(\frac{e^{\beta U\left(c^2+\frac{1}{2}\right)}}{\pi^L}\right)^{\frac{N}{2}}\int\limits_{\mathbb{R}^{N\times L}} e^{-\left|\sigma^2\right|+\mathrm{i}|\sigma|\lambda c}\,\mathrm{tr}\Bigg(\prod_{s\in\{\pm1\}}\Bigg(\prod_{l=1}^{L} e^{s(-\mathrm{i})\lambda\sum\limits_i\sigma_{il}\,n_{is}}e^{-\Delta\tau H_{\mathrm{kin}}^{s}}\Bigg)\cdot$$

$$\cdot\prod_{l=1}^{L} e^{\sum\limits_i\left(\frac{\Delta\tau\alpha^2}{2U}x_i^2+\alpha x_i\left(\Delta\tau c+\frac{\mathrm{i}\sigma_{il}\,\lambda}{U}\right)\right)}e^{-\Delta\tau\left(H_{\mathrm{ph}}-\alpha\sum\limits_i x_i\right)}\Bigg)\mathrm{d}\sigma,$$

the trace is of the form $\mathrm{tr}\left(O_\uparrow O_\downarrow O_{\mathrm{ph}}\right)$, where all three operators only act in their respective subspaces [7]. So, the trace can again be written as a product of the subtraces $\mathrm{tr}_\uparrow$, $\mathrm{tr}_\downarrow$ and $\mathrm{tr}_{\mathrm{ph}}$,

$$Z=e^{\beta\mu N}\left(\frac{e^{\beta U\left(c^2+\frac{1}{2}\right)}}{\pi^L}\right)^{\frac{N}{2}}\int\limits_{\mathbb{R}^{N\times L}} e^{-\left|\sigma^2\right|+\mathrm{i}|\sigma|\lambda c}\prod_{s\in\{\pm1\}}\Bigg(\mathrm{tr}_s\Bigg(\prod_{l=1}^{L} e^{\vec{c_s}^{\,\dagger}s(-\mathrm{i})\lambda G^{(l)}\vec{c_s}}e^{\vec{c_s}^{\,\dagger}(-\Delta\tau)(-t)h_{\mathrm{kin}}\vec{c_s}}\Bigg)\Bigg)\cdot$$

$$\cdot\,\mathrm{tr}_{\mathrm{ph}}\Bigg(\prod_{l=1}^{L} e^{\sum\limits_i\left(\frac{\Delta\tau\alpha^2}{2U}x_i^2+\alpha x_i\left(\Delta\tau c+\frac{\mathrm{i}\sigma_{il}\,\lambda}{U}\right)\right)}e^{-\Delta\tau\left(H_{\mathrm{ph}}-\alpha\sum\limits_i x_i\right)}\Bigg)\mathrm{d}\sigma=$$

$$=e^{\beta\mu N}\left(\frac{e^{\beta U\left(c^2+\frac{1}{2}\right)}}{\pi^L}\right)^{\frac{N}{2}}\int\limits_{\mathbb{R}^{N\times L}} e^{-\left|\sigma^2\right|+\mathrm{i}|\sigma|\lambda c}\left|\det\left(\mathbb{1}+\prod_{l=1}^{L} e^{-\mathrm{i}\lambda G^{(l)}}e^{\Delta\tau t h_{\mathrm{kin}}}\right)\right|^2\cdot$$

$$\cdot\,\mathrm{tr}_{\mathrm{ph}}\Bigg(\prod_{l=1}^{L} e^{\sum\limits_i\left(\frac{\Delta\tau\alpha^2}{2U}x_i^2+\alpha x_i\left(\Delta\tau c+\frac{\mathrm{i}\sigma_{il}\,\lambda}{U}\right)\right)}e^{-\Delta\tau\left(H_{\mathrm{ph}}-\alpha\sum\limits_i x_i\right)}\Bigg)\mathrm{d}\sigma. \tag{38}$$

Next, we will modify the phonon trace, which is the integral over the expectation values with respect to all phonon eigenstates $|\vec{x}\rangle$ [7]:

$$
\begin{aligned}
&\mathrm{tr}_{\mathrm{ph}}\left(\prod_{l=1}^{L} e^{\sum_i\left(\frac{\Delta\tau\alpha^2}{2U}x_i^2+\alpha x_i\left(\Delta\tau c+\frac{\mathrm{i}\sigma_{il}\lambda}{U}\right)\right)}e^{-\Delta\tau\left(H_{\mathrm{ph}}-\alpha\sum_i x_i\right)}\right)=\\
&=\int_{\mathbb{R}^N}\langle\vec{x}^{(1)}|\prod_{l=1}^{L}\left(e^{\sum_i\left(\frac{\Delta\tau\alpha^2}{2U}x_i^2+\alpha x_i\left(\Delta\tau c+\frac{\mathrm{i}\sigma_{il}\lambda}{U}\right)\right)}e^{-\Delta\tau\sum_i\left(\frac{p_i^2}{2}+\frac{\omega^2}{2}x_i^2-\alpha x_i\right)}\right)|\vec{x}^{(1)}\rangle\,\mathrm{d}\vec{x}^{(1)}\approx\\
&\approx\int_{\mathbb{R}^N}\langle\vec{x}^{(1)}|\prod_{l=1}^{L}\left(\int_{\mathbb{R}^N}|\vec{x}^{(l)}\rangle\langle\vec{x}^{(l)}|\,\mathrm{d}\vec{x}^{(l)}e^{\sum_i\left(-\frac{\Delta\tau}{2}\left(\omega^2-\frac{\alpha^2}{U}\right)x_i^2+\alpha x_i\left(\Delta\tau(c+1)+\frac{\mathrm{i}\sigma_{il}\lambda}{U}\right)\right)}\cdot\right.\\
&\qquad\left.\cdot\,e^{-\Delta\tau\sum_i\frac{p_i^2}{2}}\int_{\mathbb{R}^N}|\vec{x}^{(l+1)}\rangle\langle\vec{x}^{(l+1)}|\,\mathrm{d}\vec{x}^{(l+1)}\right)|\vec{x}^{(1)}\rangle\,\mathrm{d}\vec{x}^{(1)}=\\
&=\left|c+1=:\widetilde{c}\right|=\\
&=\int_{\mathbb{R}^{N\times L}}\prod_{l=1}^{L}\left(\langle\vec{x}^{(l)}|\,e^{\sum_i\left(-\frac{\Delta\tau}{2}\left(\omega^2-\frac{\alpha^2}{U}\right)x_i^2+\alpha x_i\left(\Delta\tau\widetilde{c}+\frac{\mathrm{i}\sigma_{il}\lambda}{U}\right)\right)}e^{-\Delta\tau\sum_i\frac{p_i^2}{2}}\,|\vec{x}^{(l+1)}\rangle\right)\mathrm{d}\vec{x}=\\
&=\int_{\mathbb{R}^{N\times L}}\prod_{l=1}^{L}\left(e^{\sum_i\left(-\frac{\Delta\tau}{2}\left(\omega^2-\frac{\alpha^2}{U}\right)x_i^{(l)2}+\alpha x_i^{(l)}\left(\Delta\tau\widetilde{c}+\frac{\mathrm{i}\sigma_{il}\lambda}{U}\right)\right)}\langle\vec{x}^{(l)}|\,e^{-\Delta\tau\sum_i\frac{p_i^2}{2}}\,|\vec{x}^{(l+1)}\rangle\right)\mathrm{d}\vec{x}\qquad,\widetilde{c}=c+1,c=\frac{\mu}{U}
\end{aligned}
$$

In order to make this integral work, i.e. to make it converge, $\frac{\Delta\tau}{2}\left(\omega^2-\frac{\alpha^2}{U}\right)$ needs to be greater than zero leading to

$$\omega^2>\frac{\alpha^2}{U}. \tag{39}$$

Now, since we have set $\hbar=1$, we have $\vec{p}=\hbar\vec{k}=\vec{k}$ and further

$$\langle\vec{p}|\vec{p}\,'\rangle=\delta(\vec{p}-\vec{p}\,')=\delta(\vec{k}-\vec{k}\,')=\langle\vec{k}|\vec{k}\,'\rangle\quad\Longleftrightarrow\quad|\vec{p}\rangle=|\vec{k}\rangle.$$

Furthermore, we have

$$\langle\vec{x}|\vec{p}\rangle=\langle\vec{x}|\vec{k}\rangle=\left(\frac{1}{2\pi}\right)^{\frac{N}{2}}e^{\mathrm{i}\vec{x}^{\mathrm{t}}\vec{k}}=\left(\frac{1}{2\pi}\right)^{\frac{N}{2}}e^{\mathrm{i}\vec{x}^{\mathrm{t}}\vec{p}},$$

where $\langle\vec{x}|\vec{p}\rangle$ is the scalar projection of $|\vec{p}\rangle$ onto $|\vec{x}\rangle$, which is an eigenstate of the (continuous) position space.

Let $\{|\vec{p}\rangle\}$ be a full set of momentum eigenstates, $\vec{p} \in \mathbb{R}^N$. Then,

$$\langle \vec{x}| e^{-\Delta\tau \sum_i \frac{p_i^2}{2}} |\vec{y}\rangle = \int_{\mathbb{R}^N} \langle \vec{x}| e^{-\frac{\Delta\tau}{2} \sum_i p_i^2} |\vec{p}\rangle \langle \vec{p}|\vec{y}\rangle \, \mathrm{d}\vec{p} = \int_{\mathbb{R}^N} e^{-\frac{\Delta\tau}{2}|\vec{p}|^2} \left(\frac{1}{2\pi}\right)^{\frac{N}{2}} e^{\mathrm{i}\,\vec{x}^{\mathrm{t}}\vec{p}} \left(\frac{1}{2\pi}\right)^{\frac{N}{2}} e^{-\mathrm{i}\,\vec{y}^{\mathrm{t}}\vec{p}} \, \mathrm{d}\vec{p} =$$
$$= \left(\frac{1}{2\pi}\right)^N \int_{\mathbb{R}^N} e^{-\frac{\Delta\tau}{2}|\vec{p}|^2 - \mathrm{i}(\vec{y}-\vec{x})^{\mathrm{t}}\vec{p}} \, \mathrm{d}\vec{p}.$$

Taking into account (6), or rather the N-dimensional "version" of it,

$$\left(\frac{1}{\sqrt{2\pi a}}\right)^N \int_{\mathbb{R}^N} e^{-\frac{1}{2a}|\vec{y}|^2 - \mathrm{i}\,\vec{x}^{\mathrm{t}}\vec{y}} \, \mathrm{d}\vec{y} = e^{-\frac{a}{2}|\vec{x}|^2},$$

we get

$$\langle \vec{x}| e^{-\Delta\tau \sum_i \frac{p_i^2}{2}} |\vec{y}\rangle = \left(\frac{1}{\Delta\tau}\right)^{\frac{N}{2}} \left(\frac{1}{2\pi}\right)^{\frac{N}{2}} \left(\frac{\Delta\tau}{2\pi}\right)^{\frac{N}{2}} \int_{\mathbb{R}^N} e^{-\frac{\Delta\tau}{2}|\vec{p}|^2 - \mathrm{i}(\vec{y}-\vec{x})^{\mathrm{t}}\vec{p}} \, \mathrm{d}\vec{p} = \left(\frac{1}{2\pi\Delta\tau}\right)^{\frac{N}{2}} e^{-\frac{1}{2\Delta\tau}|\vec{y}-\vec{x}|^2} =$$
$$= \left(\frac{1}{2\pi\Delta\tau}\right)^{\frac{N}{2}} e^{-\frac{1}{2\Delta\tau}|\vec{x}-\vec{y}|^2}. \tag{40}$$

This solution can now be used to simplify the phonon trace,

$$\mathrm{tr}_{\mathrm{ph}}\left(\prod_{l=1}^{L} e^{\sum_i \left(\frac{\Delta\tau\alpha^2}{2U} x_i^2 + \alpha x_i \left(\Delta\tau c + \frac{\mathrm{i}\sigma_{il}\lambda}{U}\right)\right)} e^{-\Delta\tau\left(H_{\mathrm{ph}} - \alpha \sum_i x_i\right)}\right) =$$
$$= \int_{\mathbb{R}^{N\times L}} \prod_{l=1}^{L} \left(e^{\sum_i \left(-\frac{\Delta\tau}{2}\left(\omega^2 - \frac{\alpha^2}{U}\right) {x_i^{(l)}}^2 + \alpha x_i^{(l)} \left(\Delta\tau\widetilde{c} + \frac{\mathrm{i}\sigma_{il}\lambda}{U}\right)\right)} \left(\frac{1}{2\pi\Delta\tau}\right)^{\frac{N}{2}} e^{-\frac{1}{2\Delta\tau}\left|\vec{x}^{(l)} - \vec{x}^{(l+1)}\right|^2} \right) \mathrm{d}\vec{x} =$$
$$= \left(\frac{1}{2\pi\Delta\tau}\right)^{\frac{NL}{2}} \int_{\mathbb{R}^{N\times L}} \prod_{l=1}^{L} \left(e^{\sum_i \left(-\frac{\Delta\tau}{2}\left(\omega^2 - \frac{\alpha^2}{U}\right) {x_i^{(l)}}^2 + \alpha x_i^{(l)} \left(\Delta\tau\widetilde{c} + \frac{\mathrm{i}\sigma_{il}\lambda}{U}\right)\right) - \frac{1}{2\Delta\tau}\sum_i \left({x_i^{(l)}}^2 + {x_i^{(l+1)}}^2 - 2x_i^{(l)} x_i^{(l+1)}\right)} \right) \mathrm{d}\vec{x} =$$
$$= \left(\frac{1}{2\pi\Delta\tau}\right)^{\frac{NL}{2}} \int_{\mathbb{R}^{N\times L}} \prod_{l=1}^{L} \left(e^{\sum_i \left(-\left(\frac{\Delta\tau}{2}\left(\omega^2 - \frac{\alpha^2}{U}\right) + \frac{1}{\Delta\tau}\right) {x_i^{(l)}}^2 + \alpha x_i^{(l)} \left(\Delta\tau\widetilde{c} + \frac{\mathrm{i}\sigma_{il}\lambda}{U}\right) + \frac{1}{\Delta\tau} x_i^{(l)} x_i^{(l+1)}\right)} \right) \mathrm{d}\vec{x}.$$

As there is no coupling between the sites i, the trace can be written as a product of traces acting only on a single site [7]. But because of the coupling between $\vec{x}$ and $\vec{y}$ in (40), this separation is not possible for the time slices l.

$$\begin{aligned}
&\mathrm{tr}_{\mathrm{ph}}\left(\prod_{l=1}^{L} e^{\sum_i\left(\frac{\Delta\tau\alpha^2}{2U}x_i^2+\alpha x_i\left(\Delta\tau c+\frac{\mathrm{i}\sigma_{il}\lambda}{U}\right)\right)} e^{-\Delta\tau\left(H_{\mathrm{ph}}-\alpha\sum_i x_i\right)}\right) = \\
&= \left(\frac{1}{2\pi\Delta\tau}\right)^{\frac{NL}{2}} \prod_i \int_{\mathbb{R}^L} e^{\sum_{l=1}^{L}\left(-\left(\frac{\Delta\tau}{2}\left(\omega^2-\frac{\alpha^2}{U}\right)+\frac{1}{\Delta\tau}\right)x^{(l)^2}+\alpha x^{(l)}\left(\Delta\tau\widetilde{c}+\frac{\mathrm{i}\sigma_{il}\lambda}{U}\right)+\frac{1}{\Delta\tau}x^{(l)}x^{(l+1)}\right)}\,\mathrm{d}\vec{x} = \left|\vec{x}\to\sqrt{\Delta\tau}\,\vec{x}\right| = \\
&= \left(\frac{1}{2\pi}\right)^{\frac{NL}{2}} \prod_i \int_{\mathbb{R}^L} e^{\sum_{l=1}^{L}\left(-\left(\frac{\Delta\tau^2}{2}\left(\omega^2-\frac{\alpha^2}{U}\right)+1\right)x^{(l)^2}+\alpha\sqrt{\Delta\tau}x^{(l)}\left(\Delta\tau\widetilde{c}+\frac{\mathrm{i}\sigma_{il}\lambda}{U}\right)+x^{(l)}x^{(l+1)}\right)}\,\mathrm{d}\vec{x}
\end{aligned}$$

Using the identity

$$\int_{\mathbb{R}^L} e^{\sum_{l=1}^{L}\left(-ax_l^2+\left(v_l+b\right)x_l+x_lx_{l+1}\right)}\,\mathrm{d}\vec{x} = \sqrt{\frac{(2\pi)^L}{\left(\Omega^L-1\right)\left(1-\Omega^{-L}\right)}}\; e^{\frac{\vec{v}^{\mathrm{t}}R\,\vec{v}}{4\left(1-\Omega^{-L}\right)\sqrt{a^2-1}}+\frac{b(2|\vec{v}|+Lb)}{4(a-1)}},$$

where $a>1$ arbitrary, $\Omega = a+\sqrt{a^2-1}$, $R=(R_{ll'})\in\mathbb{R}^{L\times L}$, $R_{ll'}=\Omega^{|l-l'|-L}+\frac{1}{\Omega^{|l-l'|}}$, $\vec{v}\in\mathbb{C}^L$, $|\vec{v}| := \sum_{l=1}^{L} v_l$ and $b\in\mathbb{R}$, the phonon trace finally becomes

$$\begin{aligned}
&\mathrm{tr}_{\mathrm{ph}}\left(\prod_{l=1}^{L} e^{\sum_i\left(\frac{\Delta\tau\alpha^2}{2U}x_i^2+\alpha x_i\left(\Delta\tau c+\frac{\mathrm{i}\sigma_{il}\lambda}{U}\right)\right)} e^{-\Delta\tau\left(H_{\mathrm{ph}}-\alpha\sum_i x_i\right)}\right) = \\
&= \left(\frac{1}{2\pi}\right)^{\frac{NL}{2}} \prod_i \sqrt{\frac{(2\pi)^L}{\left(\Omega^L-1\right)\left(1-\Omega^{-L}\right)}}\; e^{\frac{-\alpha^2\Delta\tau\lambda^2U^{-2}\,\vec{\sigma_i}^{\mathrm{t}}R\,\vec{\sigma_i}}{4\left(1-\Omega^{-L}\right)\sqrt{a^2-1}}+\frac{\alpha\sqrt{\Delta\tau^3}\,\widetilde{c}\left(2\mathrm{i}\alpha\sqrt{\Delta\tau}\lambda U^{-1}|\vec{\sigma_i}|+L\alpha\sqrt{\Delta\tau^3}\,\widetilde{c}\right)}{4(a-1)}} = \\
&= \left(\frac{1}{\left(\Omega^L-1\right)\left(1-\Omega^{-L}\right)}\right)^{\frac{N}{2}} e^{\frac{\alpha^2\widetilde{c}\left(2\mathrm{i}\Delta\tau^2\lambda U^{-1}|\sigma|+NL\Delta\tau^3\widetilde{c}\right)}{4(a-1)}}\; e^{\frac{\alpha^2\Delta\tau\lambda^2}{4U^2\left(\Omega^{-L}-1\right)\sqrt{a^2-1}}\sum_i \vec{\sigma_i}^{\mathrm{t}}R\vec{\sigma_i}} = \\
&= \left(\frac{1}{\left(\Omega^L-1\right)\left(1-\Omega^{-L}\right)}\right)^{\frac{N}{2}} e^{\frac{\alpha^2\widetilde{c}\left(2\mathrm{i}\lambda U^{-1}|\sigma|+N\beta\widetilde{c}\right)}{2\left(\omega^2-\alpha^2U^{-1}\right)}}\; e^{\frac{\alpha^2\Delta\tau^2}{2U\left(\Omega^{-L}-1\right)\sqrt{a^2-1}}\sum_i \vec{\sigma_i}^{\mathrm{t}}R\vec{\sigma_i}},
\end{aligned}$$

where $\widetilde{c} = c+1$, $c=\frac{\mu}{U}$, $a=\frac{\Delta\tau^2}{2}\left(\omega^2-\frac{\alpha^2}{U}\right)+1$, which is greater than one because of (39), $\Omega = a+\sqrt{a^2-1}$, $R=(R_{ll'})\in\mathbb{R}^{L\times L}$, $R_{ll'}=\Omega^{|l-l'|-L}+\frac{1}{\Omega^{|l-l'|}}$, $\sigma\in\mathbb{R}^{N\times L}$, $|\sigma| := \sum_{l=1}^{L}\sum_i \sigma_{il}$ and $\vec{\sigma_i} = \left(\sigma_{i*}\right)^{\mathrm{t}}$.

This is now the analytic expression of the phonon trace in (38). So, we finally obtain for the grand canonical partition function of the Hubbard-Holstein model (38)

$$
\begin{aligned}
Z &= e^{\beta\mu N}\left(\frac{e^{\beta U\left(c^2+\frac{1}{2}\right)}}{\pi^L}\right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times L}} e^{-|\sigma^2|+\mathrm{i}|\sigma|\lambda c}\left|\det\left(\mathbb{1}+\prod_{l=1}^{L} e^{-\mathrm{i}\lambda G^{(l)}} e^{\Delta\tau t h_{\mathrm{kin}}}\right)\right|^2 \cdot \\
&\qquad \cdot\left(\frac{1}{(\Omega^L-1)(1-\Omega^{-L})}\right)^{\frac{N}{2}} e^{\frac{\alpha^2\tilde{c}\left(2\mathrm{i}\lambda U^{-1}|\sigma|+N\beta\tilde{c}\right)}{2\left(\omega^2-\alpha^2U^{-1}\right)}} e^{\frac{\alpha^2\Delta\tau^2}{2U\left(\Omega^{-L}-1\right)\sqrt{a^2-1}}\sum_i \vec{\sigma_i}^{\mathrm{t}} R\vec{\sigma_i}}\,\mathrm{d}\sigma = \\
&= \left| e^{\frac{\alpha^2\tilde{c}\left(2\mathrm{i}\lambda U^{-1}|\sigma|+N\beta\tilde{c}\right)}{2\left(\omega^2-\alpha^2U^{-1}\right)}} = e^{\frac{\mathrm{i}\alpha^2\tilde{c}\lambda|\sigma|}{U\omega^2-\alpha^2}+\frac{\alpha^2\tilde{c}^2UN\beta}{2\left(U\omega^2-\alpha^2\right)}} = e^{\frac{\mathrm{i}\alpha^2(c+1)\lambda|\sigma|}{U\omega^2-\alpha^2}} e^{\frac{\alpha^2(c+1)^2UN\beta}{2\left(U\omega^2-\alpha^2\right)}} \right| = \\
&= e^{\beta\mu N}\left(\frac{e^{\beta U\left(c^2+\frac{1}{2}+\frac{\alpha^2(c+1)^2}{U\omega^2-\alpha^2}\right)}}{\pi^L(\Omega^L-1)(1-\Omega^{-L})}\right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times L}} e^{-\sum_i \vec{\sigma_i}^{\mathrm{t}}\left(\mathbb{1}-\frac{\alpha^2\Delta\tau^2}{2U\left(\Omega^{-L}-1\right)\sqrt{a^2-1}}R\right)\vec{\sigma_i}+\mathrm{i}|\sigma|\lambda c\left(1+\frac{\alpha^2}{U\omega^2-\alpha^2}+\frac{\alpha^2}{c\left(U\omega^2-\alpha^2\right)}\right)} \cdot \\
&\qquad \cdot\left|\det\left(\mathbb{1}+\prod_{l=1}^{L} e^{-\mathrm{i}\lambda G^{(l)}} e^{\Delta\tau t h_{\mathrm{kin}}}\right)\right|^2 \mathrm{d}\sigma = \\
&= \left(\frac{e^{\beta U\left(\frac{(c+1)^2U\omega^2}{U\omega^2-\alpha^2}-\frac{1}{2}\right)}}{\pi^L(\Omega^L-1)(1-\Omega^{-L})}\right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times L}} \underbrace{e^{-\sum_i \vec{\sigma_i}^{\mathrm{t}}\left(\mathbb{1}+\frac{\alpha^2\Delta\tau^2}{2U\left(1-\Omega^{-L}\right)\sqrt{a^2-1}}R\right)\vec{\sigma_i}+\mathrm{i}|\sigma|\lambda\frac{cU\omega^2+\alpha^2}{U\omega^2-\alpha^2}}}_{} \cdot \\
&\qquad \underbrace{\cdot\left|\det\left(\mathbb{1}+\prod_{l=1}^{L} e^{-\mathrm{i}\lambda G^{(l)}} e^{\Delta\tau t h_{\mathrm{kin}}}\right)\right|^2}_{=:\rho(\sigma)} \mathrm{d}\sigma = \\
&= \left(\frac{e^{\beta U\left(\frac{(c+1)^2U\omega^2}{U\omega^2-\alpha^2}-\frac{1}{2}\right)}}{\pi^L(\Omega^L-1)(1-\Omega^{-L})}\right)^{\frac{N}{2}} \int\limits_{\mathbb{R}^{N\times L}} \rho(\sigma)\,\mathrm{d}\sigma, \qquad (41)
\end{aligned}
$$

where $c=\frac{\mu}{U}$, $a=\frac{\Delta\tau^2}{2}\left(\omega^2-\frac{\alpha^2}{U}\right)+1$, $\Omega=a+\sqrt{a^2-1}$, $R=(R_{ll'})\in\mathbb{R}^{L\times L}$, $R_{ll'}=\Omega^{|l-l'|-L}+\frac{1}{\Omega^{|l-l'|}}$, $\sigma\in\mathbb{R}^{N\times L}$, $|\sigma|:=\sum\limits_{l=1}^{L}\sum\limits_i \sigma_{il}$, $\vec{\sigma_i}=\left(\sigma_{i*}\right)^{\mathrm{t}}$ and $\left(G^{(l)}\right)_{ij}=\delta_{ij}\,\sigma_{il}$.

We have again chosen the time ordering in increasing order and, with $B_l:=e^{-\mathrm{i}\lambda G^{(l)}}e^{\Delta\tau t h_{\mathrm{kin}}}$, the fermion matrix $M(l)$ is defined as

$$M(l):=\mathbb{1}+B_l\cdots B_L B_1\cdots B_{l-1}.$$

12 Ingredients for the Monte Carlo simulation

So we are having a complex continuous grand canonical partition function and we will therefore again be using normally distributed random numbers for the Hubbard-Stratonovich fields in the Monte Carlo simulations and sample them from $\mathcal{N}(0, \frac{1}{2})^{N\times L}$.
Defining a constant γ as

$$\gamma := \frac{\alpha^2 \Delta\tau^2}{2U\,(1-\Omega^{-L})\,\sqrt{a^2-1}} \tag{42}$$

and assuming $\sigma'_{\alpha\beta} \neq \sigma_{\alpha\beta}$ and $\sigma'_{il} = \sigma_{il}\ \forall\ (i,\, l) \neq (\alpha,\, \beta)$, we get for the ratio of the acceptance distributions $A(\sigma'|\sigma)$ and $A(\sigma|\sigma')$ (32)

$$\begin{aligned}
\frac{A(\sigma'|\sigma)}{A(\sigma|\sigma')} &= \frac{\rho(\sigma')}{\rho(\sigma)}\,\frac{e^{-|\sigma^2|}}{e^{-|\sigma'^2|}} = \frac{e^{-\sum\limits_i \vec{\sigma}_i'^{\mathrm{t}}(\mathbb{1}+\gamma R)\vec{\sigma}_i' + \mathrm{i}|\sigma'|\lambda\frac{cU\omega^2+\alpha^2}{U\omega^2-\alpha^2}}\,|\det(M(l)')|^2}{e^{-\sum\limits_i \vec{\sigma}_i^{\mathrm{t}}(\mathbb{1}+\gamma R)\vec{\sigma}_i + \mathrm{i}|\sigma|\lambda\frac{cU\omega^2+\alpha^2}{U\omega^2-\alpha^2}}\,|\det(M(l))|^2}\,\frac{e^{-|\sigma^2|}}{e^{-|\sigma'^2|}} = \\
&= \frac{e^{-\gamma\vec{\sigma}_\alpha'^{\mathrm{t}}R\vec{\sigma}_\alpha'}}{e^{-\gamma\vec{\sigma}_\alpha^{\mathrm{t}}R\vec{\sigma}_\alpha}}\; e^{\mathrm{i}\lambda\frac{cU\omega^2+\alpha^2}{U\omega^2-\alpha^2}\left(\sigma'_{\alpha\beta}-\sigma_{\alpha\beta}\right)}\left|\frac{\det(M(l)')}{\det(M(l))}\right|^2 = \\
&= e^{-\gamma\left(R_{\beta\beta}\left(\sigma'^2_{\alpha\beta}-\sigma^2_{\alpha\beta}\right)+\left(\sigma'_{\alpha\beta}-\sigma_{\alpha\beta}\right)\sum\limits_{l\neq\beta}\sigma_{\alpha l}\left(R_{\beta l}+R_{l\beta}\right)\right)}\; e^{\mathrm{i}\lambda\frac{cU\omega^2+\alpha^2}{U\omega^2-\alpha^2}\left(\sigma'_{\alpha\beta}-\sigma_{\alpha\beta}\right)}\left|\frac{\det(M(l)')}{\det(M(l))}\right|^2 .
\end{aligned}$$

So, we get for the acceptance probability $A(\sigma'|\sigma)$ that fulfills the condition above,

$$A(\sigma'|\sigma) = \min\left(1, \left|\frac{A(\sigma'|\sigma)}{A(\sigma|\sigma')}\right|\right) = \min\left(1, e^{-\gamma\left(R_{\beta\beta}\left(\sigma'^2_{\alpha\beta}-\sigma^2_{\alpha\beta}\right)+\left(\sigma'_{\alpha\beta}-\sigma_{\alpha\beta}\right)\sum\limits_{l\neq\beta}\sigma_{\alpha l}\left(R_{\beta l}+R_{l\beta}\right)\right)}\left|\frac{\det(M(l)')}{\det(M(l))}\right|^2\right).$$

The sign of the probability distribution for a given Hubbard-Stratonovich field value σ, $\rho(\sigma)$, is

$$\begin{aligned}
\mathrm{sgn}(\rho(\sigma)) = \frac{\rho(\sigma)}{|\rho(\sigma)|} &= \frac{e^{-\sum\limits_i \vec{\sigma}_i^{\mathrm{t}}(\mathbb{1}+\gamma R)\vec{\sigma}_i + \mathrm{i}|\sigma|\lambda\frac{cU\omega^2+\alpha^2}{U\omega^2-\alpha^2}}\,|\det(M(l))|^2}{e^{-\sum\limits_i \vec{\sigma}_i^{\mathrm{t}}(\mathbb{1}+\gamma R)\vec{\sigma}_i}\,|\det(M(l))|^2} = e^{\mathrm{i}|\sigma|\lambda\frac{cU\omega^2+\alpha^2}{U\omega^2-\alpha^2}} =: \\
&=: \mathrm{phase}(\rho(\sigma))\,,
\end{aligned} \tag{43}$$

which means that the sign has now turned into a phase factor.

It is convenient to define a dimensionless electron-phonon coupling constant Λ as the ratio of the lattice deformation energy $E_{\text{ph}} = \frac{\alpha^2}{2m\omega^2} = \frac{\alpha^2}{2\omega^2}$ to half the non-interacting bandwidth $\frac{W}{2} \approx 4$ [6],

$$\Lambda := \frac{E_{\text{ph}}}{\frac{W}{2}} = \frac{\frac{\alpha^2}{2\omega^2}}{\frac{W}{2}} = \frac{\alpha^2}{\omega^2 W}, \tag{44}$$

with which we can rewrite (43) as

$$\text{phase}(\rho(\sigma)) = e^{\mathrm{i}|\sigma|\lambda\frac{\mu+\Lambda W}{U-\Lambda W}}. \tag{45}$$

From now on we will use Λ as the measure of the electron-phonon coupling strength instead of α.

Furthermore, the matrix $\Delta(i, l)$ turns into

$$(\Delta(i,l))_{jk} = \delta_{ji}\,\delta_{ki}\left(e^{-\mathrm{i}\lambda\left(\sigma'_{il}-\sigma_{il}\right)} - 1\right).$$

Apart from everything that we have just discussed, the rest of the ingredients for our efficient update scheme stays the same as for the real continuous Hubbard-Stratonovich transformation, except that this time we are using the SVD instead of the UDR decomposition to stabilize the numerical computation of inverses (and determinants) of ill-conditioned complex matrices.

13 Sampling the average density under the asymmetric particle-hole transformation

The only thing where one really has to be careful is when sampling thermodynamic expectation values after one has used the asymmetric particle-hole transformation (34) to transform the Hamilton operator for a system. For our numerical study of the Hubbard-Holstein model we will mostly be interested in the average phase factor and the average density. The phase factor of the probability distribution for a given Hubbard-Stratonovich field value σ, $\rho(\sigma)$, is simply calculated via (45). For the average density, however, we will present two methods, with which it can be calculated.

13.1 Sampling the average density using Green's functions

The first method to calculate $\langle n \rangle$, for a given σ and hence Green's function g is the same that we used before, except that this time we need to take into account (36),

$$\begin{aligned}\langle n \rangle = \frac{\left\langle \hat{N} \right\rangle}{N} = \frac{1}{N} \sum_i \left(\langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle \right) = \frac{1}{N} \sum_i \left(\langle n_{i\uparrow} \rangle + 1 - \langle n_{i\downarrow} \rangle \right) = \\ = \frac{1}{N} \sum_i \left(1 - \left(g^{\uparrow} \right)_{ii} + 1 - \left(1 - \left(g^{\downarrow} \right)_{ii} \right) \right) = \frac{1}{N} \sum_i \left(1 - g_{ii} + (g^*)_{ii} \right).\end{aligned}$$

13.2 Sampling the average density using Hubbard-Stratonovich fields

On the other hand, we can derive an expression for $\langle n \rangle$ that only contains the Hubbard-Stratonovich fields we are sampling.

Starting out with the (transformed) Hamilton operator of the Hubbard-Holstein model (35), we get for the grand canonical partition function

$$Z = \mathrm{tr}\left(e^{-\beta \widetilde{H}} \right) = \mathrm{tr}\left(e^{-\beta \left(H_{\mathrm{kin}} - H_{\mathrm{C}} - \mu \hat{M} - \mu N + H_{\mathrm{ph}} + H_{\alpha} \right)} \right),$$

and for its partial derivative with respect to the chemical potential μ

$$\begin{aligned}\frac{\partial Z}{\partial \mu} &= \mathrm{tr}\left(e^{-\beta \left(H_{\mathrm{kin}} - H_{\mathrm{C}} - \mu \hat{M} - \mu N + H_{\mathrm{ph}} + H_{\alpha} \right)} \left(\beta \hat{M} + \beta N \right) \right) = \mathrm{tr}\left(e^{-\beta \widetilde{H}} \left(\beta \hat{M} + \beta N \right) \right) = \\ &= \beta \, \mathrm{tr}\left(e^{-\beta \widetilde{H}} \hat{M} \right) + \beta N \, \mathrm{tr}\left(e^{-\beta \widetilde{H}} \right) = \beta \, \mathrm{tr}\left(e^{-\beta \widetilde{H}} \right) \left(\frac{\mathrm{tr}\left(\hat{M} e^{-\beta \widetilde{H}} \right)}{\mathrm{tr}\left(e^{-\beta \widetilde{H}} \right)} + N \right) = \beta Z \left(\left\langle \hat{M} \right\rangle + N \right) = \\ &= \beta Z \left(\left\langle \sum_i \left(n_{i\uparrow} - n_{i\downarrow} \right) \right\rangle + \left\langle \sum_i 1 \right\rangle \right) = \beta Z \left\langle \sum_i \left(n_{i\uparrow} + 1 - n_{i\downarrow} \right) \right\rangle = \beta Z \left\langle \sum_i \left(n_{i\uparrow} + n_{i\downarrow} \right) \right\rangle = \\ &= \beta Z \left\langle \hat{N} \right\rangle = \beta Z N \langle n \rangle,\end{aligned}$$

which gives us

$$\langle n \rangle = \frac{1}{\beta N} \frac{\frac{\partial Z}{\partial \mu}}{Z} = \frac{1}{\beta N} \frac{\partial}{\partial \mu} \ln Z. \tag{46}$$

Next, we rewrite the grand canonical partition function (41) using (42), (44) and $c = \frac{\mu}{U}$:

$$\begin{aligned}
Z = &\left(\frac{e^{-\frac{\beta U}{2}}}{\pi^L \left(\Omega^L - 1\right)\left(1 - \Omega^{-L}\right)} \right)^{\frac{N}{2}} e^{\frac{\beta N U}{2} \frac{U\omega^2}{U\omega^2 - \alpha^2}\left(\frac{\mu^2}{U^2} + 2\frac{\mu}{U} + 1\right)} \int\limits_{\mathbb{R}^{N\times L}} e^{-\sum\limits_i \vec{\sigma_i}^{\mathrm{t}}(\mathbb{1}+\gamma R)\vec{\sigma_i} + \mathrm{i}|\sigma|\lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \cdot \\
&\cdot \left| \det\left(\mathbb{1} + \prod_{l=1}^{L} e^{-\mathrm{i}\lambda G^{(l)}} e^{\Delta\tau t h_{\mathrm{kin}}} \right) \right|^2 \mathrm{d}\sigma = \\
= &\underbrace{\left(\frac{e^{\beta U\left(\frac{U}{U-\Lambda W} - \frac{1}{2}\right)}}{\pi^L \left(\Omega^L - 1\right)\left(1 - \Omega^{-L}\right)} \right)^{\frac{N}{2}}}_{=:Z_0} \overbrace{e^{\frac{\beta N}{2(U-\Lambda W)}\mu^2 + \frac{\beta N U}{U-\Lambda W}\mu}}^{=:Z_1(\mu)} \underbrace{\int\limits_{\mathbb{R}^{N\times L}} e^{-\sum\limits_i \vec{\sigma_i}^{\mathrm{t}}(\mathbb{1}+\gamma R)\vec{\sigma_i}} \cdot}_{} \\
&\underbrace{\cdot \left| \det\left(\mathbb{1} + \prod_{l=1}^{L} e^{-\mathrm{i}\lambda G^{(l)}} e^{\Delta\tau t h_{\mathrm{kin}}} \right) \right|^2 e^{\mathrm{i}|\sigma|\lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \mathrm{d}\sigma}_{=:I} = \\
= &\, Z_0 \, Z_1(\mu) \, I
\end{aligned} \tag{47}$$

With that we can finally derive our alternative expression for $\langle n \rangle$,

$$\begin{aligned}
\beta N \langle n \rangle = &\frac{\partial}{\partial \mu} \ln Z = \frac{Z'}{Z} = \frac{Z_0 Z_1' I}{Z_0 Z_1 I} + \frac{Z_0 Z_1 I'}{Z_0 Z_1 I} = \\
= &\frac{\partial}{\partial \mu} \ln Z_1 + \frac{\int\limits_{\mathbb{R}^{N\times L}} |\rho(\sigma)| \, e^{\mathrm{i}|\sigma|\lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \, \frac{\mathrm{i}|\sigma|\lambda}{U-\Lambda W} \, \mathrm{d}\sigma}{\int\limits_{\mathbb{R}^{N\times L}} |\rho(\sigma)| \, e^{\mathrm{i}|\sigma|\lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \, \mathrm{d}\sigma} = \\
= &\left(\frac{\beta N}{2\left(U - \Lambda W\right)} \mu^2 + \frac{\beta N U}{U - \Lambda W} \mu \right)' + \frac{\mathrm{i}\lambda}{U - \Lambda W} \frac{\int\limits_{\mathbb{R}^{N\times L}} |\sigma| \, e^{\mathrm{i}|\sigma|\lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \, |\rho(\sigma)| \, \mathrm{d}\sigma}{\int\limits_{\mathbb{R}^{N\times L}} |\rho(\sigma)| \, \mathrm{d}\sigma} \\
&\frac{\int\limits_{\mathbb{R}^{N\times L}} e^{\mathrm{i}|\sigma|\lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \, |\rho(\sigma)| \, \mathrm{d}\sigma}{\int\limits_{\mathbb{R}^{N\times L}} |\rho(\sigma)| \, \mathrm{d}\sigma} =
\end{aligned}$$

$$= \frac{\beta N}{U - \Lambda W}(\mu + U) + \frac{\mathrm{i}\lambda}{U - \Lambda W} \frac{\left\langle |\sigma| \, e^{\mathrm{i}|\sigma|\lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \right\rangle}{\left\langle e^{\mathrm{i}|\sigma|\lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \right\rangle} \quad \Longleftrightarrow$$

$$\Longleftrightarrow \quad \langle n \rangle = \frac{\mu + U}{U - \Lambda W} + \frac{1}{\beta N} \frac{\mathrm{i}\lambda}{U - \Lambda W} \frac{\left\langle |\sigma| \, e^{\mathrm{i}|\sigma|\lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \right\rangle}{\left\langle e^{\mathrm{i}|\sigma|\lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \right\rangle}.$$

14 Analytically exact results without hopping

Here we want to analytically evaluate the grand canonical partition function and with that the average density and the average phase factor without hopping, i.e. for $t = 0$, and compare our later numerical results with the analytically exact solutions.

14.1 Analytic evaluation of the grand canonical partition function

First, we want to analytically evaluate the grand canonical partition function (47) for $t = 0$.

With the definition $B := \mathbb{1} + \gamma R$ we get

$$\widetilde{Z} := Z(t=0) = Z_0\, Z_1(\mu)\, I(t=0) = Z_0\, Z_1(\mu) \int\limits_{\mathbb{R}^{N\times L}} e^{-\sum\limits_i \vec{\sigma_i}^{\mathrm{t}} B \vec{\sigma_i} + \mathrm{i}|\sigma| \lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \left| \det\left(\mathbb{1} + \prod_{l=1}^{L} e^{-\mathrm{i}\lambda G^{(l)}} \right) \right|^2 \mathrm{d}\sigma =$$

$$= Z_0\, Z_1(\mu) \int\limits_{\mathbb{R}^{N\times L}} e^{-\sum\limits_i \left(\vec{\sigma_i}^{\mathrm{t}} B \vec{\sigma_i} - \mathrm{i} \sum\limits_{l=1}^{L} \sigma_{il} \lambda \frac{\mu+\Lambda W}{U-\Lambda W} \right)} \left| \prod_i \left(1 + e^{-\mathrm{i}\lambda \sum\limits_{l=1}^{L} \sigma_{il}} \right) \right|^2 \mathrm{d}\sigma =$$

$$= Z_0\, Z_1(\mu) \prod_i \int\limits_{\mathbb{R}^L} e^{-\vec{\sigma_i}^{\mathrm{t}} B \vec{\sigma_i} + \mathrm{i} \sum\limits_{l=1}^{L} \sigma_{il} \lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \left| 1 + e^{-\mathrm{i}\lambda \sum\limits_{l=1}^{L} \sigma_{il}} \right|^2 \mathrm{d}\vec{\sigma_i} =$$

$$= Z_0\, Z_1(\mu) \left(\int\limits_{\mathbb{R}^L} e^{-\vec{\sigma}^{\mathrm{t}} B \vec{\sigma}}\, e^{\mathrm{i} \sum\limits_{l=1}^{L} \sigma_l \lambda \frac{\mu+\Lambda W}{U-\Lambda W}} \left(2 + e^{-\mathrm{i}\lambda \sum\limits_{l=1}^{L} \sigma_l} + e^{\mathrm{i}\lambda \sum\limits_{l=1}^{L} \sigma_l} \right) \mathrm{d}\vec{\sigma} \right)^N = \left| \begin{array}{c} \sum\limits_{l=1}^{L} \sigma_l =: S \\ \mu + \Lambda W =: \widetilde{\mu} \\ U - \Lambda W =: \widetilde{U} \end{array} \right| =$$

$$= Z_0\, Z_1(\mu) \left(\int\limits_{\mathbb{R}^L} e^{-\vec{\sigma}^{\mathrm{t}} B \vec{\sigma}} \left(2 e^{\mathrm{i} S \lambda \frac{\widetilde{\mu}}{\widetilde{U}}} + e^{\mathrm{i} S \lambda \left(\frac{\widetilde{\mu}}{\widetilde{U}} - 1 \right)} + e^{\mathrm{i} S \lambda \left(\frac{\widetilde{\mu}}{\widetilde{U}} + 1 \right)} \right) \mathrm{d}\vec{\sigma} \right)^N =$$

$$= \left| \begin{array}{c} S\,\lambda\dfrac{\widetilde{\mu}}{\widetilde{U}} = 2\underbrace{\underbrace{\dfrac{\lambda}{2}\dfrac{\widetilde{\mu}}{\widetilde{U}}}_{=:\lambda_1}\vec{1}^{\,\mathrm{t}}}_{=:\vec{\lambda}_1^{\,\mathrm{t}}}\vec{\sigma} = 2\vec{\lambda}_1^{\,\mathrm{t}}\vec{\sigma} \\ S\,\lambda\left(\dfrac{\widetilde{\mu}}{\widetilde{U}}-1\right) = 2\underbrace{\underbrace{\dfrac{\lambda}{2}\left(\dfrac{\widetilde{\mu}}{\widetilde{U}}-1\right)}_{=:\lambda_2}\vec{1}^{\,\mathrm{t}}}_{=:\vec{\lambda}_2^{\,\mathrm{t}}}\vec{\sigma} = 2\vec{\lambda}_2^{\,\mathrm{t}}\vec{\sigma} \\ S\,\lambda\left(\dfrac{\widetilde{\mu}}{\widetilde{U}}+1\right) = 2\underbrace{\underbrace{\dfrac{\lambda}{2}\left(\dfrac{\widetilde{\mu}}{\widetilde{U}}+1\right)}_{=:\lambda_3}\vec{1}^{\,\mathrm{t}}}_{=:\vec{\lambda}_3^{\,\mathrm{t}}}\vec{\sigma} = 2\vec{\lambda}_3^{\,\mathrm{t}}\vec{\sigma} \end{array} \right| =$$

$$= Z_0\,Z_1(\mu)\left(\int_{\mathbb{R}^L} e^{-\vec{\sigma}^{\,\mathrm{t}}B\vec{\sigma}}\left(2e^{2\mathrm{i}\vec{\lambda}_1^{\,\mathrm{t}}\vec{\sigma}} + e^{2\mathrm{i}\vec{\lambda}_2^{\,\mathrm{t}}\vec{\sigma}} + e^{2\mathrm{i}\vec{\lambda}_3^{\,\mathrm{t}}\vec{\sigma}}\right)\mathrm{d}\vec{\sigma}\right)^N = \left|\int_{\mathbb{R}^L} e^{-\left(\vec{\sigma}^{\,\mathrm{t}}B\vec{\sigma}-2\mathrm{i}\vec{\lambda}_\alpha^{\,\mathrm{t}}\vec{\sigma}\right)}\,\mathrm{d}\vec{\sigma} =: I_\alpha\right| =$$

$$= Z_0\,Z_1(\mu)\,(2I_1 + I_2 + I_3)^N\,.$$

The argument of the exponential function in I_α can be written as

$$\vec{\sigma}^{\,\mathrm{t}}B\vec{\sigma} - 2\mathrm{i}\vec{\lambda}_\alpha^{\,\mathrm{t}}\vec{\sigma} = \left(\vec{\sigma} - \mathrm{i}\vec{\sigma_0}\right)^{\mathrm{t}} B\left(\vec{\sigma} - \mathrm{i}\vec{\sigma_0}\right) + C = \vec{\sigma}^{\,\mathrm{t}}B\vec{\sigma} - 2\mathrm{i}\vec{\sigma_0}^{\,\mathrm{t}}B\vec{\sigma} - \vec{\sigma_0}^{\,\mathrm{t}}B\vec{\sigma_0} + C \quad \Longleftrightarrow$$
$$\Longleftrightarrow \quad C = \vec{\sigma_0}^{\,\mathrm{t}}B\vec{\sigma_0} \qquad \text{and} \qquad \vec{\sigma_0}^{\,\mathrm{t}}B = \vec{\lambda}_\alpha^{\,\mathrm{t}}.$$

Because $R_{ll'} = \Omega^{|l-l'|-L} + \frac{1}{\Omega^{|l-l'|}} = \Omega^{|l'-l|-L} + \frac{1}{\Omega^{|l'-l|}} = R_{l'l}\ \ \forall\ l,\, l' \in \{1,\ldots,L\}$, B is a symmetric matrix meaning $B = B^{\mathrm{t}}$ and $B^{-1} = \left(B^{-1}\right)^{\mathrm{t}}$. Hence we get

$$\vec{\sigma_0}^{\,\mathrm{t}}B = \vec{\lambda}_\alpha^{\,\mathrm{t}} \quad \Longleftrightarrow \quad \vec{\sigma_0}^{\,\mathrm{t}} = \vec{\lambda}_\alpha^{\,\mathrm{t}}B^{-1} \quad \Longleftrightarrow \quad \vec{\sigma_0} = \left(B^{-1}\right)^{\mathrm{t}}\vec{\lambda}_\alpha = B^{-1}\vec{\lambda}_\alpha$$

and

$$C = \vec{\sigma_0}^{\,\mathrm{t}}B\vec{\sigma_0} = \vec{\lambda}_\alpha^{\,\mathrm{t}}B^{-1}\vec{\lambda}_\alpha.$$

With that we get for I_α a multidimensional Gaussian integral, which can easily be solved analytically,

$$I_\alpha = \int_{\mathbb{R}^L} e^{-\left(\vec{\sigma}-\mathrm{i}B^{-1}\vec{\lambda}_\alpha\right)^{\mathrm{t}}B\left(\vec{\sigma}-\mathrm{i}B^{-1}\vec{\lambda}_\alpha\right)-\vec{\lambda}_\alpha^{\,\mathrm{t}}B^{-1}\vec{\lambda}_\alpha}\,\mathrm{d}\vec{\sigma} = e^{-\vec{\lambda}_\alpha^{\,\mathrm{t}}B^{-1}\vec{\lambda}_\alpha}\,\frac{\left(\sqrt{\pi}\right)^L}{\sqrt{\det(B)}}.$$

And with

$$\overrightarrow{\lambda_\alpha}^{\mathrm{t}} B^{-1} \overrightarrow{\lambda_\alpha} = \underbrace{\sum_{ll'} \left(B^{-1}\right)_{ll'}}_{=:\widetilde{\kappa}} \lambda_\alpha^2 = \widetilde{\kappa}\lambda_\alpha^2$$

I_α can be simplified to

$$I_\alpha = \left(\frac{\pi^L}{\det(B)}\right)^{\frac{1}{2}} e^{-\widetilde{\kappa}\lambda_\alpha^2} \qquad ,\widetilde{\kappa} = \sum_{ll'} \left(B^{-1}\right)_{ll'}.$$

So the integral yields

$$\begin{aligned}
\widetilde{I} &:= 2I_1 + I_2 + I_3 = \left(\frac{\pi^L}{\det(B)}\right)^{\frac{1}{2}} \left(2e^{-\widetilde{\kappa}\lambda_1^2} + e^{-\widetilde{\kappa}\lambda_2^2} + e^{-\widetilde{\kappa}\lambda_3^2}\right) = \\
&= \left(\frac{\pi^L}{\det(B)}\right)^{\frac{1}{2}} e^{-\widetilde{\kappa}\lambda_1^2} \left(2 + e^{-\widetilde{\kappa}\left(\lambda_2^2-\lambda_1^2\right)} + e^{-\widetilde{\kappa}\left(\lambda_3^2-\lambda_1^2\right)}\right) = \\
&= \left(\frac{\pi^L}{\det(B)}\right)^{\frac{1}{2}} e^{-\widetilde{\kappa}\frac{\lambda^2}{4}\frac{\widetilde{\mu}^2}{\widetilde{U}^2}} \left(2 + e^{-\widetilde{\kappa}\frac{\lambda^2}{4}\left(\left(\frac{\widetilde{\mu}}{\widetilde{U}}-1\right)^2-\frac{\widetilde{\mu}^2}{\widetilde{U}^2}\right)} + e^{-\widetilde{\kappa}\frac{\lambda^2}{4}\left(\left(\frac{\widetilde{\mu}}{\widetilde{U}}+1\right)^2-\frac{\widetilde{\mu}^2}{\widetilde{U}^2}\right)}\right) = \\
&= \left(\frac{\pi^L}{\det(B)}\right)^{\frac{1}{2}} e^{-\widetilde{\kappa}\frac{\lambda^2}{4}\frac{\widetilde{\mu}^2}{\widetilde{U}^2}} \left(2 + e^{-\widetilde{\kappa}\frac{\lambda^2}{4}\left(1-2\frac{\widetilde{\mu}}{\widetilde{U}}\right)} + e^{-\widetilde{\kappa}\frac{\lambda^2}{4}\left(1+2\frac{\widetilde{\mu}}{\widetilde{U}}\right)}\right) = \\
&= \left| e^{-\widetilde{\kappa}\frac{\lambda^2}{4}\left(1-2\frac{\widetilde{\mu}}{\widetilde{U}}\right)} + e^{-\widetilde{\kappa}\frac{\lambda^2}{4}\left(1+2\frac{\widetilde{\mu}}{\widetilde{U}}\right)} = e^{-\widetilde{\kappa}\frac{\lambda^2}{4}} \left(e^{\widetilde{\kappa}\frac{\lambda^2}{2}\frac{\widetilde{\mu}}{\widetilde{U}}} + e^{-\widetilde{\kappa}\frac{\lambda^2}{2}\frac{\widetilde{\mu}}{\widetilde{U}}}\right) = e^{-\widetilde{\kappa}\frac{\lambda^2}{4}}\, 2\cosh\left(\widetilde{\kappa}\frac{\lambda^2}{2}\frac{\widetilde{\mu}}{\widetilde{U}}\right) \right| = \\
&= 2\left(\frac{\pi^L}{\det(B)}\right)^{\frac{1}{2}} e^{-\widetilde{\kappa}\frac{\lambda^2}{4}\frac{\widetilde{\mu}^2}{\widetilde{U}^2}} \left(1 + e^{-\widetilde{\kappa}\frac{\lambda^2}{4}} \cosh\left(\widetilde{\kappa}\frac{\lambda^2}{2}\frac{\widetilde{\mu}}{\widetilde{U}}\right)\right),
\end{aligned}$$

which finally leads to

$$\widetilde{Z} = Z_0\, Z_{\mathrm{I}}(\mu)\, \widetilde{I}^N.$$

14.2 Analytic evaluation of the average density and the average phase factor

With that we can now, using (46), analytically evaluate $\langle n \rangle$ for $t = 0$,

$$\begin{aligned}
\beta N \langle n \rangle_{t=0} &= \frac{\partial}{\partial\mu} \ln \widetilde{Z} = \frac{\partial}{\partial\mu} \left(\ln Z_0 + \ln Z_1 + N \ln \widetilde{I}\right) = \\
&= \frac{\beta N (\mu + U)}{U - \Lambda W} + N \frac{\partial}{\partial\mu} \left(\ln\left(2\left(\frac{\pi^L}{\det(B)}\right)^{\frac{1}{2}}\right) - \widetilde{\kappa}\frac{\lambda^2}{4}\frac{(\mu + \Lambda W)^2}{(U - \Lambda W)^2} + \right.
\end{aligned}$$

$$+\ln\left(1+e^{-\widetilde{\kappa}\frac{\lambda^2}{4}}\cosh\left(\widetilde{\kappa}\frac{\lambda^2}{2}\frac{\mu+\Lambda W}{U-\Lambda W}\right)\right)\Bigg)\Bigg) =$$

$$= \frac{\beta N(\mu+U)}{U-\Lambda W} + N\left(-\widetilde{\kappa}\frac{\lambda^2}{2}\frac{\mu+\Lambda W}{(U-\Lambda W)^2} + \frac{e^{-\widetilde{\kappa}\frac{\lambda^2}{4}}\sinh\left(\widetilde{\kappa}\frac{\lambda^2}{2}\frac{\mu+\Lambda W}{U-\Lambda W}\right)\widetilde{\kappa}\frac{\lambda^2}{2}\frac{1}{U-\Lambda W}}{1+e^{-\widetilde{\kappa}\frac{\lambda^2}{4}}\cosh\left(\widetilde{\kappa}\frac{\lambda^2}{2}\frac{\mu+\Lambda W}{U-\Lambda W}\right)}\right) =$$

$$= \frac{\beta N(\mu+U)}{U-\Lambda W} + N\widetilde{\kappa}\frac{\lambda^2}{2}\frac{1}{U-\Lambda W}\left(-\frac{\mu+\Lambda W}{U-\Lambda W} + \frac{e^{-\widetilde{\kappa}\frac{\lambda^2}{4}}\sinh\left(\widetilde{\kappa}\frac{\lambda^2}{2}\frac{\mu+\Lambda W}{U-\Lambda W}\right)}{1+e^{-\widetilde{\kappa}\frac{\lambda^2}{4}}\cosh\left(\widetilde{\kappa}\frac{\lambda^2}{2}\frac{\mu+\Lambda W}{U-\Lambda W}\right)}\right) =$$

$$= \frac{\beta N(\mu+U)}{U-\Lambda W} + N\widetilde{\kappa}\frac{\lambda^2}{2}\frac{1}{U-\Lambda W}\left(-\frac{\mu+\Lambda W}{U-\Lambda W} + \frac{\sinh\left(\widetilde{\kappa}\frac{\lambda^2}{2}\frac{\mu+\Lambda W}{U-\Lambda W}\right)}{e^{\widetilde{\kappa}\frac{\lambda^2}{4}}+\cosh\left(\widetilde{\kappa}\frac{\lambda^2}{2}\frac{\mu+\Lambda W}{U-\Lambda W}\right)}\right) \quad \Longleftrightarrow$$

$$\Longleftrightarrow \quad \langle n\rangle_{t=0} = \frac{\mu+U}{U-\Lambda W} + \frac{\widetilde{\kappa}}{L}\frac{U}{U-\Lambda W}\left(-\frac{\mu+\Lambda W}{U-\Lambda W} + \frac{\sinh\left(\widetilde{\kappa}\Delta\tau U\frac{\mu+\Lambda W}{U-\Lambda W}\right)}{e^{\widetilde{\kappa}\frac{\Delta\tau U}{2}}+\cosh\left(\widetilde{\kappa}\Delta\tau U\frac{\mu+\Lambda W}{U-\Lambda W}\right)}\right). \tag{48}$$

Next, we want to explicitly evaluate $\widetilde{\kappa}$. To this end we will first have a look at the matrix R and prove that, no matter the index l, $\sum_{l'} R_{ll'} = const$ and then explicitly calculate that constant.
So first we prove that

$$\sum_{l'} R_{ll'} = \underbrace{\sum_{l'}\Omega^{|l-l'|-L}}_{=:S_1(l)} + \underbrace{\sum_{l'}\frac{1}{\Omega^{|l-l'|}}}_{=:S_2(l)} = S_1(l)+S_2(l) =: S(l) = const$$

for all $l = 1,\ldots,L$.

Proof.
The proof will be made by induction with respect to l.

(1) Induction basis: $l = 1$

$$S(1) = \frac{1}{\Omega^L}+\frac{1}{\Omega^{L-1}}+\cdots+\frac{1}{\Omega}+1+\frac{1}{\Omega}+\cdots+\frac{1}{\Omega^{L-1}} = 1+2\left(\frac{1}{\Omega}+\cdots+\frac{1}{\Omega^{L-1}}\right)+\frac{1}{\Omega^L} =$$
$$= const =: \Gamma$$

(2) Induction step: $l \to l+1$

$$S(l+1) = \sum_{l'}\Omega^{|l+1-l'|-L} + \sum_{l'}\frac{1}{\Omega^{|l+1-l'|}} = \sum_{l'}\Omega^{|l-(l'-1)|-L} + \sum_{l'}\frac{1}{\Omega^{|l-(l'-1)|}} =$$
$$= \sum_{l''=0}^{L-1}\Omega^{|l-l''|-L} + \sum_{l''=0}^{L-1}\frac{1}{\Omega^{|l-l''|}} = S_1(l)+\Omega^{l-L}-\Omega^{-l}+S_2(l)+\frac{1}{\Omega^l}-\frac{1}{\Omega^{L-l}} =$$
$$= S_1(l)+\frac{1}{\Omega^{L-l}}-\frac{1}{\Omega^l}+S_2(l)+\frac{1}{\Omega^l}-\frac{1}{\Omega^{L-l}} = S_1(l)+S_2(l) = S(l) = \Gamma$$

□

And now we want to explicitly calculate that constant Γ,

$$S(l) = \Gamma = 1 + 2\left(\frac{1}{\Omega} + \cdots + \frac{1}{\Omega^{L-1}}\right) + \frac{1}{\Omega^L} = \frac{1 + 2\left(\Omega + \cdots + \Omega^{L-1}\right) + \Omega^L}{\Omega^L} =$$
$$= \frac{(1+\Omega)\left(1 + \cdots + \Omega^{L-1}\right)}{\Omega^L} = \frac{(1+\Omega)}{\Omega^L} \underbrace{\sum_{l''=0}^{L-1} \Omega^{l''}}_{=:\widetilde{S}(L)} = \frac{(1+\Omega)}{\Omega^L}\,\widetilde{S}(L).$$

We claim that

$$\widetilde{S}(L) = \sum_{l''=0}^{L-1} \Omega^{l''} = \frac{-1 + \Omega^L}{-1 + \Omega}.$$

Proof.
Because this is a statement depending on L, we again have to prove it by induction, but this time with respect to L.

(1) Induction basis: $L = 1$

$$\widetilde{S}(1) = 1 = \frac{-1 + \Omega}{-1 + \Omega}$$

(2) Induction step: $L \to L + 1$

$$\widetilde{S}(L+1) = \sum_{l''=0}^{L} \Omega^{l''} = \frac{-1 + \Omega^{L+1}}{-1 + \Omega} \iff \frac{-1 + \Omega^L}{-1 + \Omega} + \Omega^L = \frac{-1 + \Omega^{L+1}}{-1 + \Omega} \iff$$
$$\iff -1 + \Omega^L - \Omega^L + \Omega^{L+1} = -1 + \Omega^{L+1} \iff -1 + \Omega^{L+1} = -1 + \Omega^{L+1}$$

□

So we finally get

$$S(l) = \Gamma = \frac{(1+\Omega)\left(-1 + \Omega^L\right)}{\Omega^L\,(-1+\Omega)} \qquad \forall\ l \in \{1, \ldots, L\},$$

which of course means

$$\sum_{l'} R_{ll'} = \Gamma = \frac{(1+\Omega)\left(-1 + \Omega^L\right)}{\Omega^L\,(-1+\Omega)} \qquad \forall\ l \in \{1, \ldots, L\}.$$

Hence we get further

$$\sum_{l'} B_{ll'} = \sum_{l'} (\mathbb{1} + \gamma R)_{ll'} = 1 + \gamma\Gamma \qquad \forall\ l \in \{1, \ldots, L\}.$$

Due to symmetry we have

$$1 = \sum_{l'} \delta_{ll'} = \sum_{l'} \mathbb{1}_{ll'} = \sum_{l'} \left(BB^{-1}\right)_{ll'} = \sum_{l'} \sum_{l''} B_{ll''} \left(B^{-1}\right)_{l''l'} = \sum_{l''} B_{ll''} \sum_{l'} \left(B^{-1}\right)_{l''l'} =$$
$$= (1+\gamma\Gamma) \sum_{l'} \left(B^{-1}\right)_{l''l'} \quad \Longleftrightarrow \quad \sum_{l'} \left(B^{-1}\right)_{l''l'} = \frac{1}{1+\gamma\Gamma}.$$

So we finally get for $\widetilde{\kappa}$

$$\widetilde{\kappa} = \sum_{ll'} \left(B^{-1}\right)_{ll'} = \frac{L}{1+\gamma\Gamma}.$$

So,

$$\frac{L}{\widetilde{\kappa}} = 1 + \gamma\Gamma \overset{(42)}{=} 1 + \frac{\alpha^2\Delta\tau^2}{2U\left(1-\Omega^{-L}\right)\sqrt{a^2-1}} \frac{(1+\Omega)\left(-1+\Omega^L\right)}{\Omega^L(-1+\Omega)} =$$
$$= 1 + \frac{\alpha^2\Delta\tau^2\Omega^L}{2U\left(\Omega^L-1\right)\sqrt{a^2-1}} \frac{(1+\Omega)\left(\Omega^L-1\right)}{\Omega^L(-1+\Omega)} = 1 + \frac{\alpha^2\Delta\tau^2}{2U\sqrt{a^2-1}} \frac{1+a+\sqrt{a^2-1}}{-1+a+\sqrt{a^2-1}} =$$
$$= 1 + \frac{\alpha^2\Delta\tau^2}{2U\sqrt{a^2-1}} \frac{\left(1+a+\sqrt{a^2-1}\right)^2}{-1+\left(a+\sqrt{a^2-1}\right)^2} =$$
$$= 1 + \frac{\alpha^2\Delta\tau^2}{2U\sqrt{a^2-1}} \frac{1+a^2+a^2-1+2a\sqrt{a^2-1}+2a+2\sqrt{a^2-1}}{-1+a^2+a^2-1+2a\sqrt{a^2-1}} =$$
$$= 1 + \frac{\alpha^2\Delta\tau^2}{2U\sqrt{a^2-1}} \frac{2a^2+2a+2a\sqrt{a^2-1}+2\sqrt{a^2-1}}{-2+2a^2+2a\sqrt{a^2-1}} =$$
$$= 1 + \frac{\alpha^2\Delta\tau^2}{2U\sqrt{a^2-1}} \frac{(a+1)\left(a+\sqrt{a^2-1}\right)}{-1+a^2+a\sqrt{a^2-1}} = 1 + \frac{\alpha^2\Delta\tau^2}{2U} \frac{(a+1)\left(a+\sqrt{a^2-1}\right)}{\sqrt{a^2-1}\,(a^2-1)+a\,(a^2-1)} =$$
$$= 1 + \frac{\alpha^2\Delta\tau^2}{2U} \frac{(a+1)\left(a+\sqrt{a^2-1}\right)}{(a^2-1)\left(a+\sqrt{a^2-1}\right)} = 1 + \frac{\alpha^2\Delta\tau^2}{2U} \frac{a+1}{(a+1)(a-1)} = 1 + \frac{\alpha^2\Delta\tau^2}{2U} \frac{1}{a-1} =$$
$$= \left| a = \frac{\Delta\tau^2}{2}\left(\omega^2 - \frac{\alpha^2}{U}\right) + 1 = \frac{\Delta\tau^2}{2}\frac{\omega^2}{U}(U-\Lambda W) + 1 = \frac{\Delta\tau^2\omega^2\widetilde{U}}{2U} + 1 \right| =$$
$$= 1 + \frac{\alpha^2\Delta\tau^2}{2U} \frac{2U}{\Delta\tau^2\omega^2\widetilde{U}} = 1 + \frac{\Lambda W}{\widetilde{U}} = \frac{\widetilde{U}+\Lambda W}{\widetilde{U}} = \frac{U}{\widetilde{U}} \quad \Longleftrightarrow \quad \frac{\widetilde{\kappa}}{L} = \frac{\widetilde{U}}{U}.$$

With this relation we get for the average density in (48) the simple expression

$$\langle n \rangle_{t=0} = 1 + \frac{\sinh(\beta(\mu+\Lambda W))}{e^{\frac{\beta}{2}(U-\Lambda W)} + \cosh(\beta(\mu+\Lambda W))}.$$

One can immediately see here that $\langle n \rangle_{t=0} = 1 \quad \Longleftrightarrow \quad \mu + \Lambda W = 0.$

We can also easily evaluate the average phase factor for $t = 0$,

$$\begin{aligned}
\langle \text{phase} \rangle_{t=0} &= \frac{\prod_i \int_{\mathbb{R}^L} e^{\mathrm{i} \sum_{l=1}^{L} \sigma_{il} \lambda \frac{\mu+\Lambda W}{U-\Lambda W}} e^{-\vec{\sigma_i}^{\mathrm{t}} B \vec{\sigma_i}} \left| 1 + e^{-\mathrm{i}\lambda \sum_{l=1}^{L} \sigma_{il}} \right|^2 \mathrm{d}\vec{\sigma_i}}{\prod_i \int_{\mathbb{R}^L} e^{-\vec{\sigma_i}^{\mathrm{t}} B \vec{\sigma_i}} \left| 1 + e^{-\mathrm{i}\lambda \sum_{l=1}^{L} \sigma_{il}} \right|^2 \mathrm{d}\vec{\sigma_i}} = \frac{\widetilde{I}^N}{\left(\widetilde{I}(\mu + \Lambda W = 0) \right)^N} = \\
&= \frac{e^{-\widetilde{\kappa}\frac{\lambda^2}{4}\frac{\widetilde{\mu}^2}{\widetilde{U}^2} N} \left(1 + e^{-\widetilde{\kappa}\frac{\lambda^2}{4}} \cosh\left(\widetilde{\kappa} \frac{\lambda^2}{2} \frac{\widetilde{\mu}}{\widetilde{U}} \right) \right)^N}{\left(1 + e^{-\widetilde{\kappa}\frac{\lambda^2}{4}} \right)^N} = e^{-\widetilde{\kappa}\frac{\lambda^2}{4}\frac{\widetilde{\mu}^2}{\widetilde{U}^2} N} \left(\frac{e^{\widetilde{\kappa}\frac{\lambda^2}{4}} + \cosh\left(\widetilde{\kappa} \frac{\lambda^2}{2} \frac{\widetilde{\mu}}{\widetilde{U}} \right)}{e^{\widetilde{\kappa}\frac{\lambda^2}{4}} + 1} \right)^N = \\
&= e^{-L\frac{\widetilde{U}}{U}\frac{2\Delta\tau U}{4}\frac{\widetilde{\mu}^2}{\widetilde{U}^2} N} \left(\frac{e^{L\frac{\widetilde{U}}{U}\frac{2\Delta\tau U}{4}} + \cosh\left(L \frac{\widetilde{U}}{U} \frac{2\Delta\tau U}{2} \frac{\widetilde{\mu}}{\widetilde{U}} \right)}{e^{L\frac{\widetilde{U}}{U}\frac{2\Delta\tau U}{4}} + 1} \right)^N = \\
&= e^{-\frac{\beta N}{2(U-\Lambda W)}(\mu+\Lambda W)^2} \left(\frac{e^{\frac{\beta}{2}(U-\Lambda W)} + \cosh(\beta(\mu + \Lambda W))}{e^{\frac{\beta}{2}(U-\Lambda W)} + 1} \right)^N .
\end{aligned}$$

For $\mu + \Lambda W = 0$ the average phase factor is one. The envelope is given by a Gaussian prefactor with variance

$$\sigma^2 = \frac{U - \Lambda W}{\beta N}$$

and width

$$\sigma = \sqrt{\frac{U - \Lambda W}{\beta N}},$$

so it decreases with $\sqrt{\beta N}$.

15 Numerical results

Here we want to present some results for the Hubbard-Holstein model without and with hopping. All of the following results are obtained by generating (and saving) 400000 Hubbard-Stratonovich fields, or more precisely their sum over all their elements, and their respective Green's functions for a specific Λ and $\mu = -\Lambda W$, i.e. at half-filling.

15.1 Without hopping

We start out with the Hubbard-Holstein model without hopping, i.e. for $t = 0$, and compare our numerical results with those obtained from the analytic evaluation of the average density and the average phase factor.

In figure 5 we first show the normalized histogram of our 400000 sampled $|\sigma|$ for a 4×4 lattice for $\beta = 1$ and $\Lambda = 0.25$.

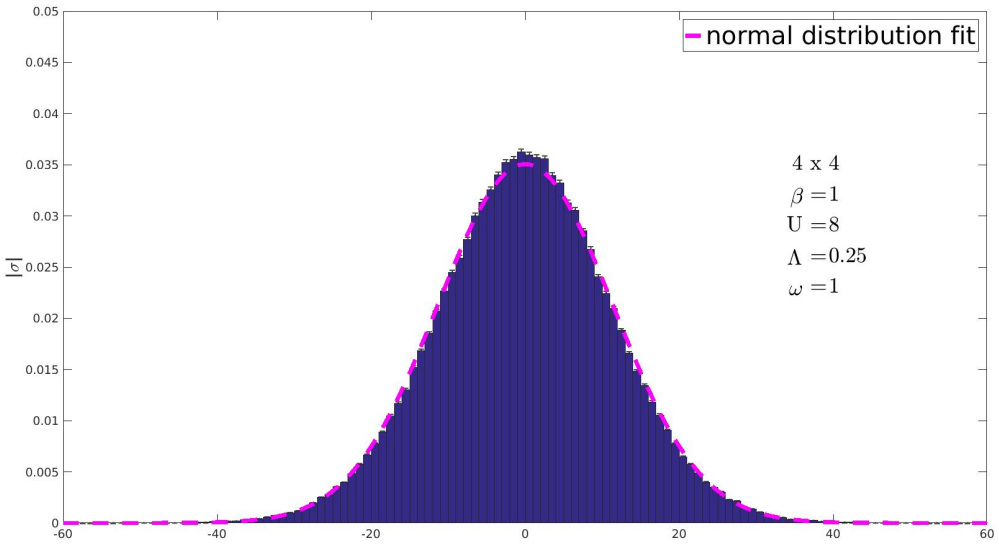

Figure 5: Normalized histogram of 400000 $|\sigma|$ for a 4×4 lattice for $\beta = 1$ and $\Lambda = 0.25$.

As one can see, the histogram follows a normal distribution with expectation value zero. Figure 6 shows the real part of the average phase factor and the analytically exact solution as a function of the chemical potential μ shifted by ΛW such that they are one at $\mu + \Lambda W = 0$.

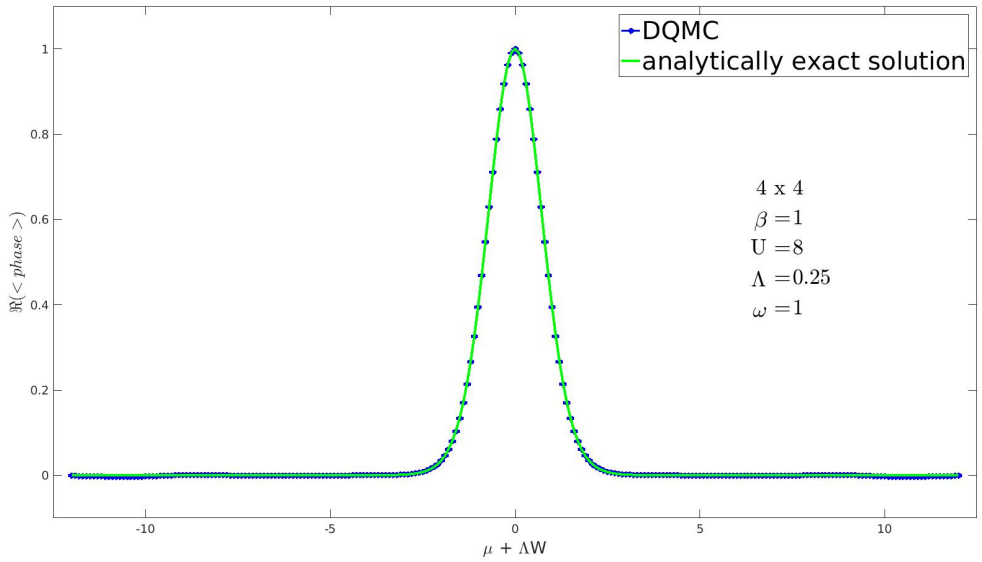

Figure 6: $\Re(\langle \text{phase} \rangle)$ vs $\mu + \Lambda W$ and comparison with the analytically exact solution.

As one can see, $\Re(\langle \text{phase} \rangle)$ and its error bars are clearly above zero only for $\mu + \Lambda W \in [-2, 2]$. Figure 7 shows the real part of the average density using both of the methods that we described before and the analytically exact solution as a function of $\mu + \Lambda W$.

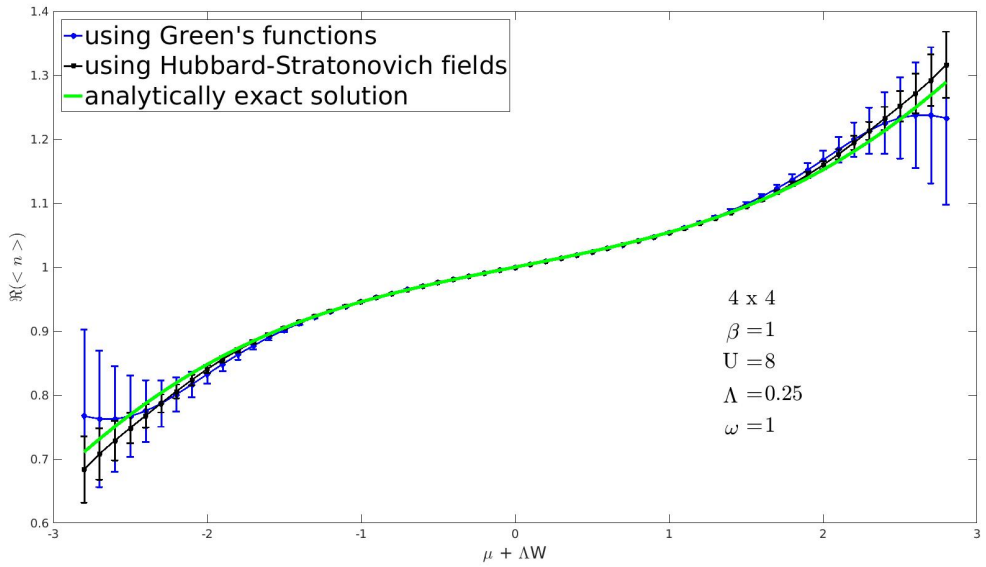

Figure 7: $\Re(\langle n \rangle)$ vs $\mu + \Lambda W$ using both methods and comparison with the analytically exact solution.

As one can see, using Hubbard-Stratonovich fields might have some advantages over using

Green's functions for the calculation of $\langle n \rangle$. Nevertheless, none of the two methods gives any useful results for $\mu + \Lambda W \notin [-2, 2]$.
What's very interesting here is that we have $\Re(\langle n \rangle) = 1$ at $\mu + \Lambda W = 0$. This is because of a shift in the equilibrium position of the lattice due to the coupled system minimizing its energy by exploiting the electron-phonon interaction energy $E_{\text{el-ph}} = -\alpha \sum_i \langle n_i \rangle \langle x_i \rangle$ at the expense of the lattice potential energy $E_{\text{ph,pot}} = \frac{\omega^2}{2} \sum_i \left\langle x_i^2 \right\rangle$ paid for the shifted equilibrium position [6].
For a uniform charge density, $\langle n_i \rangle = 1$, which one would expect for the half-filled case, this lattice shift can be obtained by minimizing the total energy (see (33)) with respect to the phonon displacement x_i for an arbitrary $i \in \{1, \ldots, N\}$.
The new equilibrium position is given by

$$\frac{\mathrm{d}}{\mathrm{d}x_i} \left(\frac{\omega^2}{2} x_i^2 - \alpha \langle n_i \rangle x_i \right) = 0,$$

which, for $\langle n_i \rangle = 1$, yields $x_i = \frac{\alpha}{\omega^2} = \frac{\sqrt{\Lambda W}}{\omega}$.
This demonstrates that at half-filling the lattice shifts to a new equilibrium position and electrons couple to fluctuations around this point.
Figure 8 shows the real part of the average phase factor as a function of the real part of the average density using Hubbard-Stratonovich fields and their respective analytically exact solutions.

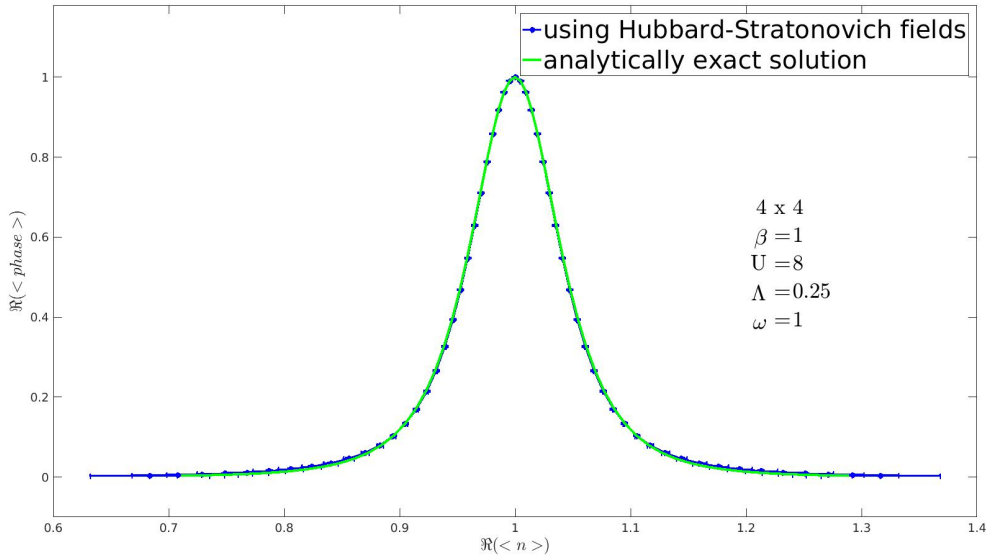

Figure 8: $\Re(\langle \text{phase} \rangle)$ vs $\Re(\langle n \rangle)$ using Hubbard-Stratonovich fields and comparison with the analytically exact solutions.

Also here the results are most accurate for $\Re(\langle \text{phase} \rangle)$ clearly above zero.

So by now we can be sure that our DQMC algorithm for the Hubbard-Holstein model works

perfectly fine as long as one considers a band-filling where $\Re(\langle \text{phase} \rangle)$ and its error bars are clearly above zero.

15.2 With hopping

Next, we consider the Hubbard-Holstein model with hopping ($t = 1$) and apply our DQMC algorithm to a 4×4 and a 2×1 lattice.

In figure 9 we show the real part of the average phase factor as a function of the shifted chemical potential $\mu + \Lambda W$ for a 4×4 lattice for $\Lambda = 0.25$ and $\Lambda = 0.5$.

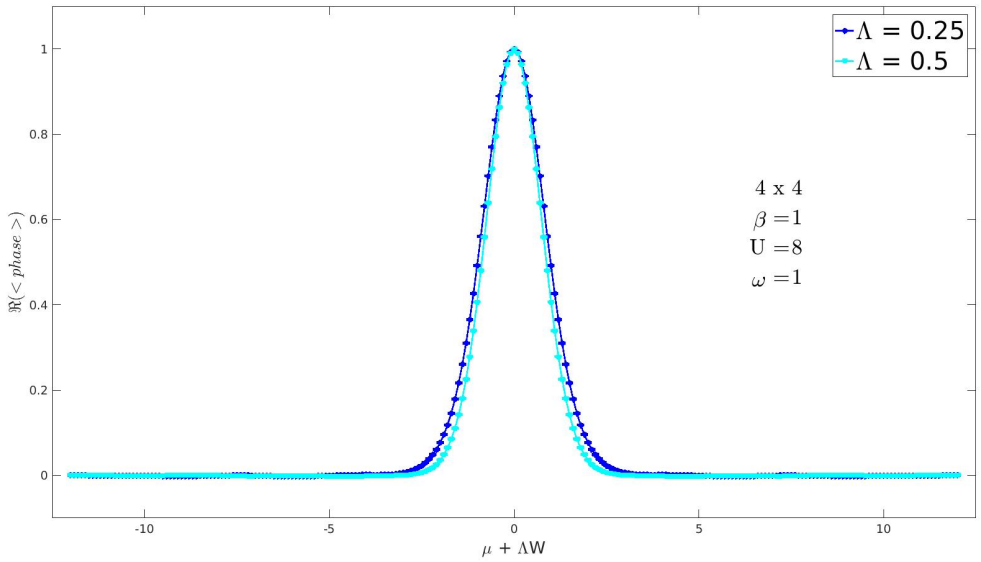

Figure 9: $\Re(\langle \text{phase} \rangle)$ vs $\mu + \Lambda W$ for a 4×4 lattice for $\Lambda = 0.25$ and $\Lambda = 0.5$.

As one can see, for $\Lambda = 0.25$ $\Re(\langle \text{phase} \rangle)$ and its error bars are clearly above zero only for $\mu + \Lambda W \in [-2.5, 2.5]$ and for $\Lambda = 0.5$ only for $\mu + \Lambda W \in [-2, 2]$.
Figure 10 shows the real part of the average density using again both methods as a function of $\mu + \Lambda W$.

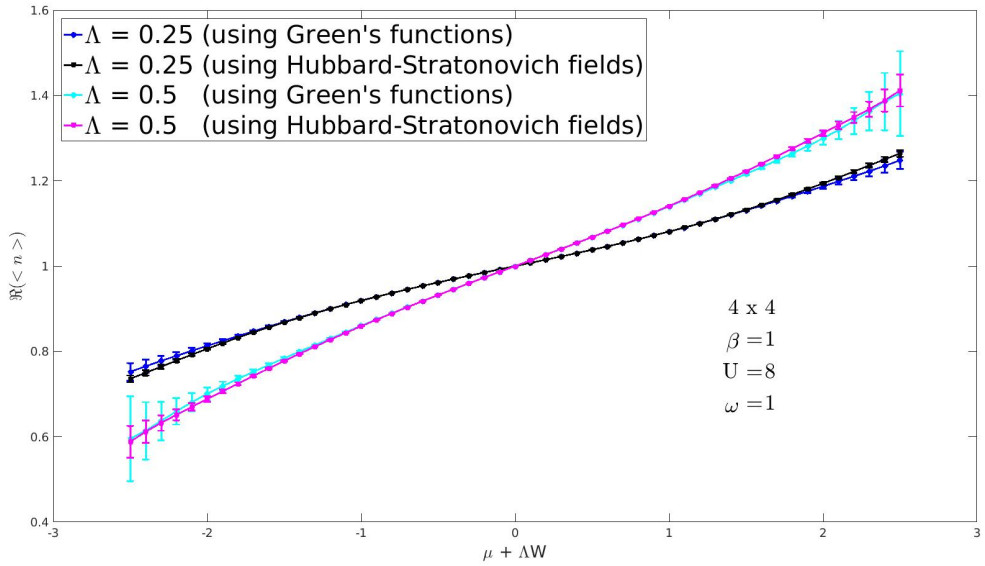

Figure 10: $\mathfrak{R}(\langle n \rangle)$ vs $\mu + \Lambda W$ using both methods.

Also here, using Hubbard-Stratonovich fields seems to have some advantages over using Green's functions for the calculation of $\langle n \rangle$.
Figure 11 shows the real part of the average phase factor as a function of the real part of the average density using Hubbard-Stratonovich fields.

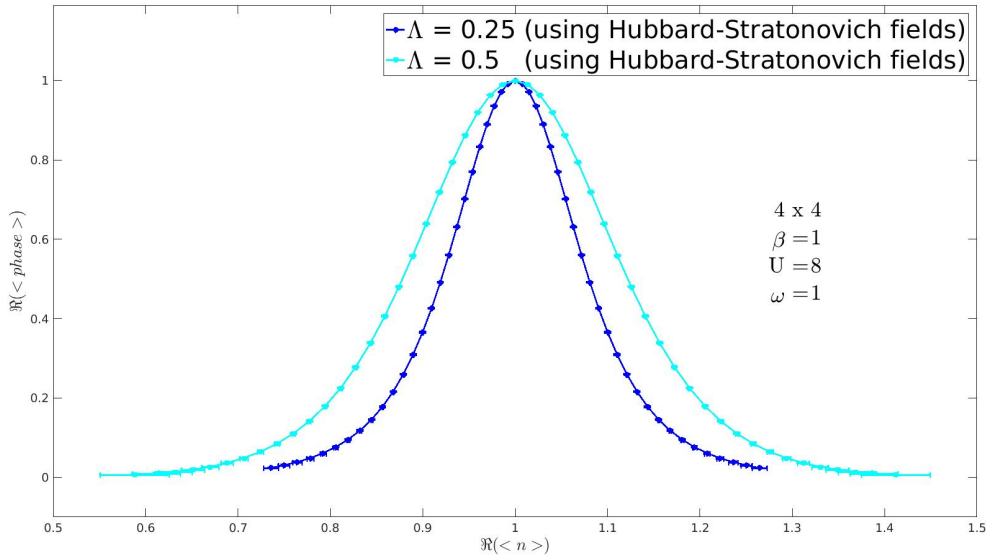

Figure 11: $\mathfrak{R}(\langle \text{phase} \rangle)$ vs $\mathfrak{R}(\langle n \rangle)$ using Hubbard-Stratonovich fields.

What's interesting here is that, although in figure 9 $\mathfrak{R}(\langle \text{phase} \rangle)$ was slightly better for

$\Lambda = 0.25$ than for $\Lambda = 0.5$, if plotted against $\mathfrak{R}(\langle n \rangle)$, it is better for the greater Λ. That's because for a given interval of $\mu + \Lambda W$, let's say $[-2.5, 2.5]$, the difference in band-filling between the two curves is greater (figure 10) than it is in $\mathfrak{R}(\langle \text{phase} \rangle)$.

In figure 12 we show again the real part of the average phase factor as a function of the shifted chemical potential $\mu + \Lambda W$, but this time for a 2×1 lattice for $\Lambda = 0.1$, $\Lambda = 0.2$ and $\Lambda = 0.3$.

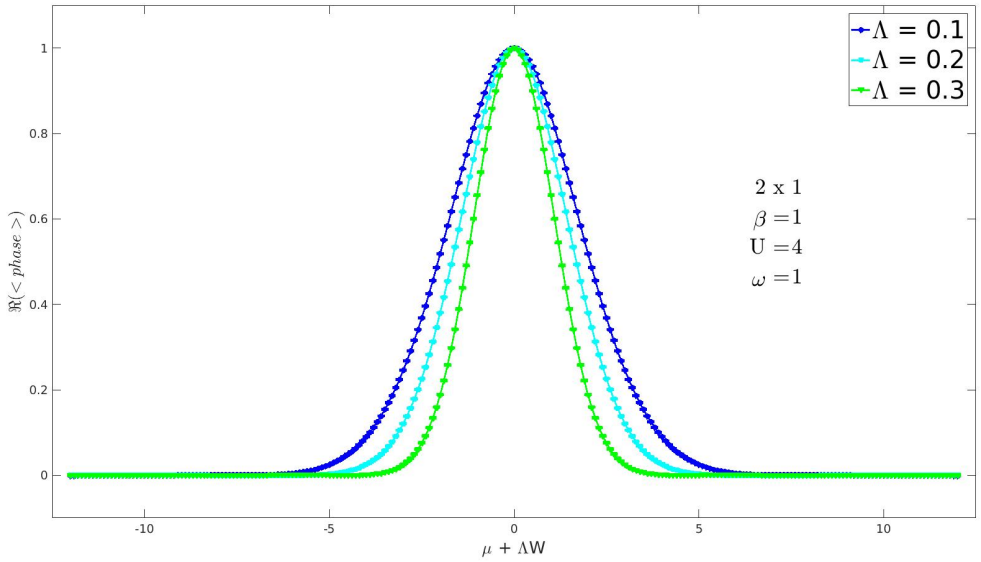

Figure 12: $\mathfrak{R}(\langle \text{phase} \rangle)$ vs $\mu + \Lambda W$ for a 2×1 lattice for $\Lambda = 0.1$, $\Lambda = 0.2$ and $\Lambda = 0.3$.

As one can see here, we won't expect any useful results for $\Lambda = 0.1$ for $\mu + \Lambda W \notin [-5, 5]$, for $\Lambda = 0.2$ for $\mu + \Lambda W \notin [-4, 4]$ and for $\Lambda = 0.3$ for $\mu + \Lambda W \notin [-3, 3]$.
Figure 13 shows the real part of the average density using Hubbard-Stratonovich fields as a function of $\mu + \Lambda W$.

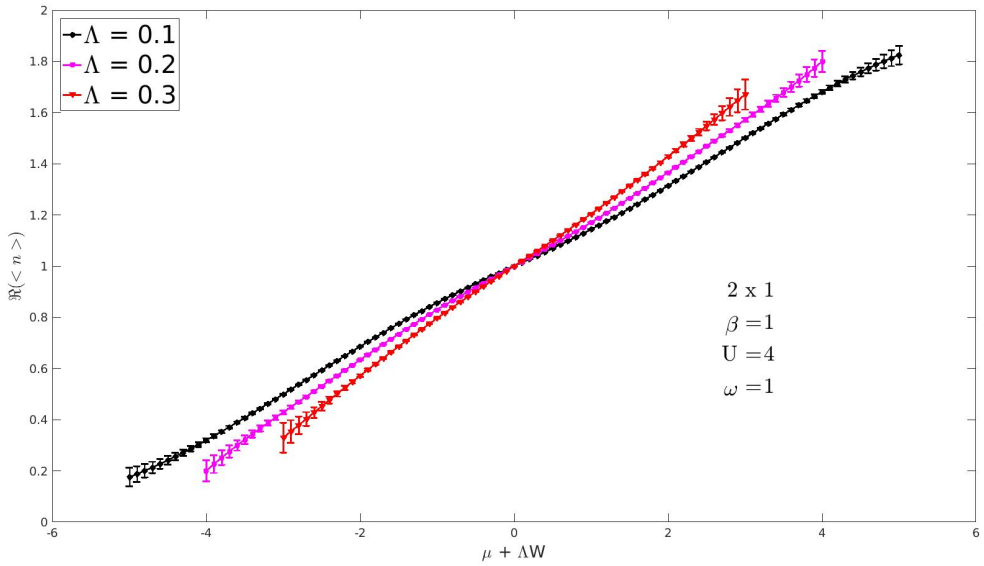

Figure 13: $\mathfrak{R}(\langle n \rangle)$ vs $\mu + \Lambda W$ using Hubbard-Stratonovich fields.

Figure 14 shows the real part of the average phase factor as a function of the real part of the average density using Hubbard-Stratonovich fields.

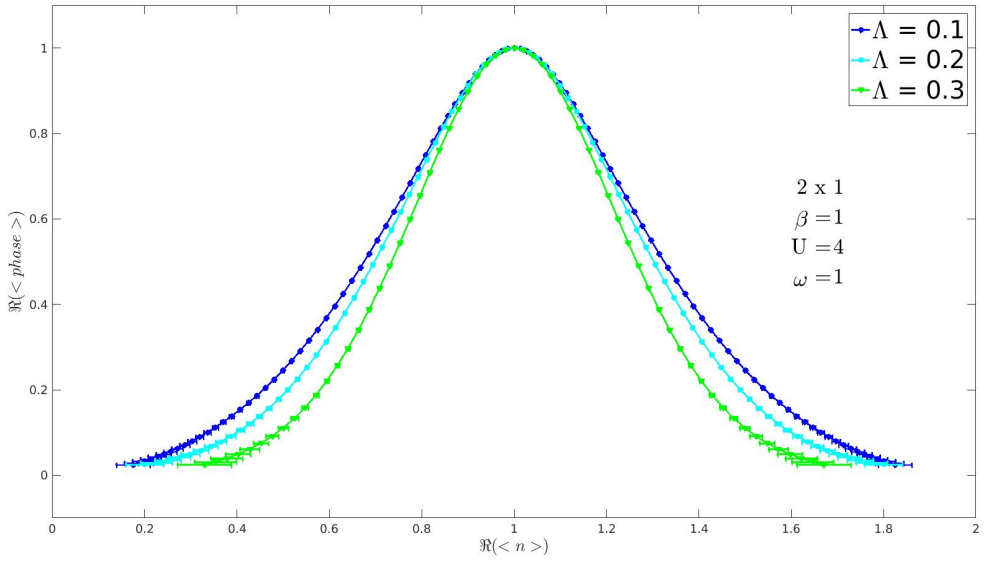

Figure 14: $\mathfrak{R}(\langle \text{phase} \rangle)$ vs $\mathfrak{R}(\langle n \rangle)$ using Hubbard-Stratonovich fields.

In contrast to the 4×4 lattice from before (figure 11), here, the greater Λ, the worse $\mathfrak{R}(\langle \text{phase} \rangle)$. And finally, figure 15 shows the compressibility $\kappa \propto \frac{\partial \langle n \rangle}{\partial \mu}$ using the data of the results in figure 13, but for smaller intervals, as a function of $\mu + \Lambda W$.

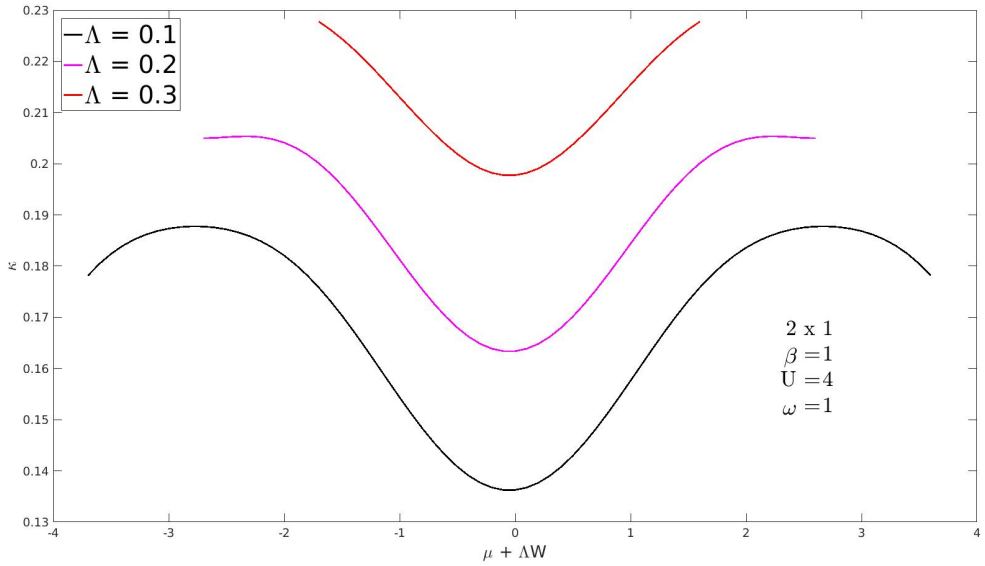

Figure 15: κ vs $\mu + \Lambda W$ using the data of the results in figure 13.

In these results one starts to see indications of competition between the attractive interaction mediated by the phonons and the Coulomb repulsion [6]. We can demonstrate this quite easily as we have explicitly integrated out the phonon degrees of freedom and obtained an effective Coulomb interaction strength $\widetilde{U} = U - \Lambda W$. For $\Lambda = 0.1$ the Coulomb repulsion dominates, showing a Mott gap in the system which manifests as a minimum located at $\mu + \Lambda W = 0$. As the electron-phonon coupling strength increases, the attractive interaction grows. This reduces the influence of the Coulomb repulsion and the size of the Mott gap diminishes. This is evident in figure 13, where the curves are the steeper and more linear the greater Λ, and in figure 15 in the rise in the minimum. Only for $\Lambda = 0.1$ we had sufficient accurate data in order to show that the system has a finite compressibility and $\kappa \to 0$ as the band completely fills or empties.

Conclusion

All the fundamental concepts that lay behind the DQMC algorithm were provided and it was applied to the Hubbard model. At the same time the real discrete and the real continuous Hubbard-Stratonovich transformations were used. Numerical results were compared with those obtained from exact diagonalization. In addition, a few results were presented for a band off half-filling.

For the Hubbard-Holstein model we presented a totally new approach where we were using the complex continuous Hubbard-Stratonovich transformation to derive an expression for the grand canonical partition function of the Hubbard-Holstein model with the phonon degrees of freedom being explicitly integrated out in order not to have had to sample the phonon fields. This solved the sign problem at half-filling for any electron-phonon coupling strength, but only there. At the end some results were presented for the Hubbard-Holstein model without and with hopping, where those for that without hopping were compared with those obtained from the analytic evaluation of the average density and the average phase factor. It turned out that our DQMC algorithm for the Hubbard-Holstein model works perfectly fine as long as one considers a band-filling where $\mathfrak{R}(\langle \text{phase} \rangle)$ and its error bars are clearly above zero.

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