Stochastic gradient approximation method applied to Hubbard model

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The two-dimensional Hubbard model is studied using the variational quantum Monte Carlo technique with Gutzwiller-type variational wave functions. In addition to the simple on-site correlated Gutzwiller wave function, we use a form with correlation between electrons on nearest- and next-nearest-neighbor sites. We show that the stochastic gradient approximation method suits very well for the optimization of the free parameters of the variational wave functions.

I. INTRODUCTION

The one-band Hubbard Hamiltonian is the simplest lattice model for studying strongly correlated electrons. It is widely studied, especially in its two-dimensional version, as a model for the high-$T_c$ superconducting cuprates. Among the various methods used for studying the Hubbard model, the quantum Monte Carlo (QMC) methods have shown to be powerful tools, both at zero and finite temperatures. The studies of the Hubbard model at zero temperature include several QMC methods, namely, the variational (VMC) \cite{4}, the fixed-node diffusion (DMC) \cite{3,4}, and the constrained path QMC (CPMC) \cite{5–7}. From these zero-temperature methods, only CPMC does not depend crucially on the variational wave function. Actually, the simple free-electron-like wave functions are rather generally found to be better importance functions for CPMC than the unrestricted Hartree-Fock wave functions \cite{11,12}. On the other hand, CPMC is limited to smaller lattice sizes than VMC. It can, however, give accurate results for system sizes far beyond the limits of exact diagonalizations \cite{13} or the subspace techniques such as stochastic diagonalization \cite{11}. Also the finite temperature QMC simulations can be used to obtain ground state properties if the temperature used is low enough \cite{10}. This approach is, however, mainly applicable for half-filled systems due to the problems related to the negative weights of the configurations, i.e., the fermion sign problem.

Compared to the other approaches, the VMC methods are very potent for studying larger system sizes. The computational cost of the VMC method is roughly an order of magnitude smaller than of the more sophisticated QMC methods. The VMC method is basically free from any methodological problems such as the fermion sign problem. There is, however, one very serious limitation in the VMC approach. This is related to the ultimate connection of the method to the many-body wave function itself. The form of the wave function is an input to the VMC simulations, and choosing the form requires human creativity and insight into the problem. Due to this, VMC can hardly be called a reliable “black-box” simulation method. However, the recent advancements in the optimization of the variational wave functions \cite{11,12} combined with the enormous increase in computing power indicate a possibility of having considerably more flexible VMC wave functions and making the VMC simulations less “human-biased”.

The crucial part of the VMC simulation is to locate the optimal values of the free parameters in the many-body wave function. An efficient optimization method allows one to have more variational parameters and thus a more flexible form of the wave function and saves computer time. In this paper, we show that the optimization method called the stochastic gradient approximation (SGA) \cite{11} suits very well for the VMC also in the case of lattice Hamiltonians. We have previously used it for continuum models, mainly quantum dots \cite{11,12}.

The goal in the VMC optimization is to minimize the cost function

$$\mathcal{F}(\alpha) = \lim_{k \to \infty} \frac{1}{k} \sum_{j=1}^{k} Q(R_j;\alpha),$$

where configuration $R_j$ contains the coordinates of the simulated particles at $j$th step of a random sequence, $\alpha = (\alpha_1, \cdots, \alpha_n)$ represents the vector of $n$ parameters to be optimized, and $Q$ is the “local” version of the cost function of a configuration $R$ and $\alpha$. One can formulate the VMC optimization problem approximately as a “standard” optimization problem by taking a finite but large $k$ in the cost function above. One can then use the resulting approximation of the function as a deterministic function during the optimization. Doing this, one approximates the whole distribution of $R$s by a finite set, and more importantly, one forgets the $\alpha$ dependence of $R$. To some extent this error can be corrected by weighting the configurations by factors that depend on the change of the probability of the configuration in question.

In the SGA optimization method such truncation is not done. In SGA, the optimal parameter vector $\alpha^*$, defined so that

$$\nabla_{\alpha} \mathcal{F}(\alpha^*) = \lim_{k \to \infty} \frac{1}{k} \sum_{j=1}^{k} \nabla_{\alpha} Q(R_j;\alpha^*) = 0,$$

is found by changing the parameters $\alpha$ to the direction
of the unbiased stochastic approximation of the negative gradient, i.e., \(-\nabla \alpha Q\). The approximate gradient \(\nabla \alpha Q(R; \alpha^*)\) is not zero even for the optimal parameters, but the average of it over configurations \(R\) vanishes. Due to this, the stochastic simulation should include damping so that it actually converges. Without damping, the simulation would end up in oscillating around the optimal parameters. The damping should, however, be so slow that the simulation is able to reach the optimal parameters. A more detailed formulation of the SGA method for VMC is given in Sec. [1].

II. METHOD

We use the two-dimensional Hubbard model given by the Hamiltonian

\[
H = -t \sum_{\langle i,j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow},
\]

where \(\langle \ldots \rangle\) stands for nearest neighbors, \(c_{i\sigma}^\dagger\) (\(c_{i\sigma}\)) creates (destroys) an electron with spin \(\sigma\) at site \(i\) of the square lattice, and \(n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}\). The electrons at the same site interact with strength \(U > 0\), and \(t\) is the hopping parameter. We use \(t\) as the energy scale, and set \(t = 1\).

The periodic boundary conditions are used for both space directions. This choice of boundary conditions leads to non-interacting single particle states that are plane-waves \(\exp(ik \cdot r)\) with energy \(\varepsilon_k = -2(\cos(k_x) + \cos(k_y))\).

A commonly used variational wave function for the Hubbard model is the Gutzwiller wave function \([1]\)

\[
\Psi(g) = g^D \Psi_0,
\]

where \(D = \sum_i n_{i\uparrow} n_{i\downarrow}\) is the number of doubly occupied sites, \(g\) is the only variational parameter, and \(\Psi_0\) is the many-body wave function for the non-interacting ground state. In this case, it is made of the plane-waves discussed above, with the \(k\) values chosen to minimize the energy. The motivation for this wave function is that the Gutzwiller factor reduces the probability to find electrons on the same site and reduces the average interaction energy. This is done, of course, with a cost of higher kinetic energy. It is also possible to correlate electrons that are not on the same site by constructing a Gutzwiller-type wave function

\[
\Psi(g) = \sum_i g_i \Psi_0,
\]

where the \(g_i\)'s are parameters and the \(C_i\)'s measure the number of nearest (and next nearest) neighbor electrons with various spin configurations, see Fig. [2] for more details.

We calculate the energy using the standard Metropolis algorithm (see, e.g., Refs. [3] for more details and Ref. [4] for a modified algorithm), giving the estimate for the energy as \(E = \langle E_L \rangle\), where the local energy is defined as

\[
E_L(R) = \frac{H \Psi(R)}{\Psi(R)},
\]

and the average in the calculation of \(\bar{E}\) is over configurations \(R\) distributed according to probability distribution \(\propto |\Psi(R)|^2\). The standard deviation of the local energy is given by

\[
\sigma = \sqrt{\langle (E_L - \bar{E})^2\rangle}.
\]

One can also define a modified version of \(\sigma\), namely,

\[
\tilde{\sigma} = \sqrt{\langle (E_L - E_T)^2\rangle} = \sigma^2 + (\bar{E} - E_T)^2,
\]

which gives the root-mean-square distance of the local energy from the target energy \(E_T\). The deviation \(\tilde{\sigma}\) is particularly useful in the optimization of the wave function.

The SGA optimization method involves stochastic simulation in two spaces: the configuration and the parameter space. These spaces are coupled via the parameter vector. In the configuration space, a set of \(m\) configurations \(\{R_i\}_1^m\) is sampled from a distribution \(|\Psi(\alpha)|^2\), where \(\alpha\) is the current parameter vector. When the parameters are changed, the set of configurations follow this change because the new sampling distribution depends on the new parameters. In practice, the set of configurations is found by the Metropolis algorithm. In the parameter space, the parameters at iteration \(i + 1\) are obtained from the previous ones by the formula:

\[
\alpha_{i+1} = \alpha_i - \gamma_i \nabla \alpha Q_i,
\]

where \(\gamma_i\) is a scaling factor of the step length. The scaling factor has an important role in averaging out the fluctuations in the approximate gradient, ensuring the convergence. On the other hand, too small a value of \(\gamma\) would damp the simulation too much. These rules can be formulated mathematically as:

\[
\sum_{i=1}^\infty \gamma_i^2 < \sum_{i=1}^\infty \gamma_i = \infty.
\]

There is a simple interpretation for these conditions. The sum of \(\gamma^2\) should be finite to dissipate the cumulative error given by the noise in the approximate gradient and the sum of \(\gamma\) should diverge, because otherwise the maximum distance from the initial parameters would be limited. If one uses a formula \(\gamma_i \propto \gamma^{\beta}\), one should have \(\frac{1}{2} < \beta \leq 1\). The choice of \(\beta = 1\), which is the maximally damped case, leads to a formula similar to the recursive calculation of a mean: \(\bar{x}_i = \bar{x}_{i-1} - \frac{1}{i}(\bar{x}_{i-1} - x_i)\).

In Eq. (11), the approximate gradient is calculated using the set of \(m\) configurations. There are several possibilities for the cost function \(Q\). For the energy minimization, the cost function is simply the mean of the local energies over the set of configurations:
and for the variance minimization one has \( Q = 1/m \sum_{j=1}^{m} E_L(R_j) \), (11)

where the points \( R_j \) are distributed according to \( |\Psi(\alpha)|^2 \), \( \tilde{m} = \sum w_j \), and \( w_j = |\Psi(R_j; \alpha + \Delta)/\Psi(R_j; \alpha)|^2 \). The 'weights' \( w_j \) of the local functions are very close to unity, because \( \Delta \) is only a small change.

It is, however, possible to calculate the gradient also analytically. In Ref. [12], Lin et al. have shown that in the case of real wave function and energy minimization, the derivative of the energy \( E \) with respect to a variational parameter \( \alpha_i \) is simply

\[
\frac{\partial E}{\partial \alpha_i} = 2 \left\{ E_L \times \frac{\partial \ln \Psi}{\partial \alpha_i} \right\} - E \times \left\{ \frac{\partial \ln \Psi}{\partial \alpha_i} \right\},
\]

where the average \( \langle \ldots \rangle \) is over the whole Metropolis simulation [12]. One can implement this simple formula also for the SGA algorithm, with the small modification that the average is taken over only the current set of \( m \) configurations. One should also note that the finite-difference formulation required calculation of the local energy with several parameters, whereas only a single evaluation is needed (for each configuration) if the analytic formula is used.

In this work, we have used the both schemes discussed above for the calculation of the gradient.

### III. RESULTS

#### A. Single Gutzwiller parameter

First, we will consider the wave function with correlation only between electrons on the same site, and thus only one free parameter \( g \). In Fig. 4, the energy and the deviations of the local energy \( \sigma \) and \( \tilde{\sigma} \) are plotted as a function of the Gutzwiller parameter \( g \). The system consists of \( 101 + 101 \) electrons on a \( 16 \times 16 \) lattice with \( U = 4 \). One can see that the minimum of the total energy is located at \( g \approx 0.56 \), and the minima of \( \sigma \) and \( \tilde{\sigma} \) are at \( g \approx 0.6 \). The energy as a function of \( g \) is in a good agreement with Fig. 2. of Ref. [3]. The predicted value of \( g \) resulting from the minimization of energy in Ref. [3] is slightly higher, around \( g \approx 0.566 \). The statistical error in the energies is too large in order to locate the optimal value of \( g \) with accuracy better than 0.01.

Next, the SGA optimization method is used to locate the optimal values of \( g \) with energy and \( \sigma \) as the cost functions. In Fig. 5, the Gutzwiller parameter \( g_i \) is plotted as a function of the SGA optimization step \( i \) for both energy and variance minimizations for the same system parameters as above. We have calculated the gradient using the original, finite-difference formulation. The simulations converge to \( g \approx 0.566 \) in the case of energy minimization, and to \( g \approx 0.603 \) in the optimization of \( \tilde{\sigma} \) with the target energy \( E_T = -280.5 \). Both parameter values are in a good agreement with the independent simulations presented above, and with the estimate of the optimal value of Ref. [3]. One can also see that around 1000 steps are enough to estimate the optimal parameter values with a reasonable accuracy. The computational task of this is smaller than of one independent simulation presented in Fig. 4 for a single value of \( g \). On the other hand, it seems that the accuracy of the optimal parameters found by SGA is one order of magnitude higher than in using the polynomial fit to the independent points. We have performed several simulations starting from different values of \( g_0 \). In every case, the performance of SGA is similar to those shown in Fig. 5.

Fig. 6 shows the first 200 values of the Gutzwiller parameter \( g_i \) for the simulation using the analytic derivative of Eq. (13). This simulation converges also very accurately to the optimal value found above. The most important feature are that the fluctuations in the value of \( g \) during the optimization process is much smaller than in the simulation where the finite-difference formula was used. This leads to a faster convergence.

To summarize, the performance of the SGA method has been found very satisfactory in finding the optimal parameter of the simple single-parameter Gutzwiller wave function. This is especially true in the case where the gradient is calculated analytically.

#### B. Generalized Gutzwiller wave function

Next, we will consider the generalized Gutzwiller wave function, defined in Eq. (9). We consider only the generalization with 4 parameters related to typical configurations shown in Fig 1. The aim of these parameters is to capture partially the missing correlations. The generalization made to the Gutzwiller wave function is bosonic in the sense that it does not change the nodal structure of the one-parameter Gutzwiller wave function. The energy gain of this extra correlation could directly be compared to the energy of the fixed-node DMC simulations of Ref. [3] as the nodal structure used there is also given by
the simple Gutzwiller wave function. This DMC energy is lower than the corresponding VMC energy by \(\approx 2.5\) units. One should note that in the lattice formulation of DMC, unlike in the continuum formulation, the energy depends also on the bosonic correlation factor which does not change the nodes. This dependence is much smaller than the dependence of the VMC energy on \(g\). There are also correlations that change the nodal structure, and the estimate for the importance of these can be estimated from the CPMC energy which is lower than the VMC energy by more than 6 units [1].

We have optimized the 4 free parameters of the generalized Gutzwiller wave function using the SGA and the analytic formulation of the gradient. The latter choice is due to better results in the one-parameter case. One should note that setting the parameter \(g_1 = g\) and \(g_2 = g_3 = g_4 = 1\) one obtains the simple Gutzwiller wave function. We have again studied 101 + 101 electrons on a 16 \(\times\) 16 lattice with \(U = 4\) as above.

The optimization of the energy leads to a reduced on-site correlation factor of \(g_1 \approx 0.51\). The other parameters are \(g_2 \approx 0.92\) and \(g_3 \approx g_4 \approx 0.98\). The smaller value of \(g_1\) does not cost as much kinetic energy in this case as in the case of a simple Gutzwiller wave function, because the values of \(g_2\) and \(g_3\) are also smaller than one. It is also interesting to compare the optimal value of \(g_1\) found here with the optimal \(g \approx 0.52\) of the simple Gutzwiller wave function determined from the \(g\) dependence of the DMC energy [1]. The optimization converges again in few hundred steps, in similar fashion as shown in Fig. 2.

The energy calculated with the optimal parameters is presented in the Table 1 with corresponding one-parameter VMC, DMC, and CPMC results. One can see that the generalization of the Gutzwiller wave function is able to lower the energy by 1.1 units, which is less than half of the difference to the DMC energy. The CPMC energy is still around 5 units lower in energy.

There are still important ingredients missing from the variational wave function. Possible extensions are three- and higher-particle correlation factors, modified single-particle states, and multiple-determinant wave functions. The good performance of the SGA method combined with the simple calculation of the energy gradient could be extremely useful in the studies exploring these directions.

**IV. CONCLUSIONS**

We have shown that the SGA optimization method finds the optimal values of the Gutzwiller wave function parameter in a reliable and efficient fashion. The computational cost of the optimization process is comparable to a single calculation of the expectation values with a fixed parameter value. The good performance is very important particularly if a variational wave function with several parameters is used. Due to this, SGA is very useful in finding more accurate wave functions for the Hubbard model.

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FIG. 1. Typical configurations measured by the correlation factors in the Gutzwiller-type wave function. For example, \( C_3 \) counts the number of electron pairs that have opposite spin electrons differing in both coordinates by one.

FIG. 2. Energy as a function of the Gutzwiller parameter \( g \). The solid line shows a fourth-order polynomial fit. The inset shows the deviations of the local energy, defined as \( \sigma \) and \( \tilde{\sigma} \) in the text, marked with ‘o’ and ‘+’, respectively. In \( \tilde{\sigma} \), \( E_T = -280.5 \) has been used.

FIG. 3. The Gutzwiller parameter \( g_i \) for the optimization step \( i \). The solid (dashed) line corresponds to the variance (energy) minimization, respectively. Both simulations are started from \( g_0 = 0.65 \).

FIG. 4. The Gutzwiller parameter \( g_i \) for the first 200 optimization steps \( i \) using the analytic calculation of the gradient. Simulation is started from \( g_0 = 0.65 \). The solid line show the optimal parameter value, and the dotted ones show a range of parameter value that gives results with energy error within the statistical uncertainty of the Fig. 2. The fluctuation of the parameter value is much smaller than in Fig. 3.

TABLE I. Energy of 101+101 electrons on a 16×16 lattice with \( U = 4 \) for different methods. Numbers in the parenthesis are statistical errors in energy. The number of VMC parameters is also given. The DMC energy is from Ref. [3] and CPMC from Ref. [5].

| Method   | Energy   |
|----------|----------|
| VMC 1    | -280.3(1) |
| VMC 4    | -281.4(1) |
| DMC      | -283.0(5) |
| CPMC     | -286.55(8) |