Comparison of Calculations for the Hubbard model obtained with Quantum-Monte-Carlo, exact and stochastic Diagonalization

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Abstract

In this paper we compare numerical results for the ground state of the Hubbard model obtained by Quantum-Monte-Carlo simulations with results from exact and stochastic diagonalizations. We find good agreement for the ground state energy and superconducting correlations for both, the repulsive and attractive Hubbard model. Special emphasis lies on the superconducting correlations in the repulsive Hubbard model, where the small magnitude of the values obtained by Monte-Carlo simulations gives rise to the question, whether these results might be caused by fluctuations or systematic errors of the method. Although we notice that the Quantum-Monte-Carlo method has convergence problems for large interactions, coinciding with a minus sign problem, we confirm the results of the diagonalization techniques for small and moderate interaction strengths. Additionally we investigate the numerical stability and the convergence of the Quantum-Monte-Carlo method in the attractive case, to study the influence of the minus sign problem on convergence. Also here in the absence of a minus sign problem we encounter convergence problems for strong interactions.
I. INTRODUCTION

The Quantum-Monte-Carlo-Algorithms (QMC) are a well established tool in theoretical many particle physics [1] [2]. They have been successfully used to investigate the spin and charge degrees of freedom for the attractive and repulsive Hubbard model [3]. There are several kinds of QMC algorithms. We focus here on the Projector Quantum-Monte-Carlo-Algorithm (PQMC) [4]. In the case of the repulsive Hubbard model (RHM) the sign problem severely restricts the parameter space one can calculate. One goal of this paper is to show, what parameters of the RHM can be calculated using state of the art QMC-methods and which of the observables still give meaningful results when a sign problem occurs. Concerning the minus sign free attractive Hubbard model (AHM) we also want to distinguish numerical instabilities and convergence problems from well-”behaved” runs.

Inspired by results of de Raedt et al. [5] for the Heisenberg model we additionally investigate whether the choice of the elementary move in the Monte-Carlo procedure will have influence on the results.

We show that exact diagonalization (ED) [6], the stochastic diagonalization(SD) [7] and PQMC [4] give consistent results for a broad range of the simulated parameters.

In our paper we investigated a modified version of the Hubbard model the $t$-$t_p$-Hubbard model that is defined on a square lattice by the Hamiltonian:

$$H = -t \sum_{\langle i, j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) - t_p \sum_{\langle\langle i, j \rangle\rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$  \hspace{1cm} (1)

The number operator $n_{i\sigma}$ and the fermion creation operator $c_{i\sigma}^\dagger$ are defined as the ones with spin $\sigma$ at site $i$. $\sigma$ is the summation of spin up and spin down particles. The summation with respect to $\langle i, j \rangle$ is over the nearest neighbor pairs, whereas the summation with respect to $\langle\langle i, j \rangle\rangle$ is over the next nearest neighboring pairs. Taking $t_p = 0$ reproduces the usual single band Hubbard model [8]. The hopping parameter $t = 1$ is taken as the energy unit throughout this paper.
II. NUMERICAL METHODS

A. Exact Diagonalization

A basic technique to determine the ground state properties is the exact diagonalization. Here one writes the quantum problem as an eigenproblem

\[ H |\Psi\rangle = E |\Psi\rangle \]  

and searches for the lowest eigenvalue and eigenvector (eigenstate) of the Hamiltonian \( H \). We use for this paper the well-known Lanczos-method [6].

As basis states for the matrix formalism of the Hamiltonian we use plane waves, i.e. we take basis states \( |\Psi_i\rangle \) of the form:

\[ |\Psi_i\rangle := c_{k_1\uparrow}^\dagger c_{k_2\uparrow}^\dagger \ldots c_{k_n\uparrow}^\dagger c_{k_1'\downarrow}^\dagger c_{k_2'\downarrow}^\dagger \ldots c_{k_n'\downarrow}^\dagger |0\rangle, \]  

where \( |0\rangle \) is the vacuum state. To reduce the amount of the basis states we apply the translation symmetry, and restrict the calculation to the subspace where the total momentum \( K := \sum_i (k_i + k_i') = 0 \). As initial-vector for the Lanczos-procedure we use a random vector with the norm 1.

As Lanczos iteration we use [8]:

\[ H q_j = \beta_j q_{j-1} + \alpha_j q_j + \beta_j q_{j+1} \quad \text{with} \quad \beta_0 q_0 = 0 \]  

with \( q_j \) being the Lanczos-vector in the \( j \)-th iteration.

The limitation of the exact diagonalization is the amount of memory that is dramatically increasing with increasing system-size. For a lattice with \( N = n_x \cdot n_y \) points and \( n_e \) particles with spin up and \( n_e \) particles with spin down the Hilbert-space has the dimension \( D \):

\[ D = \left( \frac{N}{n_e} \right)^2 \]  

This means, that a system with \( N = 4 \cdot 4 = 16 \) lattice-points and \( n_e = 5 \) electrons per spin has the dimension \( D = \left( \frac{16}{5} \right)^2 = 4368^2 \approx 1.9 \cdot 10^7 \) and can be solved with the Lanczos-method.
on state of the art computers. But a system with $N = 6 \cdot 6 = 36$ and $n_e = 13$ electrons per spin direction has $D = \binom{36}{13}^2 \approx (2.3108 \cdot 10^9)^2 \approx 5.3398 \cdot 10^{18}$ and can not be solved by exact diagonalization with computer systems available today.

One method that circumvents some of these limitations is the stochastic diagonalization method.

B. Stochastic Diagonalization

For the stochastic diagonalization one also writes the physical quantum problem as an eigenproblem to extract the ground state properties. But one does not use all basis-states \[ \text{from the view of memory consumption it would be possible to handle all system-sizes with this technique. But due to a dramatic growth of the CPU-consumption with system-size it is so far only possible to determine the Hubbard-model for systems up to } 8 \times 8 \text{ sites for small and intermediate interactions.}

Sketching the basic ideas of the algorithm we consider $n$ basis-states, which are orthonormal. The matrix (Hamiltonian) for these $n$ basis-states is then denoted as $H^{(n)}$. The problem is to find the eigenvalues $E_i^{(n)}$. It is assumed, that they are ordered: $E_1^{(n)} \leq E_2^{(n)} \leq \ldots \leq E_n^{(n)}$. They can be obtained from $H^{(n)}$ with an unitary transformation $U^{(n)}$

$$E^{(n)} = U^{(n)} H^{(n)} U^{(n)^T}, \quad (6)$$

where $E^{(n)}$ is a diagonal matrix with the eigenvalues $E_1^{(n)}, E_2^{(n)}, \ldots, E_n^{(n)}$. There are several standard algorithms for obtaining this unitary transformation. In the classical Jacobi algorithm \[ \text{for example the transformation } U^{(n)} \text{ is a product of plane rotations } U^{(n,m)}(i_m, j_m). \]

$$U^{(n)} = \lim_{m \to \infty} \prod_m U^{(n,m)}(i_m, j_m). \quad (7)$$

Each plane rotation annihilates two off-diagonal elements $H_{i_m,j_m}^{(n,m)}$ and $H_{j_m,i_m}^{(n,m)}$, but also zeros in the off-diagonal elements can become nonzero after a rotation. Only the sum over all
off-diagonal elements converges to zero. This means that, it is very important for the convergence, in which order the rotations are performed. Usually one always annihilates the largest off-diagonal element in the following step. It is impossible to perform the infinite number of plane rotations in equation 7 with a computer, which is necessary for the exact diagonalization of $H^{(n)}$. Therefore one only performs so many plane rotations, until the absolute value of the largest off-diagonal matrix elements is smaller than a threshold $T_R$.

In the modified Jacobi scheme [7] one only computes the smallest eigenvalue of $H^{(n)}$ i.e. one keeps $i_m$ to be 1. This has the advantage, that it is not necessary to store the whole matrix and to make less rotations. One can prove [7] that the diagonal-element $H_{1,1}^{(n)}$ is the smallest eigenvalue of the matrix $H^{(n)}$, if the rotations are performed as described in [7].

A short description of the algorithm is given by:

1. choose one basis state as an initialization.

2. generate a set of new trial-states.

3. search the best trial-state for expanding the $(n \times n)$-matrix to an $((n + 1) \times (n + 1))$-matrix. The best trial-state, is the state, for which the energy reduction $\Delta_m$ with the unitary transformation $U^{(n+1,1)}(1, n + 1)$ is the largest.

4. if the reduction $\Delta_m$ of the best state is bigger than a threshold $T_A$, than this best state is added to the matrix and we apply plane rotations $U^{(n+1,m)}$ ($m \geq 1$) to the matrix $H^{(n+1)}$ until the size of all off-diagonal elements $H_{1,j}^{(n+1,m)}$ with $j = 2, \ldots, (n + 1)$ is smaller than a given threshold $T_R$.

5. if the reduction $\Delta_m$ of the best trial-state is smaller than the threshold $T_A$ reduce the threshold $T_A$.

6. if the convergence criteria are satisfied stop the iterations.

7. goto step 2.
One problem of the algorithm is: what are good convergence criteria? One is the convergence of the ground state energy $E^{(n)}_1$ (the smallest eigenvalue of the matrices $H^{(n)}$) with increasing number of states $n$. Others are the convergence of the physical properties one is interested in, like correlation-functions. An additional good criterion for the convergence of the algorithm is the norm $N^{(n,m)}_1$ of the first column of the matrix $H^{(n,m)}$:

$$N^{(n,m)}_1 := \sqrt{\sum_{i=1}^{n} H^{(n,m)}_{i,1}^2} \quad (8)$$

C. The Projector Quantum Monte Carlo Method

The QMC-algorithm used in this paper to investigate the ground state properties of the Hubbard model is the Projector-Quantum-Monte-Carlo (PQMC) algorithm. The basic idea of this algorithm is to use a projection operator $e^{-\theta H}$ to extract the ground state $|\Psi_0\rangle$ of the Hamiltonian $H$ from the trial wave function $|\Psi_T\rangle$ [4]:

$$|\Psi_0\rangle = \lim_{\theta \to \infty} e^{-\theta H} |\Psi_T\rangle \quad (9)$$

The trial wave function $|\Psi_T\rangle$ is chosen to be a Slater determinant.

Sorella et al. [10] have developed a stable algorithm for this purpose. We give a short description to introduce the notation. The Hubbard Hamiltonian [11] then reads as:

$$H = H_{\text{kin}} + H_{\text{hub}} \quad (10)$$

$$H_{\text{kin}} = -t \sum_{\langle i,j \rangle,\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) - t_p \sum_{\langle\langle i,j \rangle\rangle,\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma})$$

$$H_{\text{hub}} = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Using the Trotter-Suzuki formula [1] the exponential of the Hubbard Hamiltonian is rewritten as:

$$e^{-\theta(H_{\text{kin}}+H_{\text{hub}})} = \lim_{m \to \infty} \left( e^{-\frac{\theta}{m}H_{\text{kin}}} e^{-\frac{\theta}{m}H_{\text{hub}}} \right)^m \quad (11)$$

For the interaction term $H_{\text{hub}}$ we introduce the discrete Hubbard Stratonovich transformation [11] to eliminate the quartic term as:
\[ e^{-\tau H_{\text{hub}}} = \prod_i e^{-\tau U n_{i\uparrow} n_{i\downarrow}} \]  
\[ = \sum_{\sigma=\pm 1} e^{-\tau \sum_l \hat{n}_l U c^{\lambda} \sum_i \sigma_i \hat{m}_i} \]  
\[ \equiv \sum_{\sigma=\pm 1} e^{h_{\text{hub}}(\sigma)} \]  

where the following definitions have been used:

\[ \hat{n}_i \equiv \begin{cases} 
    n_{i\uparrow} + n_{i\downarrow} - 1 & \text{if } U \leq 0 \\
    n_{i\uparrow} + n_{i\downarrow} & \text{if } U > 0 
\end{cases} \quad \text{and} \quad \hat{m}_i \equiv \begin{cases} 
    n_{i\uparrow} + n_{i\downarrow} - 1 & \text{if } U \leq 0 \\
    n_{i\uparrow} - n_{i\downarrow} & \text{if } U > 0 
\end{cases} \]  

and

\[ \cosh(\lambda) \equiv e^{\frac{\tau}{2}|U|} \]  
\[ \tau = \frac{\theta}{m} . \]  

The elements of the discrete Hubbard Stratonovich field \( \sigma \) can only take the values \( \sigma_i = \pm 1 \). The Hubbard Stratonovich field is often referred to as Ising-spins or \( \sigma \)-spins.

The projection of the ground state then reads as:

\[ e^{-\theta H} |\Psi_T\rangle = \sum_{\sigma} \prod_{l=1,m} e^{-\frac{\theta}{2} H_{\text{kin}} e^{h_{\text{hub}}(\sigma(l))}} |\Psi_T\rangle \]  
\[ \equiv \sum_{\sigma} |\sigma\rangle \]  

The expectation value of an observable \( A \) in the ground state is now given by:

\[ \langle \langle A \rangle \rangle = \frac{\sum_{\sigma,\sigma'} \langle \sigma | A | \sigma' \rangle}{\sum_{\sigma} \langle \sigma | \sigma' \rangle} . \]  

Normalizing the expectation value \( \langle \sigma | A | \sigma' \rangle \) with \( \langle \sigma | \sigma' \rangle \) and using the following definitions

\[ \langle A \rangle = \frac{\langle \sigma | A | \sigma' \rangle}{\langle \sigma | \sigma' \rangle} \]  
\[ w(\sigma, \sigma') = \frac{|\langle \sigma | \sigma' \rangle|}{\sum_{\sigma,\sigma'} |\langle \sigma | \sigma' \rangle|} \]  

the expectation value reads as:
\begin{align}
\langle\langle A\rangle\rangle &= \frac{\sum_{\sigma, \sigma'} w(\sigma, \sigma') \text{sign}(\langle\sigma|\sigma'\rangle\langle A\rangle)}{\sum_{\sigma, \sigma'} w(\sigma, \sigma') \text{sign}(\langle\sigma|\sigma'\rangle)} \quad .
\end{align}

The sum over $\sigma, \sigma'$ is now calculated by an importance sampling Monte-Carlo procedure. The algorithm can be sketched in the following way:

1. create a new configuration $(\sigma, \sigma')_{n+1}$ from the old configuration $(\sigma, \sigma')_n$ by an elementary move.

2. calculate the transition probability

\begin{align}
P((\sigma, \sigma')_n \rightarrow (\sigma, \sigma')_{n+1}) &= \frac{w(\sigma, \sigma')_{n+1}}{w(\sigma, \sigma')_n}
\end{align}

3. calculate a random number $z$ between 0 and 1

4. if $z < P((\sigma, \sigma')_n \rightarrow (\sigma, \sigma')_{n+1})$ accept the new configuration $(\sigma, \sigma')_{n+1}$ else keep the old configuration $(\sigma, \sigma')_n$

5. with this procedure one generates the Monte Carlo configurations with the probability $w(\sigma, \sigma')$. The expectation value of an observable $A$ is then given by:

\begin{align}
\langle\langle A\rangle\rangle = \frac{\sum_{\sigma, \sigma'} \text{sign}(w(\sigma, \sigma'))\langle A\rangle}{\langle\text{sign}\rangle}
\end{align}

with the average sign $\langle\text{sign}\rangle$:

\begin{align}
\langle\text{sign}\rangle = \sum_{\sigma, \sigma'} \text{sign}(w(\sigma, \sigma'))
\end{align}

In order to use the determinant $\langle\sigma|\sigma'\rangle$ as a probability one has to take the absolute value. The sign of this determinant then becomes part of the expectation value which causes the so called Minus-Sign problem.

We implemented three different kinds of elementary moves, acting on the $N \times m$ array of the $\sigma$-configurations ($\sigma$-spins), where $N$ is the system-size and $m$ the number of Trotter slices. We are motivated by results obtained for QMC-Simulations of the Spin $\frac{1}{2}$ Heisenberg
model where evidence was presented that the elementary move influences the convergence of the algorithms and can even lead to wrong results [5].

1. The Cluster move flips a certain number $S$ of randomly chosen $\sigma$-spins. The criteria for the choice of the number $S$ was, that the acceptance rate of these moves was at least 40%.

2. The Slice move flips a certain number $S$ of randomly chosen $\sigma$-spins only on a single Trotter slice. By visiting the slices in consecutive order and storing intermediate results of the calculation the amount of computations can be reduced significantly. Details of the implementation will be given elsewhere [12].

3. The Single Spin elementary move only flips one randomly chosen single $\sigma$-spin. This allows a significant simplification of the algorithm [13].

For the efficient implementation of the algorithm the elementary move is more than a minor detail and the execution time depends significantly on the choice of the elementary move [12].

QMC simulations of the Hubbard model are in general very time consuming. The calculations were carried out on a parallel computer. Details of the parallelized algorithm have already been published elsewhere [14].

Finally we define two important quantities, the Monte-Carlo steps and the error bars in the QMC algorithm. One Monte Carlo step (MCS) is completed when the program has tried to flip all $N \cdot m$ $\sigma$-spins ($N$ is the size of the lattice and $m$ is the number of Trotterslices).

If after one run through the lattice the acceptance rate is too low, additional runs are performed until the acceptance rate is reached. Second the error bars are taken over bins, i.e. typically 50 measurements are sampled in one average $\bar{A}$. The error bar is now calculated as the fluctuations of these averages $\bar{A}$. 
III. OBSERVABLES

As a check whether the different programs are correct we compare different observables. The definitions of these observables will be presented in this section.

The observable commonly used for the check of a correct ground state determined with a method is the ground state energy per lattice site $E_0/N$.

A common way to study superconductivity in the Hubbard model is to examine the two particle correlation functions for the occurrence of Off Diagonal Long Range Order (ODLRO) in the model \cite{15}. In order to do this we calculate the full correlation function with $d_{x^2-y^2}$ symmetry \cite{17}

$$C^{Full}_{d_{x^2-y^2}}(r) = \frac{1}{N} \sum_{i,\delta,\delta'} g_\delta g_{\delta'} \langle \hat{c}_{i+\delta\downarrow}^\dagger \hat{c}_{i+\delta'\uparrow}^\dagger \hat{c}_{i+\delta'\downarrow} \hat{c}_{i+\delta\uparrow} \rangle$$  \hspace{1cm} (26)

that measures superconducting correlations as a function of lattice vector $r$. The phase factors $g_\delta, g_{\delta'}$ are 1 in $x$-direction and $-1$ in $y$-direction. The sum over $i$ goes over the whole lattice. The sums with respect to $\delta$ and $\delta'$ are the independent sums over the nearest neighbors of $i$.

When studying the superconducting properties of small Hubbard-Clusters the full correlation function is not a very appropriate measure as this expectation value also contains contributions from the one-particle Greens functions $C_{\sigma}^{single}(r) = \frac{1}{N} \sum_i \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{i+r\sigma} \rangle$. In principle these one particle contributions can be neglected as they decrease to zero with increasing distance $|r|$. But when studying small clusters their influence on the results has to be taken into account \cite{16}. Therefore we study the vertex correlation function

$$C^{Vertex}_{d_{x^2-y^2}}(r) = C^{Full}_{d_{x^2-y^2}}(r) - \sum_{\delta,\delta'} (g_\delta g_{\delta'} C_{\uparrow}^{single}(r) C_{\downarrow}^{single}(r + \delta' - \delta))$$  \hspace{1cm} (27)

$$= \frac{1}{N} \sum_{i,\delta,\delta'} g_\delta g_{\delta'} \langle \hat{c}_{i+\delta\downarrow}^\dagger \hat{c}_{i+\delta'\uparrow}^\dagger \hat{c}_{i+\delta'\downarrow} \hat{c}_{i+\delta\uparrow} \rangle - g_\delta g_{\delta'} \langle \hat{c}_{i+\delta\uparrow}^\dagger \hat{c}_{i+\delta'\downarrow} \rangle \langle \hat{c}_{i+\delta\downarrow}^\dagger \hat{c}_{i+\delta'\uparrow} \rangle .$$
IV. COMPARISON

In this section we compare the results obtained with ED, SD and PQMC. We restrict ourselves to the case of the $4 \times 4$ system. This is the largest square lattice that can be solved with the exact diagonalization. The goal is to check the correct convergence of the QMC-algorithms. By this we mean for the PQMC, that we check, whether the Monte Carlo procedure converges correctly and whether the projection parameter $\Theta$ and the Trotter decomposition $m$ are chosen sufficiently large to obtain the true ground state. Special emphasis lies on various technical problems that come with the application of the QMC method as there are the minus sign problem, numerical instabilities and statistical fluctuations. In the case of the SD we investigate whether the number of basis states accumulated is sufficient to be a good approximation of the "true" ground state.

Inspired by the results for the RHM [17] for larger lattice sizes we first turn our attention to the RHM. The most common indicator for reaching the ground state is the ground state energy per lattice site $E_0/N$. In table I and II we present a comparison of the ground state energies of the ED, SD and the three different implementations of the PQMC-algorithm (section II.C). The error bars on the QMC results can be estimated to be 0.25%. The result of ED, SD and QMC are the same within these error bounds. We find excellent agreement between these different methods for the ground state energy even when a minus sign problem is present in the calculations. This can be seen from table III where we list the average sign ($\langle \text{sign} \rangle$, eq. 25) for the simulations presented in table I and II. The $\langle \text{sign} \rangle$ has the same value in all three PQMC-algorithms we used. The SD method gives in contrast to the PQMC algorithm an upper bound for the exact ground state energy $E_0$. Therefore comparing two energies obtained with SD it is clear, that the lower energy is closer to the exact energy. For the PQMC the error bar gives a bound for the ground state energy, but it is not possible to deduce from the PQMC value whether the energy is above or below the exact energy.

It has turned out that comparing ground state energies is not a very sensitive indicator
whether the PQMC has reached the true ground state [18], [19].

Our interest lies on the expectation values of the superconducting correlation function for the RHM in the $d_{x^2-y^2}$-channel.

In figure 1 we present the comparison of $C_{d_{x^2-y^2}}^{\text{Full}}(r)$ (eq. 26) for five different methods namely the ED, SD, single-PQMC, slice-PQMC and cluster-PQMC. For a $4 \times 4$ Hubbard system with $t_p = -0.22$, $N_e = 5 + 5$ and $U = 2, 4, 5$ and 6 respectively we observe perfect agreement of all five programs. The points for all five methods fall on identical positions and cannot be distinguished.

As we outlined in the previous section the more appropriate indicator for the existence of ODLRO in small clusters is the vertex correlation function $C_{d_{x^2-y^2}}^{\text{Vertex}}(r)$ (eq. 27). The absolute values of this vertex correlation function compared to the full correlation function turned out to be very small for the RHM [17] giving rise to the question whether these small results might be artifacts of the various problems that come with the application of the QMC-method.

In figure 2 a-d we present a systematic investigation of the $4 \times 4$-system with $5 + 5$ electrons for various values of $U$. In contrast to the case of the full correlation function $C_{d_{x^2-y^2}}^{\text{Full}}(r)$ we observe that in the case of the vertex correlation function $C_{d_{x^2-y^2}}^{\text{Vertex}}(r)$ (eq. 27) only simulations with $U = 2$ and $U = 4$ show again a perfect agreement. For larger interactions $U = 5$ and $U = 6$ we find strong fluctuations of the different PQMC methods coinciding with the occurrence of a minus sign problem in the simulations (table III). Thus we have shown that whereas the ground state energy and the full correlation function seem perfectly converged this is no proof that the vertex correlation function is converged in these runs. The fluctuations in the correlation functions have increased dramatically with interaction $U$ despite the significant higher number of MCS, as shown in table IV.

We now turn our attention to the AHM. Here we consider both the cluster and the single spin dynamics in the PQMC algorithm. The AHM shows superconductivity in the on-site s-wave channel. In this case there is no summation over the nearest neighbors, i.e. no sum with respect to $\delta$ and $\delta'$ in the eq. 26 and 27. Of course the phasefactors $g_\delta = g_{\delta'}$ are equal
First we compare the ground state energy for PQMC with ED and SD (table V). Note
that for the SD deviations from the ED values develop with increasing interaction strength\(|U|\). For interactions \(U = -6\) and \(U = -8\) the SD algorithm has convergence problems. For these high values of \(|U|\) the k-space representation of the basis states is no longer appropriate. This can be seen from figure 3. The SD algorithm is able to find almost every important state (i.e. all states with a large weight) for the interaction \(U = -2\). In the interval 0.0001 to 0.00032 there are 6276 states in the ground state of the exact diagonalization. 6012 states are in the same interval in the basis of important states of the SD. For \(U = -2\) the SD has collected almost every state with a weight larger than \(10^{-4}\).

The number of states with a relatively large weight increases for stronger interactions \(|U|\). In the interval 0.001 to 0.0032 the number of states in the ground state of the exact diagonalization goes from 1082 (\(U = -2\)) to 24003 (\(U = -8\)) (fig. 3). Therefore more states are necessary as a good approximation of the ground state in the SD. These convergence problems can be demonstrated even clearer in table VI. This table shows additionally to the number of states \(N_{SD}\) in the basis of the SD (plotted in fig. 3) the norm \(N_1^{(n,m)}\) of the first column (eq. 8) and the threshold \(T_A\) for the acceptance of new states. Because the CPU-time is limited in practice the number of states \(N_{SD}\) can not exceed to some hundred thousand. From table VI one can see, that \(N_{SD}\) and \(N_1^{(n,m)}\) as well as \(T_A\) are increasing with \(|U|\). For practical purposes the SD is not able to find a good approximation of the exact ground state beyond a certain interaction. We were not able to resolve these problems by the use of a real space representation of the basis states.

As a second step we compare the superconducting correlation function with on-site s-wave symmetry for the AHM. Figure 4 shows \(C_{Full}^{F}\) and figure 5 shows \(C_{Full}^{Vertex}(r)\) for \(U = -2, -4, -6\) and \(-8\) for a \(4 \times 4\) system with \(t_p = 0\). The comparison of the vertex correlation function with the Lanczos method clearly indicates that for \(U = -6\) and especially for \(U = -8\) the cluster program shows deviations from the ED values. These deviations are comparable to the case of the RHM, where we also observe convergence problems for increasing interaction...
We tried to find out where these convergence problems might come from. On the one hand we investigated the dependence on the projection parameter $\Theta$. In figure 7 and 8 we show the dependence of the cumulated plateau of the vertex correlation function $C^{\text{Vertex}}_\Theta(r)$ and of the ground state energy per site $E_0/N$ of the projection parameter $\Theta$. It clearly indicates that a projection parameter of $\Theta = 8$ as it was used throughout the rest of the paper is sufficient to reach the ground state. Note that especially the ground state energy does not depend very strongly on the projection parameter.

Furthermore we investigated whether numerical instabilities might cause the convergence problems. In table VII we compare the ground state energy for different numbers of stabilizations $n_{\text{stab}}$. To reduce numerical instabilities the product of $m$ imaginary time slices is being stabilized by a modified Gram-Schmidt orthogonalization [10].

A stabilization is performed every $n_{\text{stab}}$ slices of the Trotter decomposition. The results agree perfectly so we conclude that the simulations were numerically stable.

Finally we checked whether the MC process depends on the starting seed of the random number generator. Figure 9 shows the ground state energy for different seeds. Here we also cannot discover any unusual behaviour.

Thus even in the absence of a minus sign problem for the AHM the PQMC algorithms have convergence problems. An even more striking result is seen comparing table IV and VIII. The number of MCS needed for convergence both in the RHM as well as in the AHM increase with interaction strength $|U|$ for both the single and the cluster algorithm in the same manner. As a comparison we show in fig. 6 the results for unconverged runs. The corresponding number of MCS (PQMC) and number of basis state (SD) are listed in table X.

Given only limited CPU power, we come to the result, that even when there is no minus sign problem as for the example in the case of the PQMC algorithm for the attractive Hubbard model or of the SD the presented numerical algorithms cannot handle values of $U$ beyond a critical interaction, because of convergence problems.
V. CONCLUSION

We presented a detailed comparison of the results of exact diagonalization, stochastic diagonalization and the PQMC. For the PQMC we implemented three different elementary moves, namely the single spin flip move, the slice move and the cluster move. We showed that there is perfect agreement between all five methods for the ground state energies and the full correlation function for the RHM and the AHM. Also for the vertex correlation functions, that are very small in magnitude in the repulsive case, the exact diagonalization results can be confirmed by PQMC and stochastic diagonalization. But for large interactions it is necessary to perform dramatically more MCS in the PQMC respectively to collect much more states in the SD. The observation that with an increase of $|U|$ the amount of CPU-time is enhanced dramatically leads to the problem that these calculations cannot be performed with state of the art computers for large interaction strengths $|U|$. This increase in CPU-time was found both, in the RHM where it was expected due to the occurrence of the well-known minus sign problem and in the AHM that is minus sign free.

VI. ACKNOWLEDGMENT

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TABLE I. Comparison of the ground state energies per lattice site for a Hubbard model of system size \( N = 4 \times 4 \), number of electrons \( N_e = 5 + 5 \), diagonal hopping-matrix element \( t_p = 0.0 \) for various interactions \( U \). In column 1 we show the interaction \( U \), in column 2 we present the results for the exact diagonalization \( (E_{ED}/N) \), in column 3 we show the stochastic diagonalization results \( (E_{SD}/N) \), in column 4-6 we present the results obtained with the PQMC-Algorithms for different elementary moves. Details of these moves are given in the text.

| U   | \( E_{ED}/N \) | \( E_{SD}/N \) | \( E_{\text{single}}/N \) | \( E_{\text{slice}}/N \) | \( E_{\text{cluster}}/N \) |
|-----|----------------|----------------|-----------------|----------------|----------------|
| 2.0 | -1.336059      | -1.3360        | -1.337 ± 0.001  | -1.335 ± 0.001| -1.332 ± 0.003|
| 4.0 | -1.223808      | -1.2237        | -1.224 ± 0.002  | -1.224 ± 0.002| -1.22 ± 0.01   |
| 5.0 | -1.182000      | -1.1819        | -1.180 ± 0.003  | -1.184 ± 0.003| -1.19 ± 0.02   |

TABLE II. Comparison of the ground state energies per lattice site for a Hubbard model of system size \( N = 4 \times 4 \), number of electrons \( N_e = 5 + 5 \), diagonal hopping-matrix element \( t_p = -0.22 \) for various interaction \( U \). In column 1 we show the interactions \( U \), in column 2 we present the results for the exact diagonalization \( (E_{ED}/N) \), in column 3 we show the stochastic diagonalization result \( (E_{SD}/N) \), in column 4-6 we present the results obtained with the PQMC-Algorithms for different elementary moves. Details of these moves are given in the text.

| U   | \( E_{ED}/N \) | \( E_{SD}/N \) | \( E_{\text{single}}/N \) | \( E_{\text{slice}}/N \) | \( E_{\text{cluster}}/N \) |
|-----|----------------|----------------|-----------------|----------------|----------------|
| 2.0 | -1.230034      | -1.2300        | -1.2301 ± 0.0003| -1.2306 ± 0.0008| -1.229 ± 0.001|
| 4.0 | -1.126160      | -1.1261        | -1.125 ± 0.003  | -1.125 ± 0.002 | -1.13 ± 0.02   |
| 5.0 | -1.088907      | -1.0887        | -1.089 ± 0.004  | -1.087 ± 0.004 | -1.10 ± 0.02   |
| 6.0 | -1.058717      | -1.0581        | -1.061 ± 0.005  | -1.058 ± 0.007 | -1.06 ± 0.02   |
\[ U = 2 \quad U = 4 \quad U = 5 \quad U = 6 \]
\[
t_p = -0.22 \quad 1.0 \quad 0.92 \quad 0.69 \quad 0.42 \\
t_p = 0.0 \quad 1.0 \quad 0.99 \quad 0.95 \quad 0.85
\]

TABLE III. Average sign \( \langle \text{sign} \rangle \) for \(4 \times 4\) Hubbard cluster with \(N_e = 5 + 5\), \(\langle \text{sign} \rangle\) is in the given precision the same in all three implementations of the PQMC algorithm.

| U  | cluster | single | slice |
|----|---------|--------|-------|
| 2.0 | 790 000 | 49 000 | 23 400 |
| 4.0 | 890 000 | 79 000 | 50 000 |
| 5.0 | 4 490 000 | 199 000 | 65 200 |
| 6.0 | 5 390 000 | 599 000 | 72 900 |

TABLE IV. Monte Carlo Sweeps MCS for cluster and single spin flip algorithm for the \(4 \times 4\) Hubbard model with \(N_e = 5 + 5\), \(t_p = -0.22\) and interaction \(U\) of the runs in figure 1, 2, 4 and 5

| U  | \(E_{ED}/N\) | \(E_{SD}/N\) | \(E_{single}/N\) | \(E_{cluster}/N\) |
|----|---------------|---------------|-----------------|-----------------|
| -2.0 | -1.731689     | -1.7316       | -1.731 ± 0.003  | -1.732 ± 0.006  |
| -4.0 | -2.045849     | -2.0453       | -2.045 ± 0.002  | -2.048 ± 0.01   |
| -6.0 | -2.458782     | -2.4568       | -2.460 ± 0.004  | -2.47 ± 0.01    |
| -8.0 | -2.956890     | -2.9545       | -2.952 ± 0.01   | -2.969 ± 0.05   |

TABLE V. Comparison of the ground state energies per lattice site for an attractive Hubbard model of system size \(N = 4 \times 4\), number of electrons \(N_e = 5 + 5\), diagonal hopping matrix element \(t_p = 0\) for various interactions \(U\). In column 1 we show the interaction \(U\), in column 2 we present the results for the exact diagonalization \(E_{ED}/N\), in column 3 we show the stochastic diagonalization result \(E_{SD}/N\), in column 4-5 we present the results obtained with the PQMC-Algorithms for different elementary moves. Details of these moves are given in the text.
| $U$  | $t_p$  | $N_{SD}$  | $N_1^{(n,m)}$ | $T_A$        |
|------|--------|-----------|---------------|--------------|
| 6.0  | −.22   | 307 324   | 0.0491        | 0.381·10⁻⁷   |
| 5.0  | −.22   | 285 872   | 0.0426        | 0.381·10⁻⁷   |
| 4.0  | −.22   | 228 172   | 0.0334        | 0.381·10⁻⁷   |
| 2.0  | −.22   | 141 742   | 0.0062        | 0.954·10⁻⁸   |
| 1.0  | −.22   | 60 638    | 0.0020        | 0.238·10⁻⁸   |
| −1.0 | 0.0    | 20 974    | 0.0040        | 0.954·10⁻⁸   |
| −2.0 | 0.0    | 28 034    | 0.0094        | 0.298·10⁻⁸   |
| −2.0 | 0.0    | 115 304   | 0.0140        | 0.191·10⁻⁷   |
| −4.0 | 0.0    | 179 755   | 0.1117        | 0.153·10⁻⁶   |
| −6.0 | 0.0    | 253 275   | 0.1297        | 0.153·10⁻⁶   |
| −8.0 | 0.0    | 246 862   | 0.1514        | 0.153·10⁻⁶   |

**TABLE VI.** Number of states $N_{SD}$ used for the stochastic diagonalization method in a $4 \times 4$ system with $N_e = 5 + 5$ electrons and $t_p = 0$ for different interaction $U$. $N_1^{(n,m)}$ is the norm of the first column in the transformed matrix $H^{(n)}$, and $T_A$ is the threshold for the acceptance of a new basis states to the basis of important states.

| $nstab$ | MCS     | $E_{\text{cluster}}$         |
|---------|---------|------------------------------|
| 1       | 1745000 | $-2.45282 \pm 0.00607$       |
| 2       | 1745000 | $-2.45282 \pm 0.00607$       |
| 4       | 1745000 | $-2.45282 \pm 0.00607$       |
| 8       | 1745000 | $-2.45282 \pm 0.00607$       |
| 16      | 1745000 | $-2.45282 \pm 0.00607$       |

**TABLE VII.** Groundstate energy for $4 \times 4$ Hubbard cluster with $N_e = 5 + 5$, $t_p = 0.0$ and $U = -6$ for different numbers of stabilizations $nstab$. 

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TABLE VIII. Monte Carlo Sweeps MCS for the cluster and the single spin flip algorithm for
a 4 × 4 Hubbard model with $N_e = 5 + 5$, $t_p = 0$. The interactions $U$ are the same of the runs in
figure 4 and 5.

| U   | $E_{\text{cluster}}$ | single |
|-----|----------------------|--------|
| -2.0| 39 000               | 4 000  |
| -4.0| 189 000              | 9 000  |
| -6.0| 2 909 000            | 109 000|
| -8.0| 7 750 000            | 149 000|

TABLE IX. Comparison of the ground state energies per lattice site for an attractive Hubbard
model of system size $N = 4 \times 4$, number of electrons $N_e = 5 + 5$, diagonal hopping matrix element
t_p = 0 for various interactions $U$. Here we compare unconverged runs. In column 1 we show
the interaction $U$, in column 2 we present the results for the exact diagonalization ($E_{\text{ED}}/N$), in
column 3 we show the stochastic diagonalization result ($E_{\text{SD}}/N$), in column 4-5 we present the
results obtained with the PQMC-Algorithms for different elementary moves. Details of these moves
are given in the text.

| U       | $E_{\text{ED}}/N$ | $E_{\text{SD}}/N$ | $E_{\text{single}}/N$ | $E_{\text{cluster}}/N$ |
|---------|------------------|------------------|----------------------|-----------------------|
| -2.0    | -1.731689        | -1.7314          | $-1.731 \pm 0.003$   | $-1.732 \pm 0.006$    |
| -4.0    | -2.045849        | -2.0419          | $-2.035 \pm 0.003$   | $-2.078 \pm 0.078$    |
| -6.0    | -2.458782        | -2.4451          | $-2.457 \pm 0.002$   | $-2.439 \pm 0.006$    |
| -8.0    | -2.956890        | -2.9432          | $-2.952 \pm 0.001$   | $-2.977 \pm 0.000$    |
| U    | state in SD | cluster | single |
|------|-------------|---------|--------|
| -2.0 | 12122       | 39000   | 4000   |
| -4.0 | 23510       | 50000   | 5000   |
| -6.0 | 32587       | 1000000 | 49000  |
| -8.0 | 46583       | 1500000 | 109000 |

**TABLE X.** Number of basis states in the SD and Monte Carlo Sweeps MCS for the cluster and the single spin flip algorithm for a $4 \times 4$ Hubbard model with $N_e = 5 + 5$, $t_p = 0$ and attractive interaction $U$ of the unconverged runs of figure 6.
FIGURES

FIG. 1. Comparison of the full correlation function with $d_{x^2-y^2}$ symmetry $C_{d_{x^2-y^2}}^{\text{Full}}(r)$ for a $4 \times 4$ Hubbard cluster with $N_e = 5 + 5$, $t_p = -0.22$ and $U = 2, 4, 5$ and 6. ($\Theta = 8, \tau = 0.125$)

FIG. 2. Comparison of the vertex correlation function with $d_{x^2-y^2}$ symmetry $C_{d_{x^2-y^2}}^{\text{Vertex}}(r)$ for a $4 \times 4$ Hubbard cluster with $N_e = 5 + 5$, $t_p = -0.22$ and $U = 2, 4, 5$ and 6. ($\Theta = 8, \tau = 0.125$)

FIG. 3. Comparison of the weights of the basis states in the exact diagonalization (ED) and the stochastic diagonalization (SD) in a $4 \times 4$ system with $N_e = 5 + 5$ electrons for the interaction $U = -2$ and $U = -8$ and $t_p = 0.0$.

FIG. 4. Comparison of the full correlation function with on-site s-wave symmetry $C_{os}^{\text{Full}}(r)$ for a $4 \times 4$ Hubbard cluster with $N_e = 5 + 5$, $t_p = 0$ and $U = -2, -4, -6$ and $-8$. ($\Theta = 8, \tau = 0.125$)

FIG. 5. Comparison of the vertex correlation function with on-site s-wave symmetry $C_{os}^{\text{Vertex}}(r)$ for a $4 \times 4$ Hubbard cluster with $N_e = 5 + 5$, $t_p = 0$ and $U = -2, -4, -6$ and $-8$. ($\Theta = 8, \tau = 0.125$)

FIG. 6. Comparison of the vertex correlation function with on-site s-wave symmetry $C_{os}^{\text{Vertex}}(r)$ for a $4 \times 4$ Hubbard cluster with $N_e = 5 + 5$, $t_p = 0$ and $U = -2, -4, -6$ and $-8$. ($\Theta = 8, \tau = 0.125$), The runs are unconverged meaning that for $|U| > -2$ the number of Monte Carlo Steps was chosen significantly lower than in figure 5. Details are given in table X

FIG. 7. Investigation of the behaviour of the vertex correlation function with on-site s-wave symmetry $C_{os}^{\text{Vertex}}(r)$ for a $4 \times 4$ Hubbard cluster with $N_e = 5 + 5$, $t_p = 0$ and $-6$ for $\Theta = 1, 2, 4, 8$ and 16. ($\tau = 0.125$) Dashed line is the value of the exact diagonalization.

FIG. 8. Investigation of the behaviour of the ground state energy for a $4 \times 4$ Hubbard cluster with $N_e = 5 + 5$, $t_p = 0$ and $-6$ for $\Theta = 1, 2, 4, 8$ and 16. ($\tau = 0.125$) Dashed line is the value of the exact diagonalization.
FIG. 9. Investigation of the behaviour of the ground state energy for a $4 \times 4$ Hubbard cluster with $N_e = 5 + 5$, $t_p = 0$ and $U = -6$ for different seeds of the random number generator. ($\Theta = 8$, $\tau = 0.125$) Dashed line is the value of the exact diagonalization and the full line is to guide the eyes.
REFERENCES

[1] M. Suzuki: Prog. Theor. Phys. 56 1454 (1976)

[2] W. van der Linden: Phys. Reports 220 53 (1992)

[3] J.E. Hirsch: Phys. Rev. B31 4403 (1984)

[4] S.E. Koonin, G. Sugiyama, H. Friederich: In: Proceedings of the International Symposium Bad Honnef, K. Goeke, P. Greinhard (Eds.), Springer Verlag Heidelberg (1982)

[5] H. de Raedt, B. de Raedt, A. Lagendijk: Z. Phys. B57 209 (1984)

[6] J. Cullum and R.A. Wiloughby: Lanczos Algorithms for Large Symmetric Eigenvalue Computations, Birkhäuser, Boston (1985)

[7] H. de Raedt, M. Frick: Comp. Phys. Rep. 7 1 (1992)

[8] J. Hubbard: Proc. Roy. Soc. A276 238 (1963)

[9] G.H. Golub, Ch.F. Van Loan: Matrix Computations, The John Hopkins University Press, Baltimore and London, 2. Ed. (1989)

[10] S. Sorella, S. Baroni, R. Car, M. Parinello: Europhys. Lett. 8 663 (1989)

[11] J.E. Hirsch: Phys. Rev. B28 4059 (1983)

[12] Th. Husslein, W. Fettes, I. Morgenstern: unpublished

[13] M. Imada, Y. Hatsugai: J. Phys. Soc. Jpn. 58 3752 (1989)

[14] U. Kleis, J.M. Singer, I. Morgenstern, Th. Husslein, H.-G. Matuttis: Par. Comp. 20 399 (1994)

[15] C.N. Yang: Rev. Mod. Phys. 34 694 (1962)

[16] S.R. White, D.J. Scalapino, R.L. Sugar, N.E. Bickers, R.T. Scalettar: Phys. Rev. B39 839 (1989)
[17] Th. Husslein, I. Morgenstern, D.M. Newns, P.C. Pattnaik, J.M. Singer, H.G. Matuttis: submitted to Phys. Rev B (1996)

[18] K. Michielsen, H. De Raedt: preprint, (1996)

[19] W. Fettes, I. Morgenstern, Th. Husslein: preprint (1996)

[20] results are unpublished
fig. 1
fig. 2
(a) \( U = -2 \)

(b) \( U = -8 \)

fig. 3
fig. 4
fig. 5
fig. 6
fig. 7
