Extension of Fixed-Node Monte Carlo for Lattice Fermions

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Abstract

In a previous paper, we have described a method to perform Fixed-Node Quantum Monte Carlo calculations for lattice fermions. In this paper, we present an extension of this method, by which it is possible to find information on the properties of the exact ground-state wave function. We give some further illustrations of the FNMC and the extended methods.

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I. INTRODUCTION

Recently, we described a method to perform Quantum Monte Carlo (QMC) calculations for lattice fermions\textsuperscript{1,2}. We introduced an effective Hamiltonian, by which the sign problem that is usually encountered in such systems, can be avoided. We proved that it leads to an upper bound for the ground-state energy. This Fixed-Node Monte Carlo (FNMC) method for lattice systems is very much inspired by the similar method, developed by Ceperley et al.\textsuperscript{3,4}, for continuous systems.

In this paper we want to show that, in analogy to the method for continuum problems, it is possible to extend the FNMC method for lattice systems in order to obtain approximate information about the true ground state of the system. This nodal relaxation method, as it is called by Ceperley et al.\textsuperscript{5}, can be straightforwardly implemented also on lattice systems. We will give a formalism for this method, using the (theoretical) results of the FNMC method described in\textsuperscript{1,2}. Also, we will give a few more examples of applications of these methods, in comparing our results to those presented by other authors, for a few systems frequently used in the literature.

In the next section we will recall the basic formulas of the Green Function Monte Carlo (GFMC) formalism, and give our notation and interpretation of the concept of importance sampling. After a few summarizing remarks on the Fixed-Node Monte Carlo method, we will show in Section III how the results of this method can be used to calculate properties of the true ground state of the system. In Section IV we present a few examples of applications of both methods, and we conclude this paper by a discussion on the applicability of the methods and the need for further investigation of possible wave functions.

A much more elaborate explanation and discussion of the FNMC method and the extended method, information on the implementation of both methods, and some more examples of applications, have been given in Refs. 6 and 7.

II. BASIC FORMULAS OF GREEN FUNCTION MONTE CARLO

The GFMC method, as we use it, is based on the projection operator

\[ \mathcal{F} = 1 - \tau(\mathcal{H} - w), \]

by which the ground state of the Hamiltonian \( \mathcal{H} \) is filtered from a trial state \( |\Psi_T\rangle \), which is known or can be calculated for each configuration \( R \) in the configuration space \( \{R\} \). The parameters \( \tau \) and \( w \) are to be chosen appropriately. After applying this operator \( n \) times, an approximation

\[ |\Psi^{(n)}\rangle = \mathcal{F}^n |\Psi_T\rangle \]

of the ground state is obtained, which closely resembles the ground state for large \( n \). The energy of this state can be formally calculated as

\[ E^{(n)} = \frac{\langle \Psi_T | \mathcal{H} | \Psi^{(n)} \rangle}{\langle \Psi_T | \Psi^{(n)} \rangle} \]

\[ = \frac{\sum_R \langle \Psi_T | H | R_n \rangle \prod_{i=1}^{n} \langle R_i | F | R_{i-1} \rangle \langle R_0 | \Psi_T \rangle}{\sum_R \langle \Psi_T | R_n \rangle \prod_{i=1}^{n} \langle R_i | F | R_{i-1} \rangle \langle R_0 | \Psi_T \rangle}, \]

for large \( n \).
where $\mathcal{R} = \{R_0, R_1, R_2, \ldots, R_n\}$ is a path in the configuration space. As we will see in the actual implementation of this calculation, the wave function has to be known in the end point of each path, and therefore $\langle \Psi_T |$ must be used in this expression in stead of $\langle \Psi^{(n)} |$. This is called a mixed estimate of the energy.

The expression (4) can usually not be calculated exactly. In the Monte Carlo scheme, only a limited number of paths $\mathcal{R}$ is used for the calculation of this expression. We can rewrite (4) as

$$E^{(n)} = \frac{\sum_{\mathcal{R}} E_T(R_n) m(\mathcal{R}) p(\mathcal{R})}{\sum_{\mathcal{R}} m(\mathcal{R}) p(\mathcal{R})},$$

where

$$E_T(R) = \frac{\langle \Psi_T | H | R \rangle}{\langle \Psi_T | R \rangle}$$

is the local energy in the configuration $R$. The quantity $p(\mathcal{R})$ can be interpreted as the probability of choosing a complete path $\mathcal{R}$, and each path carries a weight or multiplicity $m(\mathcal{R})$. If one makes sure that $p$ and $m$ satisfy

$$p(\mathcal{R}) m(\mathcal{R}) = \langle \Psi_T | R_n \rangle \prod_{i=1}^n \langle R_i | F | R_{i-1} \rangle \langle R_0 | \Psi_T \rangle,$$

the energy $E^{(n)}$ can be calculated as

$$E^{(n)}_{GFMC} = \frac{\sum'_{\mathcal{R}} E_T(R_n) m(\mathcal{R})}{\sum'_{\mathcal{R}} m(\mathcal{R})},$$

where the summation is now restricted to some number of paths, chosen according to the probability $p(\mathcal{R})$. In the limit of using infinitely many paths, this calculation becomes exact; in case of a finite number of paths, a statistical error bar can be defined.

In the definition of $p$ and $m$ one can include ways to make the sampling of the wave function more efficient. This is called importance sampling, and usually refers to the idea that one should try to sample more often in regions where the trial wave function has a large absolute value. We give a description which includes the possibility of performing importance sampling by means of a guiding function $\Psi_G$. This function must be positive everywhere; often, it is taken to be the absolute value of the trial wave function. We denote the probability for choosing a path as

$$p_{\text{guiding}}(\mathcal{R}) = p_0(\mathcal{R}) \prod_{i=1}^n p(R_i \leftarrow R_{i-1}),$$

Here, the probability for the first configuration of the path to be $R$ is

$$p_0(R) = \langle \Psi_T | R \rangle \langle R | \Psi_T \rangle,$$

and the probability of each subsequent step of the path is defined by
\[
p(R' \leftarrow R) = \frac{\langle \Psi_G | R' \rangle \langle R'| F | R \rangle}{\langle \Psi_G | R \rangle m(R)}.
\]

When using this probability for the paths, one has to take \( m \) as \( m \) guiding,

\[
m_{\text{guiding}}(R) = \frac{\langle \Psi_G | R_0 \rangle}{\langle \Psi_T | R_0 \rangle} \left[ \prod_{i=1}^{n} m(R_{i-1}) \right] \frac{\langle \Psi_T | R_n \rangle}{\langle \Psi_G | R_n \rangle},
\]

where the weight factors \( m(R_{i-1}) \) can be calculated for each step \( R_i \leftarrow R_{i-1} \) separately as

\[
m(R) = \sum_{R'} \frac{\langle \Psi_G | R' \rangle \langle R'| F | R \rangle}{\langle \Psi_G | R \rangle} = \frac{\langle \Psi_G | F | R \rangle}{\langle \Psi_G | R \rangle}.
\]

These relations basically define the Monte Carlo procedure. Additionally, one can make use of branching, to avoid that the variance of the calculated result increases too rapidly.

In the Monte Carlo scheme, one can thus choose the starting configurations of the paths according to \( p_0 \), and each subsequent configuration according to the stochastic matrix defined by \( p(R' \leftarrow R) \). Interpreting the paths as random walks in the configuration space, one usually calls the configurations chosen walkers. In our interpretation, the starting set of walkers that one uses in the Monte Carlo calculations is distributed according to the square of the trial wave function. One can calculate how the walkers are redistributed after \( n \) steps, considering also the weight they carry:

\[
p(R) = \sum_{\{\mathcal{R}\}|R_n = R} m(\mathcal{R}) p(\mathcal{R}).
\]

This expression can be easily evaluated using the relation (2) for \( p \) and \( m \):

\[
p(R) = \langle \Psi_T | R \rangle \sum_{\{R_0, R_1, \ldots, R_{n-1}\}} \left[ \prod_{i=1}^{n} \langle R_i | F | R_{i-1} \rangle \right] \langle R_0 | \Psi_T \rangle
\]

\[
= \langle \Psi_T | R \rangle \langle R | F^n | \Psi_T \rangle
\]

\[
= \langle \Psi_T | R \rangle \langle R | \Psi^{(n)} \rangle.
\]

Thus, after a sufficiently large number of steps the walkers are distributed according to the product of the trial wave function and the ground-state wave function of the Hamiltonian considered.

**III. EXTENSION OF THE FNMC FORMALISM**

The Fixed-Node Monte Carlo method uses in fact the same formalism as the general Green Function Monte Carlo, presented in the previous section, but with a modified Hamiltonian \( H_{\text{eff}} \) to avoid steps that could introduce a change of sign in the weights or the probabilities (the sign problem). The GFMC procedure is straightforwardly applied to this effective Hamiltonian, for which a prescription has been given in Refs. 1 and 2. Thus, by the FNMC method, information is obtained not on the ground state of the Hamiltonian \( H \) one is interested in, but on the ground state of \( H_{\text{eff}} \). It has been proven that the ground-state energy
of $H_{\text{eff}}$ provides an upper bound for the ground-state energy of $H$. Of course, it would be better to obtain information directly on $H$. As we will see, under certain circumstances this is possible, using the FNMC result as input for a new calculation, called nodal relaxation. It strongly resembles the method described by Ceperley and Alder\cite{Ceperley:1983} for a continuum problem. The method suffers from the sign problem, but it may yield convergent results before the fluctuations destroy the accuracy of the calculations.

Let us rewrite the expression (17) to give the distribution of the configurations in the FNMC procedure after $n$ steps:

$$p^{(n)}_{\text{FN}}(R) = \langle \Psi_T | R \rangle \langle R | \Psi^{(n)}_{\text{eff}} \rangle,$$  

(18)

where $| \Psi^{(n)}_{\text{eff}} \rangle$ is supposed to be a good approximation of the ground state $| \Psi_{\text{eff}} \rangle$ of $H_{\text{eff}}$. The idea is now that $| \Psi_{\text{eff}} \rangle$ is sufficiently close to the ground state $| \Psi_0 \rangle$ of $H$, such that in GFMC procedure used on $H$ convergence can be obtained within a relatively small number of steps. Thus, we modify (2) in the following way:

$$| \Psi^{(n)}_P \rangle = F^n | \Psi_{\text{eff}} \rangle.$$  

(19)

Then, we also have to modify the expression (4) for the mixed estimate of the energy:

$$E^{(n)}_P = \frac{\langle \Psi_T | H | \Psi^{(n)}_P \rangle}{\langle \Psi_T | \Psi^{(n)}_P \rangle} = \frac{\sum_R \langle \Psi_T | H | R_n \rangle \prod_{i=1}^n \langle R_i | F | R_{i-1} \rangle \langle R_0 | \Psi_{\text{eff}} \rangle}{\sum_R \langle \Psi_T | R_n \rangle \prod_{i=1}^n \langle R_i | F | R_{i-1} \rangle \langle R_0 | \Psi_{\text{eff}} \rangle},$$  

(20)

Note that we still have to put $\langle \Psi_T |$ in this expression, as that is the only available information we have in each configuration. However, in the starting configurations of the paths, the trial wave function has been replaced by the effective ground-state wave function, of which we have information through the distribution of the walkers in the FNMC procedure. We have to pay further attention to the fact that sign changes can now occur, which have to be embedded in the transition probabilities and multiplicities. We can use the following guiding procedure, adapted from the regular GFMC scheme described in the previous section: the probability to start in a configuration $R$ is given by the fixed-node resulting distribution:

$$p_0(R) = p^{(n)}_{\text{FN}}(R).$$  

(22)

The transition probabilities are given by

$$p(R' \leftarrow R) = \frac{\langle \Psi_G | R' \rangle \langle R' | F | R \rangle}{\langle \Psi_G | R \rangle m(R)},$$  

(23)

with the modified weight factor

$$m(R) = \sum_{R'} \frac{\langle \Psi_G | R' \rangle \langle R' | F | R \rangle}{\langle \Psi_G | R \rangle}.$$  

(24)
The absolute value has to be taken to make sure that the transition probabilities remain positive, such that the procedure can still be interpreted as a stochastic walk. With these expressions replacing (10), (11), and (13), the equations (9) and (12) can again be used for the total probability and the total “weight” of a path, respectively. Note that the weights can now be negative, due to the possibly different signs of the wave function in the starting and end configurations of the path.

By this formalism, one can thus try to obtain information directly on the true ground state of the Hamiltonian, using the fixed-node result as a starting point. In the following section, we will show a few examples of applications of this method.

IV. APPLICATIONS

First, we visualize how the FNMC and the nodal-relaxation method work for the Hubbard model on a small system, the $2 \times 2 \times 2$ cube, with $U = 2.5$. We have performed exact calculations for this system, in order to be able to compare the Monte Carlo results and check whether the program has been correctly implemented. In Figures and , we show calculations for this system at half filling and with zero total spin in the $z$-direction. In Figure , the first 250 steps in the Fixed-Node Monte Carlo calculation, using a homogeneous mean-field wave function as trial wave function, are shown. As can be seen, after some 100 steps the energy measured starts fluctuating around the exact ground-state energy of the effective Hamiltonian (indicated by the drawn line). The square at the right indicates the energy that one obtains after averaging over several thousands of steps (not shown in this figure), with a statistical error which is smaller than the symbol size. In Figure , two separate calculations of nodal relaxation are shown; one using the same trial wave function as in Figure (indicated by H), the other using a mean-field wave function with antiferromagnetic ordering imposed on the spins (indicated by AF). The horizontal lines indicate the exact ground-state energies of the effective (FN) Hamiltonians using the H and the AF trial functions, respectively, and of the true Hamiltonian. The resulting energy after each step is indicated by an error bar (the energy measured being the middle value of the error bar). As can be seen, the size of the error bars in both calculations first decreases with increasing number of steps, and then starts increasing, indicating the existence of the sign problem. The calculation marked H seems to converge to the correct value before the sign problem arises; the AF calculation does not has not converged at that point. Clearly, this is due to the fact that the fixed-node energy found when using the AF wave function is significantly higher than the resulting energy in the other fixed-node calculation. This nicely demonstrates that the exact result can be reached, but only if the fixed-node result is close enough to the true ground state.

We have performed some more calculations for the Hubbard model. In Table , we compare results of calculations of the ground-state energy for a $4 \times 4$ square with periodic boundary conditions (PBC), with 5 spins up and 5 down, and $U = 4$. For this system, exact and approximate results are available in the literature. As can be seen, in the case of $U = 4$, the fixed-node method yields an upper bound for the ground-state energy which is quite close to the exact value, and nodal relaxation leads to the exact result with an error bar of only 0.05% . In Table , we show the results of various calculations of the ground-state
energy in a 10 \times 10 system (PBC), at half filling and with zero total spin in the z-direction, also for \( U = 4 \). There are no exact results available for this system, but several results of mean-field and quantum Monte Carlo calculations can be found in the literature. As can be seen, our results are in very good agreement with previous QMC results by Hirsch and White et al.

V. DISCUSSION AND OUTLOOK

First we would like to make a few additional remarks on the calculations we have performed. As one can see from Table I, adding a Gutzwiller factor to the bare mean-field wave function greatly improves the (variational) energy obtained from the mean-field calculation. In the fixed-node calculation, however, the energy is hardly improved by adding the Gutzwiller factor to the trial wave function. Considering also other calculations we performed, we feel that this is a rather general feature of the fixed-node method. In the fixed-node method, the energy that is obtained is determined by the sign structure of the trial wave function, via the ratios of the wave function in neighboring configurations with different signs. In order to significantly improve the energy, one must be able to change the sign of the trial wave function in individual configurations, as that is the most important factor determining the energy that can be obtained. By a Gutzwiller factor (or, similarly, a Jastrow factor) one does not change the sign, but only the ratios of the wave function.

Another interesting point is that the Monte Carlo calculations become less stable for larger \( U \). This is due to the fact that the parameter \( \tau \) has to be taken smaller in that case, such that convergence is slowed down. For the fixed-node method this is not a very big problem, as one can simply sample for a longer time to obtain a result with desired accuracy, but in the nodal-relaxation method one can not afford to have longer paths in the calculations, as the sign problem starts showing up after a certain number of steps.

Another problem concerns the observables that can be calculated. For operators that commute with the Hamiltonian, similar formulas as have been given for the energy in Section II can be used, although (in fixed node) the results obtained for operators other than the Hamiltonian itself can not present a bound to the exact result. For operators that do not commute with the Hamiltonian, however, there is a more serious problem; in that case, the mixed estimate does not yield the correct value of the observable for the ground state of the (effective or true, depending on the method) Hamiltonian. Usually, one uses an extrapolated estimate in that case, taking two times the mixed estimate minus the variational result (i.e., the value of the observable in the trial state). In practice, this leads to rather good results; however, one is unable to check how good the approximation is.

Recently, Zhang et al. presented the Constrained Path Monte Carlo method for lattice fermions, which they claim to be a better method than fixed node. Like we, they apply some kind of fixed-node principle, but in a continuous space of Slater determinants, which seems to cause that the CPMC energy is a better approximation of the true energy than the fixed-node energy. Also, they claim that they have a better method (backtracing) to perform calculations for non-commuting operators. It is not very clear to us how CPMC compares to fixed node combined with nodal relaxation. It seems to us that our method is more generally applicable, as we can use any wave function as trial wave function (as long
as it can be calculated relatively easily) and we can also treat systems of frustrated bosons or spins, while their method restricts the trial wave function to be a Slater determinant. In any case, it would be very interesting to make a better comparison of both methods for some different systems.

Finally, we state that the most important ingredient of our method is the trial wave function. The quality of the trial function, i.e., its sign structure, determines how good the approximation is that can be obtained. This is not a trivial problem, for, as Ceperley states, ‘...little progress [has been made] in stating exact conditions that nodes must obey.’ Most studies of wave functions aim at improving the energy of the wave function itself, while for our purposes it would be necessary to explore its sign structure, in order the improve the energy that results after a fixed-node Monte Carlo simulation. We still not have a clear understanding, yet, of the requirements that a wave function must fulfill to make a good fixed-node trial wave function. However, we feel that the fixed-node method combined with nodal relaxation offers great new opportunities to tackle problems of lattice Hamiltonians.

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TABLE I. Comparison of the exact ground-state energy to the energy of mean-field and Gutzwiller wave functions, and to the energy obtained by MC simulations, for the $4 \times 4$ square (PBC), with 5 spins up and 5 down, for $U = 4$. A mean-field (MF) homogeneous (H) wave function has been used. The Gutzwiller wave function (GMF) was used with $g = 0.6$; its energy was calculated by variational Monte Carlo. For the fixed-node (FN) and nodal relaxation (NR) Monte Carlo calculations, a trial wave function has been used as indicated. Energies are given per site and in units of $t$. Constrained Path Monte Carlo (CPMC) results were taken from Ref. 11, exact results from Ref. 12.

| $U$ | MF  | GMF | FN/MF     | FN/GMF   | NR/GMF   | CPMC     | exact   |
|-----|-----|-----|-----------|----------|----------|----------|---------|
| 4   | -1.109 | -1.212 | -1.2186(4) | -1.2201(4) | -1.2234(6) | -1.2238(6) | -1.2238 |

TABLE II. Various mean-field and quantum Monte Carlo calculations (QMC) of the exact ground-state energy of a $10 \times 10$ square (PBC), at half filling and with zero total $S^z$, for $U = 4$. Slave Boson MF result has been taken from Ref. 13. QMC results from Refs. 14 and 15.

| method                  | energy per site |
|-------------------------|-----------------|
| Mean Field (AF)         | -0.797          |
| Slave Boson MF          | -0.839          |
| Gutzwiller VMC          | -0.842          |
| QMC (Hirsch ’85)       | -0.88(3)        |
| QMC (White ’89)        | -0.864(1)       |
| FNMC                    | -0.852(2)       |
| Power MC                | -0.860(5)       |
FIGURES

FIG. 1. First part of a FNMC simulation, for a $2 \times 2 \times 2$ cube (see text for details). Each star indicates the average of the energy samples in 10 Monte Carlo steps. The drawn line indicates the exact ground-state energy of the fixed-node effective Hamiltonian. The square at the right indicates the resulting energy, obtained after averaging over several thousands of steps, with a statistical error which is smaller than the symbol size.

FIG. 2. Nodal relaxation for the system as in Fig. 1. Two calculations using different trial wave functions are shown (see text for details). Error bars indicate the estimated values of the ground-state energy after each step of the calculation.
