Corrigendum: A Simple Monte Carlo Simulation For the Two Dimensional Attractive Hubbard Model (2020 Journal of Physics: Conf. Series 1483 012002)

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Page 2:
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A Simple Monte Carlo Simulation For the Two Dimensional Attractive Hubbard Model

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Abstract. We use the Auxiliary Field Quantum Monte Carlo technique to perform a simple study of the two dimensional attractive Hubbard model and calculate the total ground state energy to compare with another technique in the literature for \( U = -4t \). Our finite size extrapolated result corroborate the approximated lattice density-functional theory method for this value of \( U \) at half-filling. To stabilize the Auxiliary Field Quantum Monte Carlo algorithm one must resort to one of the two decomposition methods: the modified Grand-Schmidt decomposition and the singular value decomposition. Two characteristics like accuracy and total execution time were considered to compare the decomposition algorithms, and the results are presented bellow.

1. Introduction

Since it was proposed the Hubbard model[1, 2] has been intensively studied as a minimal model to describe electron-electron correlations in narrow band solids. In one dimension this model can be solved exactly by means of Bethe ansatz[3] wave functions leading to a set of Lieb and Wu equations[4]. By contrast, the two dimensional Hubbard model has no general exact
solution and several approaches have been employed to characterize the physical properties in real systems.

Although it seems a simple model in its Hamiltonian form (as we will see below), the set of parameters \((t, U, \mu)\) introduces new challenges in characterizing the physical properties like magnetic phases, electronic properties, and Mott transitions in two dimensions. For negative \(U\), it is well known that in the one-band \(U < 0\) attractive Hubbard model (AHM), the s-wave superconductivity transition manifests itself for a wide range of the attractive coupling strength. At half-filling, the competition between a charge density wave and s-wave superconductivity long-range orders renders the transition temperature to zero. For other fillings a finite superconducting transition temperature occurs. This is confirmed by the fact that off half-filling the AHM transition line can be mapped approximately onto the classical XY model. As a result, an effective Kosterlitz-Thouless transition temperature can be found\[5\]. This fact allowed that several well known techniques could be employed to determine the physical properties of the AHM, and, among them, we can cite the Auxiliary Field Quantum Monte Carlo (AFQMC)\[6\], the Renormalization Group Theory (RG)\[7\], and the Dynamical Mean Field Theory (DMFT)\[8\].

In all these techniques the Green’s function plays a central role and is used to calculate all physical quantities. We are particularly interested in performing a study of the AHM using the AFQMC technique for \(U = -4t\). The Green’s function for a given temperature is obtained through a procedure involving a multiplication of a certain number of matrices, simulating the propagation through the imaginary time direction. This matrix multiplication is a bottleneck of the method and one must take some care in dealing with it because numerical instabilities can arise for moderate values of \(|U|\). Two algorithms are commonly used to deal with it and we want to compare their performance (accuracy and total execution time) in the calculation of the Green’s function: the modified Grand-Schmidt decomposition (MGD) and the singular value decomposition (SVD)\[9\]. As we will see, both algorithms can be used to decompose the product of matrices in the imaginary time direction to stabilize the AFQMC algorithm when \(\beta\) grows beyond 4/t. The physical quantity used for our calculations was the total ground state energy. After finite size extrapolation we compare our results at half-filling with the lattice density-functional theory result\[10\]. Finally, we discuss about accuracy and total execution time of our program to give an idea about which algorithm must be chosen depending on the optimization of total execution time and accuracy of interest.

2. Auxiliary Field Quantum Monte Carlo

The starting point to the AFQMC simulations is the Hubbard Hamiltonian

\[
H = -t \sum_{<i,j>,\sigma} \left( a_{i,\sigma}^\dagger a_{j,\sigma} + h.c. \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} - \mu \sum_i (n_{i,\uparrow} + n_{i,\downarrow})
\]

(1)

where \(<i,j>\) stands for nearest neighbors, \( \{a_{i,\sigma}, a_{j,\sigma}'\} = \delta_{ij} \delta_{\sigma\sigma'} \), \(U\) the on-site electron-electron interaction strength (\(U < 0\) in the AHM case), \(n_{i,\sigma} = a_{i,\sigma}^\dagger a_{i,\sigma}\), and \(\mu\) the chemical potential responsible for the doping.

Once the total number of particles operator \((N = \sum_i (n_{i,\uparrow} + n_{i,\downarrow}))\) does commute with the Hamiltonian operator, one can add to the Hamiltonian a term \((N/2 - N_s/4)U\), where \(N_s = L^d\) (we will only consider the situation in which the number of sites, \(L\), is the same in any direction, with \(d\) being the space dimension in consideration) is the number of lattice sites, to rewrite it conveniently as
\[ H = -t \sum_{<i,j>,\sigma} (a_{i,\sigma}^\dagger a_{j,\sigma} + h.c.) + U \sum_i \left( n_{i,\uparrow} - \frac{1}{2} \right) \left( n_{i,\downarrow} - \frac{1}{2} \right) - \mu \sum_i (n_{i,\uparrow} + n_{i,\downarrow}) \]  

(2)

This additional term causes only a shift in the energy which cancels out in the process of calculating averages. The advantage to rewrite the Hamiltonian above will be clear when one calculates the partition function as we will see below.

The kinetic part of the Hamiltonian (2), \( K = -t \sum_{<i,j>,\sigma} (a_{i,\sigma}^\dagger a_{j,\sigma} + h.c.) \), does not commute with the interaction part, \( V = U \sum_i \left( n_{i,\uparrow} - \frac{1}{2} \right) \left( n_{i,\downarrow} - \frac{1}{2} \right) - \mu \sum_i (n_{i,\uparrow} + n_{i,\downarrow}) \). Nevertheless, one can use the Suzuki-Trotter decomposition\[11, 12\] to accomplish this task and write

\[ e^{-\beta H} = \left( e^{-\Delta \tau (K + V)} \right)^M = \left( e^{-\Delta \tau K} e^{-\Delta \tau V} \right)^M + O \left( \Delta \tau^2 U \right) \]

(3)

where \( \Delta \tau = \beta / M \). This is the analogue version of the path integral formulation of Quantum Mechanics with the imaginary-time interval \((0, \beta)\), discretized into \( M \) time slices.

Now we can use the fact that \( n_{i,\sigma}^2 = n_{i,\sigma} = 0, 1 \), when acting on a lattice site, to write the following relation for \( U < 0 \)

\[ \left( n_{i,\uparrow} - \frac{1}{2} \right) \left( n_{i,\downarrow} - \frac{1}{2} \right) = \frac{1}{2} (n_{i,\uparrow} + n_{i,\downarrow} - 1)^2 - \frac{1}{4} \]

(4)

With the aid of the relation above it is possible to rewrite the four operator interaction appearing in Hamiltonian, \( \left( n_{i,\uparrow} - \frac{1}{2} \right) \left( n_{i,\downarrow} - \frac{1}{2} \right) \), in terms of the double operator \( n_{i,\sigma} = a_{i,\sigma}^\dagger a_{i,\sigma} \). To this end, one must use the discrete version of the Hubbard-Stratonovich transformation\[13\]

\[ e^{-\Delta \tau U (n_{i,\uparrow} - \frac{1}{2}) (n_{i,\downarrow} - \frac{1}{2})} = \frac{1}{2} e^{\Delta \tau U / 4} \sum_{\lambda = \pm 1} e^{\lambda \Delta (n_{i,\uparrow} + n_{i,\downarrow} - 1)} \]

(5)

which introduces the discrete auxiliary field \( s = \pm 1 \), and \( \lambda \) is such that \( \cosh \lambda = \exp(\Delta \tau |U| / 2) \). The auxiliary field \( s \) can assume two values not only for each site \( i \), but also for each time slice \( \ell \). For this reason, the \( s \) variable must go through \( N_s \times M \) sites which from now on we will refer to them as space-time lattice, representing this dependence by \( s_i(\ell) \), where \( i = 1 \) to \( N_s \) and \( \ell = 1 \) to \( M \).

The grand partition function can be calculated through \( Tr e^{-\beta H} \), and using the relations above one gets

\[ Z = C^{MN_s} \sum_{\{s\}} \exp \left[ -\sum_{i,\ell} s_i(\ell) \lambda \right] \prod_{\ell=1}^M e^{-\Delta \tau \sum_{i,j,\sigma} K_{ij} a_{i,\sigma}^\dagger a_{j,\sigma}} e^{-\sum_{i} (\lambda s_i(\ell) + \Delta \tau \mu) n_{i,\sigma}} \]

(6)

where \( C = \frac{1}{2} e^{-\frac{1}{2} |U| \Delta \tau} \), \( Tr \) stands for trace over all \( \{s\} \) configurations, and \( T r \) stands for trace over all fermion configurations (number of particles and site occupation).

The relations above allow us to perform the trace over the fermions degrees of freedom in the partition function for \( U < 0 \) to get\[6, 12, 14\]
\[ Z = C^{MN_s} \sum_{\{s\}} \exp \left\{ - \sum_{i,\ell} s_i(\ell) \lambda \right\} \prod_{\sigma} \det \left[ 1 + B^\sigma_M B^\sigma_{M-1} \cdots B^\sigma_1 \right] \equiv \text{Tr}_{\{s\}} \rho(\{s\}) \] (7)

where \( B^\sigma_\ell \) is a \( N_s \times N_s \) matrix given by

\[ B^\sigma_\ell = e^{-\Delta \tau K} e^{V^\sigma(\ell)} \] (8)

with the hopping matrix \( K \) and potential matrix \( V^\sigma \) defined as

\[ K_{ij} = \begin{cases} -t & \text{for } i,j \text{ nearest neighbors,} \\ 0 & \text{otherwise,} \end{cases} \]

\[ V^\sigma_{ij}(\ell) = \delta_{ij} (\lambda s_i(\ell) + \Delta \tau \mu) \] (9)

The expression for the potential matrix \( V^\sigma \) in Eq. (9) reveals another advantage of working with the modified Hamiltonian (2). The half-filling case will occur at \( \mu = 0 \). Otherwise, the Hamiltonian (1) would imply in a term proportional to \( (\mu - U/2) \), which would set the half-filling case to \( \mu = U/2 \). Notice that the potential matrix entries at RHS in Eq. (9) do not depend on the spin index \( \sigma \). In fact, the auxiliary fields couple to the charge degrees of freedom instead of the spin ones. As a consequence, the partition function (7) is free of the sign problem because the product of determinants due to spin index is the same, unlike the \( U > 0 \) case.

The hopping matrix must be calculated using periodic boundary conditions. In one dimension, it will be a \( L \times L \) matrix, and \( L^2 \times L^2 \) in two dimensions given by

\[ K_{1D} = \begin{pmatrix} 0 & -t & 0 & \cdots & 0 & -t \\ -t & 0 & -t & \cdots & 0 & 0 \\ 0 & -t & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \cdots & 0 & -t \\ -t & 0 & \cdots & \cdots & -t & 0 \end{pmatrix} \]

\[ K_{2D} = \mathbb{1}_y \otimes K_{1D,x} + K_{1D,y} \otimes \mathbb{1}_x \]

To evaluate the respective exponential of the Kinetic matrix one can resort to the checkerboard pattern of the lattice, which is more suitable for numerical purposes or diagonalize the matrices above and calculate the exponential of the respective eigenvalues. Except when we comment in the text, we will set \( t = 1 \) to express our numerical results which means all physical quantities must be understood in units of \( t \).

The quantity \( \rho(\{s\}) \) appearing in Eq. (7) stands for the effective “density matrix”. As a result, an operator \( \mathcal{O} \) will have an average value given by

\[ \langle \mathcal{O} \rangle = \frac{1}{Z} \text{Tr}_{\{s\}} \rho(\{s\}) \] (10)

with \( \langle \mathcal{O} \rangle_{\{s\}} \) being the average with respect to a specific set of auxiliary fields configuration through the space-time lattice

\[ \langle \mathcal{O} \rangle_{\{s\}} = \frac{\text{Tr} \left\{ \mathcal{O} \prod_{t=1}^M \prod_{\sigma} e^{-\Delta \tau \sum_{i,j} a^\dagger_{i,\sigma} K_{ij} a_{j,\sigma} \sum_{\ell} (\lambda s_i(\ell) + \Delta \tau \mu) n_{i,\sigma} } \right\} \rho(\{s\}) }{\rho(\{s\})} \] (11)
Finally, the trace over the auxiliary fields \( s \) can be performed using the Monte Carlo importance sampling.

For the calculations of the physical quantities the single particle Green’s function plays a central role. For a specific configuration \( \{s\} \) one finds for the equal time Green’s function\(^6,\,^{14}\)

\[
\mathcal{g}_{ij}^\sigma(\ell) = \langle a_{i,\sigma}(\ell)a_{j,\sigma}^\dagger(\ell) \rangle_{\{s\}} = \left[ (1 + B_{\ell-1}^\sigma B_{\ell-2}^\sigma \cdots B_1^\sigma B_M^\sigma \cdots B_\ell^\sigma)^{-1} \right]_{ij}
\]

(12)

It is convenient to assess the change in the \( B_\ell^\sigma \) matrix due to \( s_i(\ell) \rightarrow -s_i(\ell) \): \( \delta V_{ij}^\sigma(\ell) \equiv V_{ij}^\sigma(\ell; -s) - V_{ij}^\sigma(\ell; s) = -2\lambda s_i(\ell)\delta_{ij} \). This allows us to write \( B_\ell^\sigma \rightarrow [B_\ell^\sigma]' = B_\ell^\sigma \Delta^\sigma_\ell(i) \), with

\[
[\Delta^\sigma_\ell(i)]_{jk} = \begin{cases} 
0 & \text{if } j \neq k \\
1 & \text{if } j = k \\
e^{\delta V_{ii}^\sigma(\ell)} & \text{if } j = k
\end{cases}
\]

In trying to flip an auxiliary field \( s_i(\ell) \) one must calculate the acceptance probability in the \textit{heat bath algorithm} \( r = r’/(1 + r’) \), with \( r’ = \rho(\{s\}’)/\rho(\{s\}) \). The configurations \( \{s\}’ \) and \( \{s\} \) are the same, except the \( s_i(\ell) \) which has the opposite sign in the \( \{s\}’ \) configuration. Using Eq. (7) it is not difficult to show that

\[
r = \frac{e^{2s_i(\ell)\lambda}R_\uparrow R_\downarrow}{1 + e^{2s_i(\ell)\lambda}R_\uparrow R_\downarrow}
\]

(13)

where \( R_\sigma = 1 + (1 - g_i^\sigma(\ell))(e^{-2s_i(\ell)\lambda} - 1) \), with \( \sigma = \uparrow, \downarrow \). Now, for a given space-time lattice site \( (i, \ell) \) one must accept to flip the auxiliary field \( s_i(\ell) \rightarrow -s_i(\ell) \) if a pseudorandom number generator \( \eta \in [0, 1] \) is such that \( \eta < r \). After the change in \( B_\ell^\sigma \) the Green’s function must be updated using the iteration

\[
\mathcal{g}_{jk}^\sigma(\ell) \leftarrow \mathcal{g}_{jk}^\sigma(\ell) + \frac{\mathcal{g}_{ik}^\sigma(\ell) \left( \mathcal{g}_{ij}^\sigma(\ell) - \delta_{ij} \right)}{e^{\delta V_{ii}^\sigma(\ell)} - 1 + (1 - g_i^\sigma(\ell))}
\]

(14)

The propagation of the change in the Green’s function can be performed by wrapping the old one

\[
\mathcal{g}^\sigma(\ell + 1) = B_\ell^\sigma \cdot \mathcal{g}^\sigma(\ell) \cdot [B_\ell^\sigma]^{-1}
\]

(15)

The propagated Green’s function through Eq. (15) is responsible for great part of imprecision during the calculations. Consequently, one must refresh the Green’s function by scratch at certain number of time slices \( \ell \) through Eq. (12).

Once particles do interact only with the auxiliary field, one can apply the Wick’s theorem to multi-particle Green’s functions. As a result, for instance, the two-particle Green’s function can be written in terms of the single-particle Green’s function

\[
\langle a_{i_1}^\dagger a_{i_2}^\dagger a_{i_3} a_{i_4} \rangle_{\{s\}} = \langle a_{i_1}^\dagger a_{i_2} \rangle_{\{s\}} \langle a_{i_3}^\dagger a_{i_4} \rangle_{\{s\}} + \langle a_{i_1}^\dagger a_{i_4} \rangle_{\{s\}} \langle a_{i_2}^\dagger a_{i_3} \rangle_{\{s\}}.
\]

(16)

This last result and the fact that \( n_{i,\sigma} = a_{i,\sigma}^\dagger a_{i,\sigma} = 1 - a_{i,\sigma} a_{i,\sigma}^\dagger \) allow us to write the on-site occupation number \( n_i = n_{i,\uparrow} + n_{i,\downarrow} \), and the double occupation as
\[
\langle n_i \rangle = 2 - \left( \langle g_{ii}^\uparrow \rangle + \langle g_{ii}^\downarrow \rangle \right)
\]
\[
\langle n_{i,\uparrow} n_{i,\downarrow} \rangle = 1 - \left( \langle g_{ii}^\uparrow \rangle + \langle g_{ii}^\downarrow \rangle \right) + \langle g_{ii}^\uparrow g_{ii}^\downarrow \rangle
\]  

(17)

where, for \( N_a \) auxiliary field configurations, we have

\[
\langle g_{ii}^\sigma \rangle = \frac{1}{MN_a} \sum_\ell \sum_{\{s\}} g_{ii}^\sigma(\ell)
\]  

(18)

We are particularly interested in the total energy per site given by the Hamiltonian (1) defined as

\[
\frac{E}{N_s} = \frac{\langle H \rangle}{N_s}
\]  

(19)

which must be calculated with the aid of Eqs. (17) and (18).

2.1. Matrix Stabilization

As mentioned above, the process of updating the Green’s function through Eq. (14) after a flip in an auxiliary field in a specific space-time lattice site \((i, \ell)\) causes no harm to the Green’s function matrices. The problem arises when we propagate the Green’s function by wrapping it through Eq. (15). To circumvent this situation we refresh the Green’s function for each certain number of time slices \(\ell\), let’s call it \(\ell_{\text{stab}}\). Thus, when \(\ell = \ell_{\text{stab}}\) the product of all \(B_{\ell}^\sigma\) matrices, \(A^\sigma(\ell)\), must be performed to calculate the refreshed Green’s function. The way we calculate the scratch (12) is important to avoid numerical instabilities, since it involves an inversion of a resulting matrix. For instance, for \(d = 2\) these instabilities often appears for calculations in which \(\beta > 4/t\) because \(A^\sigma(\ell)\) becomes very ill-conditioned for moderate values of \(U\). For those temperatures \(A^\sigma(\ell)\) can have eigenvalues as large as \(\exp(4\beta t)\) and as small as \(\exp(-4\beta t)\). The correct way to deal with this situation is to use a \(UDV\) decomposition of \(A^\sigma(\ell)\). To this end we will consider two possibilities: one is the modified Grand-Schmidt decomposition (MGD), and the other is the singular value decomposition (SVD).

In MGD a matrix can be decomposed in a product \(UDV\) in which \(U\) is a well behaved column othonormal matrix, \(D\) is a diagonal matrix containing the diverse scales, and \(V\) an upper-unit triangular matrix. If one wants to invert this matrix, it is easy to transpose the \(U\) matrix and is trivial to calculate the inverse of \(D\). To invert the \(V\) matrix one needs only to solve the linear system \(VV^{-1} = I\) by back-substitution. In SVD a matrix can be decomposed in a product \(UDV^T\) with \(U\) and \(V^T\) being orthogonal matrices, and \(D\) contains the singular values in decreasing order in its diagonal. The columns of \(U\) are the left singular vectors and the rows of \(V^T\) are the right singular vectors. To invert a matrix with non-zero singular value in SVD is very simple, since \(U\) and \(V^T\) are both orthogonal and \(D\) is diagonal. However, as we will see, the choice of the decomposition method must be made with care if the computation time is an issue to be considered. For simplicity we will use the notation \(UDV\) for general purposes and one must remember that in SVD we have \(V^T\) instead of \(V\).

The MGD algorithm is simple to implement and, under certain conditions, combine both precision and low computation time for a considerable range of temperatures and moderate values of \(U\). Although more precise the SVD algorithm involves a more complex implementation to reach high precision and lower computation time. In our calculations we use the well optimized \(DGESVD\) subroutine from the linear algebra package (lapack)[15].
Once the decomposition method is chosen we can proceed with the matrix multiplication. We will follow the procedure well described in the White et al. paper[16]. Let’s say we can multiply \( p \) matrices without losing the numerical precision. After the multiplication we must decompose the resulting matrix in the \( UDV \) form

\[
A_1^\sigma(\ell) = B_{\ell+p}^\sigma B_{\ell+p-1}^\sigma \cdots B_{\ell}^\sigma = U_1^\sigma D_1^\sigma V_1^\sigma \tag{20}
\]

and then, from the left, we multiply other \( p \) matrices to obtain

\[
A_2^\sigma(\ell) = B_{\ell+2p}^\sigma B_{\ell+2p-1}^\sigma \cdots B_{\ell+p+1}^\sigma U_1 D_1 V_1 = U_2^\sigma D_2^\sigma V_2^\sigma \tag{21}
\]

First we multiply all \( B^\sigma \) matrices by \( U_1 \) and then by \( D_1 \). This procedure rescales the product causing no harm to it. Finally we perform another \( UDV \) decomposition of this product generating \( U_2^\sigma M/p D_2^\sigma V_2^\sigma \). The last procedure is very important, since it involves to add an identity matrix, \( I \), to obtain the Green’s function. We use the fact that \( U_2^\sigma M/p \cdot U_2^\sigma M/p = I \) to substitute the identity matrix in Eq. (12) by this product and write

\[
g(\ell)^{-1} = U_2^\sigma M/p (U_2^\sigma M/p V_2^\sigma M/p + D_2^\sigma M/p V_2^\sigma M/p) = U_2^\sigma M/p \cdot U_2^\sigma V_2^\sigma M/p V_2^\sigma M/p = U_2^\sigma D_2^\sigma V_2^\sigma \tag{22}
\]

where we performed another \( UDV \) decomposition for the term in parenthesis.

3. Numerical Results

All simulations were performed at half-filling, \( \langle n \rangle = 1 \) or \( \mu = 0 \), and \( U = -4.0t \). The physical quantity of interest is the total ground state energy per site calculated through Eq. (19). First, we tested the assertion that \( t_\Delta \tau p \leq 1.5 \) as a margin of safety without loosing precision as pointed out in Ref.[16]. We can confirm this hypothesis for the one band attractive Hubbard model. We also found that \( \ell_{\text{stab}} \approx 10 \) is a good value of \( \ell \) to refresh the Green’s function for all simulations in the range of the inverse of temperatures up to \( \beta = 20/t \). Our results for the total energy per site using both MGD and SVD decompositions can be seen in Figs. (1) and (2) for \( \Delta \tau = 0.125/t \) and \( \Delta \tau = 0.1/t \). The resulting extrapolation behaved as \( \Delta \tau^2 \) as expected in analogy with the repulsive counterpart in Ref.[16]. We also assumed the same hypothesis that \( \Delta \tau \) errors in energy vary slowly with temperature, and used the same expression to correct the infinite-system limit for the two dimensional attractive Hubbard model given by

\[
E(\Delta \tau, L) = E(0, \infty) + c_1 \Delta \tau^2 + c_2/L^3 \tag{23}
\]
As a consequence, we can use the $\Delta \tau \to 0$ extrapolation to correct the energy scale as shown in the axis on the right in these figures. For both simulations, using MGD and SVD, we obtained the following extrapolated energy in units of $t$

$$E(0, \infty) = \begin{cases} -2.874 \pm 0.001 & \text{if MGD} \\ -2.877 \pm 0.001 & \text{if SVD} \end{cases}$$

(24)

(25)

with $c_1^{\text{MGD}} = -1.32 \pm 0.20$, $c_2^{\text{MGD}} = 1.81 \pm 0.11$, $c_1^{\text{SVD}} = -1.046 \pm 0.014$, and $c_2^{\text{SVD}} = 1.14 \pm 0.12$ respectively. The resulting corrections on the right scales in Figs. (1) and (2) are 0.020 and 0.016. These results are consistent with recent calculations in the work of Saubanère and Pastor[10], investigated in the framework of lattice density-functional theory in which the ground state energy for $U = -4.0t$ is about -2.86 in units of $t$.

![Figure 1. Total energy per site using $UDV$ decomposition with MGD algorithm, $\Delta \tau = 0.125/t$.](image1)

![Figure 2. Total energy per site using $UDV$ decomposition with SVD algorithm, $\Delta \tau = 0.125/t$.](image2)

In one dimension the lattice density-functional theory results are remarkably close to the exact Bethe-ansatz results for $U = -4.0t$. Although a thorough investigation is needed, we corroborate the total energy ground state result for $U = -4.0t$ as a good approximation at half-filling.

Now we move on to the accuracy and execution time of MGD and SVD algorithms. In Fig. (3) we display the plots of the total energy per site for a $4 \times 4$ lattice at half-filling, and $U = -4.0t$, using MGD and SVD algorithms. If accuracy is an issue, one can see that SVD algorithm is more suitable, and we can also say that is more stable. Although MGD can capture both the small scales and the large ones, it is not so accurate than SVD as one can see through the total ground state energy per site in Eqs. (24) and (25).

This was expected since, among other reasons, the SVD algorithm uses Givens rotations during the process of orthogonalization and therefore is more stable than MGD[9]. However, before we choose SVD as the main algorithm for auxiliary field Monte Carlo simulations, we must take into account the execution time as well. In Fig. (4) we plot the total execution time of our program depending on the number of matrices to be multiplied $M = \beta/\Delta \tau$. Once the most part of time consuming is due to scratch involving $M$, the total execution time is a good measure to compare both algorithms. As can be seen, the gain in accuracy through Eqs. (24) and (25) might not be so attractive if we look at Fig. (4). Insofar as $M$ grows, the total execution time grows very fast, which is a drawback depending on the physical properties we are interested in. As pointed out in Ref.[16] for most physical properties of interest, in one band Hubbard model, the MGD algorithm can combine both accuracy and optimized execution time.
4. Conclusion

We have tested the auxiliary field Monte Carlo algorithm to simulate the one band attractive Hubbard model. To stabilize the algorithm with respect to the number of matrices to be multiplied, one must resort to one of the decomposition methods discussed in our results. We tested two algorithms: the modified Grand-Schmidt decomposition (MGD) and singular value decomposition (SVD). We chose the total ground state energy as the physical quantity to be determined. After finite size extrapolation, we obtained good results compared with the lattice density-functional theory method. In comparing both algorithms, we could see that SVD is more accurate than MGD. However, although more accurate and stable, SVD can increase the execution time significantly, while MGD can combine both relatively good accuracy and optimized execution time, which must be taken into account through the simulations.

Acknowledgments

One of us (EC) thanks to Dr. David P. Landau for valuable discussions and the organizing committee for the kind hospitality in the XBMSP held in Ouro Preto-MG, Brazil.

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