Adaptive Sampling Approach to the Negative Sign Problem in the Auxiliary Field Quantum Monte Carlo Method

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We propose a new sampling method to calculate the ground state of interacting quantum systems. This method, which we call the adaptive sampling quantum monte carlo (ASQMC) method, utilises information from the high temperature density matrix derived from the monte carlo steps. With the ASQMC method, the negative sign ratio is greatly reduced and it becomes zero in the limit \( \Delta \tau \) goes to zero even without imposing any constraint such like the constraint path (CP) condition. Comparisons with numerical results obtained by using other methods are made and we find the ASQMC method gives accurate results over wide regions of physical parameters values.

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The negative sign problem in quantum monte carlo simulations has been an extremely serious problem. In the case of the auxiliary field quantum monte carlo (AFQMC) method \([1\,2]\), applied to the two-dimensional (2D) Hubbard model, we always have this problem in the ground state and in low temperature regions except at half-filling, where we have particle-hole symmetry. \([3]\) The negative sign difficulty is somewhat reduced and calculations become more feasible only when the filling is far away from half-filling, and/or when we use a smaller value of \( U/t \), and/or when we use a smaller value of the inverse temperature \( \beta \) or the projecting time \( \tau \). Such a reduction is also observed when the electron filling is such that the corresponding non-interacting model has a closed-shell electronic structure and the system size is small. The quantum monte carlo results on the 2D models \([4\,5]\) and the Hubbard ladder model \([6\,7]\) obtained so far are in regimes where the above conditions are satisfied. However, to get more insight into the physics of strongly correlated electrons, it is highly desirable to develop more robust numerical methods whose applicability and accuracy do not depend on the details of the system to be studied.

Recently, Zhang, Carlson and Gubernatis developed the constrained path quantum monte carlo (CPQMC) method. \([8\,9]\) Their method consists of the two ideas: the random walker in the configuration space (RWCS) and the constrained path (CP) conditions, which is local. The latter is a variant of the nonlocal positive projection condition proposed by Fahy and Hamman \([10\,11]\) but is simpler to impose. Both of their methods are variational but the rate of convergence to the ground state of the CPQMC method against a variation of the trial wavefunction has been reported to be very fast in weak and intermediate regions of \( U/t \) and the closed shell case. We will demonstrate that the CP condition is not necessary to reduce the negative sign ratio, if we adopt the adaptive sampling method which we propose here in the standard projector AFQMC (PAFQMC) algorithm.

In applying the PAFQMC method to the Hubbard model: \( H = T + V_2, \ T = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j + H.C.), \ V_2 = U \sum_j n_{1j} n_{Lj}, \) where \( \langle i,j \rangle \) indicates the sum is taken over the pairs of nearest-neighbor sites, we use the density matrix: \( \langle \Psi_1 | \exp (-\tau H) | \Psi_i \rangle \). The density matrix is expressed by using the Suzuki-Trotter (ST) formula and the Stratonovich-Hubbard (SH) transformation in the following way:

\[
\langle \Psi_1 | \exp (-\tau H) | \Psi_i \rangle = \text{Tr}_{\sigma(1),\sigma(2),\ldots,\sigma(L)} [B_1(\sigma(L)) \cdots B_\tau(\sigma(1)) | \Psi_i \rangle | \Psi_1 \rangle \times \langle \Psi_1 | B_1(\sigma(L)) \cdots B_\tau(\sigma(1)) | \Psi_i \rangle,
\]

where \( L = \tau/\Delta \tau \) and \( \Delta \tau \) is the discretized projecting time \( \tau \), \( B_\alpha(l) = \exp (-\Delta \tau U_\alpha(l)) \exp (-\Delta \tau V_{1\alpha}(l)) \) and \( V_{1\alpha}(l) = \delta_{lj} (\alpha \sigma_l \sigma_j(l) \pm (1/2) \Delta \tau U(1/2) \Delta \tau U) \). In the \( V_{1\alpha}(l) \) factor \( \alpha U \) is defined to be \( \tanh^{-1} \sqrt{\tanh(\Delta \tau U/4)} \) and \( \alpha = +1 \) for up spins and \( -1 \) for down spins. Hereafter, we denote \( U_\rho(\tau, \alpha) = B(\sigma(L)) \cdots B(\sigma(1)) \) and the spin indices will be suppressed. Products of both up-spin and down-spin elements are implicit throughout this letter. \( \tau \) is the total projection time. The trace over the Ising SH fields: \( \sigma(1),\sigma(2)\ldots,\sigma(L) \) is achieved by using the importance sampling method. The site index \( i \) of the SH fields is suppressed here. After we take the trace over the SH fields, we can calculate any ground state expectation value and the ground state wavefunction: \( | \Psi_{\text{exact}} \rangle \simeq \text{Tr}_{\sigma(1),\sigma(2),\ldots,\sigma(L)} [B(\sigma(L)) \cdots B(\sigma(1)) | \Psi_i \rangle \times \langle \Psi_1 | B(\sigma(L)) \cdots B(\sigma(1)) | \Psi_i \rangle \).

There remains freedom how we take the trace. In the standard AFQMC method, the trace over the SH fields is taken simultaneously and we use the weight function: \( P = \langle n_\rho | U_\rho(\tau, 0) | \Psi_i \rangle \). There remains another choice in how we take the trace. If we define: \( | \Psi_1 \rangle = \text{Tr}_{\sigma(i)} [B(\sigma(i)) | \Psi_{i-1} \rangle, \) and \( | \Psi_0 \rangle = | \Psi_i \rangle \),

\[
| \Psi_{\text{exact}} \rangle \simeq \text{Tr}_{\sigma(2),\ldots,\sigma(L)} [B(\sigma(L)) \cdots B(\sigma(2)) | \Psi_1 \rangle = \text{Tr}_{\sigma(3),\ldots,\sigma(L)} [B(\sigma(L)) \cdots B(\sigma(3)) | \Psi_2 \rangle = \cdots = \text{Tr}_{\sigma(L)} [B(\sigma(L)) | \Psi_{L-1} \rangle.
\]
We can then take the trace sequentially. This is similar to the propagation process in RWCS and both this method and the standard AFQMC method should give identical results, if proper monte carlo sampling is done.

To take the sequential trace properly, we introduce the adaptive sampling method and we define the weight function as follows:

\[ P_{\tau^o} = \left\langle \Psi_{t} | U_\sigma (\tau, \tau^o) | \Psi_{t} \right\rangle \left\langle \Psi_{t} | U_\sigma (\tau^o, 0) | \Psi_{t} \right\rangle, (0 \leq \tau^o \leq \tau), \]

rather than the standard weight function: \( P = \left\langle \Psi_{t} | U_\sigma (\tau, 0) | \Psi_{t} \right\rangle \). \( \tau^o \) is an imaginary time whose SH field is tried to be updated and \( \tau^o \) changes during the simulation; the SH field to be updated belongs to the \( l = \tau^o/\Delta \tau\)-th imaginary-time slice. We use the local-flip update scheme and the field is updated from \( l = 1 \) to \( l = L \) (from \( \tau^o = \Delta \tau \) to \( \tau^o = \tau \)). The ratio used in judging to accept or to reject the update of the SH field of the \( i \)-th site and of the \( l = \tau^o/\Delta \tau\)-th imaginary-time slice is given as follows:

\[ r_{\tau^o} = \left| \left\langle \Psi_{t} | U_{-\sigma, (\tau^o)} (\tau^o, 0) | \Psi_{t} \right\rangle / \left\langle \Psi_{t} | U_{\sigma, (\tau^o)} (\tau^o, 0) | \Psi_{t} \right\rangle \right|. \]

We use the heat bath method and the acceptance probability is given by \( R_{\tau^o} = r_{\tau^o}/(1 + r_{\tau^o}) \). The \( \tau^o \)' dependent weight function is the unique feature of our adaptive sampling method. The update of the SH field is initiated by using the "high temperature density matrix" (the projecting time \( \tau' = \Delta \tau \)). All the \( N \) SH fields on the imaginary-time \( \tau^o \) are tried to be updated, where \( N \) is the number of sites. The series of trial updates on the imaginary-time \( \tau^o \) is repeated \( M \) times. After the trials have completed, \( \tau^o \) increases by \( \Delta \tau \). The procedure is repeated until \( \tau^o \) becomes \( \tau \). All these constitute a sweep. The next sweep starts with \( \tau^o = \Delta \tau \), again. We call our method the adaptive sampling quantum monte carlo (ASQMC) method.

Measurements may be done with the re-weighting function: \( R_w (\tau') = |W_\sigma / \tilde{W}_\sigma (\tau')|, \)

where \( \tilde{W}_\sigma = \left( \left\langle \Psi_{t} | U_\sigma (\tau, 0) | \Psi_{t} \right\rangle \right), W_\sigma (\tau') = \left( \left\langle \Psi_{t} | U_\sigma (\tau, \tau') | \Psi_{t} \right\rangle \left\langle \Psi_{t} | U_\sigma (\tau', 0) | \Psi_{t} \right\rangle \right) \). Let \( O \) be one-body operators such like: \( O = c_{\vec{k} \sigma}^\dagger c_{\vec{k}' \sigma} \), where \( \vec{k} \) is the wave vector and \( \sigma \) is the spin variable. The expectation value of \( O \) can be calculated as follows:

\[ \left\langle \left\langle O \right\rangle \right\rangle = \frac{\text{Tr}_\sigma (O) \text{Sign}W_\sigma R_w (\tau') (|\tilde{W}_\sigma (\tau')|/\text{Tr}_\sigma |\tilde{W}_\sigma (\tau')|)}{\text{Tr}_\sigma \text{Sign}W_\sigma R_w (\tau') (|W_\sigma (\tau')|/\text{Tr}_\sigma |W_\sigma (\tau')|)}. \]

We may make measurements only by use of configurations of the SH field obtained just after the trial updates at \( \tau^o = \tau \) \((l = L)\) and then the re-weighting function \( R_w (\tau) = 1 \). In this case, we may evaluate the expectation value as follows:

\[ \left\langle \left\langle O \right\rangle \right\rangle = \frac{\sum_{n_s} \text{Sign}W_\sigma \left\langle \Psi_{t} | O U_\sigma (\tau, 0) | \Psi_{t} \right\rangle}{\sum_{n_s} \text{Sign}W_\sigma \left\langle \Psi_{t} | U_\sigma (\tau, 0) | \Psi_{t} \right\rangle}, \]

and \( n_s \) is the number of samples. For the two-body (or more) physical quantities, we use the Wick theorem. The measurements in this form are called a mixed estimator: \( \left( \Psi_{t} | O | \Psi_{\text{exact}} \right) \). One of the difficulties of the ASQMC method is measurements because the mixed estimator does not give exact expectation values other than for energy and sign. To remedy the situation, we may use the following weight function:

\[ P_{\tau^o} = \left| \left\langle \Psi_{t} | U_\sigma (\tau, 0) | \Psi_{t} \right\rangle \right| (0 \leq \tau^o \leq \tau_c), \]

\[ P_{\tau^o} = \left| \left\langle \Psi_{t} | U_\sigma (\tau, \tau^o) | \Psi_{t} \right\rangle \left\langle \Psi_{t} | U_\sigma (\tau^o, 0) | \Psi_{t} \right\rangle \right|, (\tau_c \leq \tau^o \leq \tau). \]

Measurements in this case are made only when \( 0 \leq \tau^o \leq \tau_c \). In this interval \( Rw (\tau') = 1 \) and measurements such as:

\[ \left\langle \left\langle O \right\rangle \right\rangle = \frac{\sum_{n_s} \text{Sign}W_\sigma \left\langle \Psi_{t} | O U_\sigma (\tau') \right\rangle \left\langle \Psi_{t} | U_\sigma (\tau^o, 0) | \Psi_{t} \right\rangle}{\sum_{n_s} \text{Sign}W_\sigma \left\langle \Psi_{t} | U_\sigma (\tau, 0) | \Psi_{t} \right\rangle}, \]

may be done there. We call this measurement the standard measurement.

Instead of using \( \tilde{W}_\sigma (\tau') \) to define \( Rw (\tau') \), we may be able to use any weight function which does not necessarily have any physical correspondence to the original problem. For example, we may use the weight function of the half-filled Hubbard model \( \Omega_\sigma \) to study the doped Hubbard model. The re-weighting function in this case is \( Rw = |W_\sigma / \Omega_\sigma| \). The expectation value of any one-body operator is given:

\[ \left\langle \left\langle O \right\rangle \right\rangle = \frac{\text{Tr}_\sigma (O) \text{Sign}W_\sigma \text{Rw} (|\Omega_\sigma| / \text{Tr}_\sigma |\Omega_\sigma|)}{\text{Tr}_\sigma \text{Sign}W_\sigma \text{Rw} (|\Omega_\sigma| / \text{Tr}_\sigma |\Omega_\sigma|)} \]

As the re-weighting procedures do not introduce any approximation to the theory, both of the mathematical expressions for the expectation value of operator \( O \) are exact. The numerical effectiveness of the re-weighting methods depends on whether \( \text{Sign}W_\sigma \) is mostly positive and if the re-weighting function \( Rw \) is not very small. Unless the two conditions are satisfied, numerical application of re-weighting methods will not be successful.

The ergodicity is guaranteed in our method. The ASQMC method is one of the exact algorithms like the standard AFQMC method and some other re-weighting
methods applied to it, irrespective of the sign problem. This can be checked numerically at half-filling, where there is no sign problem and comparisons of results obtained by using the ASQMC method and the standard AFQMC method are possible. We compared calculated results of the spin-spin correlation function: 

\[ S(q) = 1/N \sum_{i,j} \exp[-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)]S_i^z S_j^z \]

of the 4 × 4 Hubbard model at the half-filling. The results are Fourier transformed into the real space and they are plotted against the distance \( R \) in Fig. 4. We find nice agreement over all the distances within the cluster.

With our adaptive sampling method, we improve the trial wavefunction \( \Psi_i \) (\( i = 0, 1, \ldots, L - 1 \)) sequentially so that the final short time projection: \( \exp(-\Delta \tau H)\Psi(\tau_{\text{f}}) \) extracts out the ground state and therefore ASQMC method is expected to be less affected by the negative sign problem. Our method is easily implemented by modifying the standard AFQMC code. We do not use the population control procedure in our implementation so that \( \Delta \tau \) needs to be small. Here, we have studied the minimal case \( M = 1 \).

The benefit of our ASQMC method is that it greatly reduces the negative sign ratio without imposing any constraint such like the CP condition. We calculated the expectation value of the sign \( \langle \text{Sign} \rangle \) as a function of \( \Delta \tau \). \( \tau_c \) was set to be zero and we used the mixed estimator method to calculate the sign expectation value \( \langle \text{Sign} \rangle \).

We used the projecting time \( \tau/t = 10 \). Calculations were made with various physical parameters values of the 4 × 4 Hubbard model, but we show the result obtained with \( U/t = 8 \) and with the density \( \rho = N_e/N_s = 0.875 \), where there is very serious negative sign problem when we use the standard AFQMC method. The result is shown in Fig. 2. When \( \Delta \tau \to 0 \), \( \langle \text{Sign} \rangle \to 1 \). We have no negative sign problem in the limit of \( \Delta \tau \to 0 \). Over a wide range of finite \( \Delta \tau \), the negative sign ratio obtained with our ASQMC method is much reduced in comparison with the standard AFQMC method. When we use smaller value of \( U/t \) or when we study the closed shell filling case, \( \langle \text{Sign} \rangle \) tends to become much closer to 1 with the same value of \( \Delta \tau \). The rate of convergence to \( \langle \text{Sign} \rangle \to 1 \) depends on values of physical parameters.

Our ASQMC method is expected to give accurate numerical results, because \( \text{Sign} W_{\sigma} \) is mostly positive and \( \text{Re}(\mathbf{r}^\prime) = 1 \). (Measurements are done either at \( \mathbf{r}' = \mathbf{r} \) or \( 0 \leq \mathbf{r}' \leq \mathbf{r}_c \).) We prefer to use the standard measurement here to reduce the \( \Delta \tau \) error, which comes not only from the Trotter error but also from the finite step size \( \Delta \tau \) used in taking the sequential trace of the auxiliary fields. The ground state wavefunction obtained by using finite \( \Delta \tau \) may be expanded by powers of \( \Delta \tau \): \( \Psi(\Delta \tau) = \Psi_{\text{exact}} + \Delta \tau \Psi'(0) \), where \( \Psi'(0) = (\partial/\partial \Delta \tau)\Psi(\Delta \tau)|_{\Delta \tau = 0} \) and \( \Psi(0) \) is orthogonal to \( \Psi_{\text{exact}} \). If we use the mixed estimator measurement, we obtain the expression: 

\[ \langle \Psi_i | H | \Psi(\Delta \tau) \rangle = E_{\text{exact}} \langle \Psi_i | \Psi_{\text{exact}} \rangle + \Delta \tau \langle \Psi_i | H | \Psi'(0) \rangle. \]

On the other hand if we use the standard measurement, we get: 

\[ \langle \Psi(\Delta \tau) | H | \Psi(\Delta \tau) \rangle = E_{\text{exact}} \langle \Psi_{\text{exact}} | \Psi_{\text{exact}} \rangle + \Delta \tau^2 \langle \Psi'(0) | H | \Psi'(0) \rangle, \]

where \( E_{\text{exact}} \) is the exact ground state energy of the Hamiltonian \( H \). We notice that larger \( \Delta \tau \) error remains in the mixed estimator measurements than in the standard measurements, which is also observed in numerical simulations. So the standard measurement is the better choice even when one calculates energies. The negative sign ratio obtained by using the standard measurement method is somewhat larger than that obtained by using the mixed estimator method, but it is still far more reduced than that obtained by using the standard AFQMC algorithm. Hereafter throughout this article, we adopt the standard measurement method in our ASQMC calculations.

We compared calculated total energies, one and two-body correlation functions obtained by using the ASQMC method with those obtained by using the Lanczos exact diagonalization (ED) method and other quantum monte carlo methods. Values of \( \Delta \tau \) used are 0.025 and 0.0125. A 5000 sweep run on the 8 × 8 lattice takes almost 80 hours of CPU time on the Alpha workstation with the Alpha 21164 / 533MHz CPU chip. We found the ASQMC method gives accurate results over wide range of physical parameters values on 4 × 4, 6 × 6, and 8 × 8 lattices. In the following paragraph, we show results of such comparisons.

First, we compare total energies of \( U/t = 4 \) Hubbard model of various lattice size: 4 × 4, 6 × 6, 8 × 8. Fillings \( \rho \) are such that both the closed shell case and open shell case are included. Agreements of the total energies calculated by using the ASQMC method with those obtained by using ED, the CPQMC, and the AFQMC methods are rather nice up to 3 digits over the wide range of fillings and lattice size. This is shown in Fig. 3. To see this in more detail, we have plotted relative errors of the total energies in Fig. 5. The CPQMC results agrees with our ASQMC results within 0.1% of errors in the all cases studied here, but the AFQMC results does not always agree with our ASQMC results very precisely. The largest error we found is 0.5%. It seems that the extrapolation procedure used to make inferences of the ground state energies without taking in to account of statistical errors described in Ref. 4 does not work so well.

We next compare total energies of the 4 × 4 Hubbard model for various \( U/t \) values calculated by using the ASQMC, the CPQMC, and ED methods. \( U/t \) We set the filling \( \rho = 14/16 \). Agreements between the ASQMC and ED results are very good but we found small systematic increase of deviation of the CPQMC results from the other two results, as we increase \( U/t \). To see in more detail this tendency found in Fig. 3, we have plotted relative errors of the total energies in Fig. 6. While the CPQMC results deviate from the ED results systematically, the ASQMC results do not. Because we do not impose any constraint such like the CP condition, the ASQMC method does not have any systematic bias.
even in the large $U/t$ region. This demonstrates that our ASQMC method is superior to the CPQMC method in the large $U/t$ region.

To provide other benchmark of our ASQMC method, we have calculated the d-wave pairing correlation function of the $4 \times 4$ Hubbard model defined by: $<O(R)O^\dagger(0)>$ with $O^\dagger(R) = c_{\uparrow}^\dagger(R)c_{\downarrow}^\dagger(R+x) + c_{\uparrow}^\dagger(R)c_{\downarrow}^\dagger(R-x) - c_{\downarrow}^\dagger(R)c_{\uparrow}^\dagger(R+y) - c_{\downarrow}^\dagger(R)c_{\uparrow}^\dagger(R-y)$ and compared it with the result obtained with the Lanczos diagonalization method. [14] The result is shown in Fig. 7. We again, obtained a good agreement with the Lanczos diagonalization result over all the distances within the cluster studied.

As far as the present author knows, there are no other reliable numerical methods than ED, the AFQMC and the CPQMC methods to compare with our ASQMC methods for the 2D Hubbard model. Our ASQMC results always agree well with the best of the results obtained by using the other methods. Thus our ASQMC method turns out to be a very accurate method. The ASQMC method will be useful to study a wider physical parameter region including the large $U/t$ region, many more cases of filling and band structures, including the open shell cases, and larger lattice sizes that have not yet been explored by the quantum monte carlo methods.

To summarize, we have proposed the adaptive sampling method to utilize information from the "high temperature density matrix" in the thermalization process of monte carlo steps to calculate the ground state. With the adaptive sampling method, the negative sign ratio decreases to 0 when $\Delta \tau \to 0$ without imposing any constraint such as the CP condition. Over a wide range of finite $\Delta \tau$, the negative sign ratio is far more reduced than that in the standard AFQMC method. We compared calculated energies and two-body correlation functions obtained by using our method and with those obtained by using the Lanczos diagonalization method and other quantum monte carlo methods found in the literature and we found the ASQMC method gives accurate results over a wide range of physical parameters values.

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FIG. 1. The spin-spin correlation function as a function of the distance $R$ calculated by the ASQMC and the standard AFQMC methods at half-filling. The calculations were made on the $4 \times 4$ lattice. $U/t = 4$. Open circles and crosses are data obtained by the ASQMC and the standard AFQMC methods, respectively.

FIG. 2. The sign expectation value $\langle \text{Sign} \rangle$ as a function of $\Delta \tau$ calculated with the ASQMC method. We put $\tau_c = 0$ and $U/t = 8$ and $\rho = 0.875$. $\tau/t = 10$. The calculation is made on the $4 \times 4$ Hubbard model.
FIG. 3. Total energies per site of the two dimensional Hubbard model with various system size calculated by the ASQMC, ED, the CPQMC, and the AFQMC methods. $t = 1$ and $U = 4$. We plot the energies as a function of electron density $\rho$. Open circles, open squares, and open triangles denote results obtained by the ASQMC method with $4 \times 4$, $6 \times 6$, and $8 \times 8$ lattices, respectively. Crosses, asterisks, and closed diamonds denote ED, CPQMC, and AFQMC results, respectively.

FIG. 4. Relative errors of total energies per site calculated by the CPQMC and the AFQMC methods. They are compared with the ASQMC results. The physical parameters and fillings are the same as Fig.3. Crosses and closed diamonds denote the relative errors of the CPQMC and the AFQMC results, respectively.
FIG. 5. Total energies per site as a function of $U/t$ calculated by the ASQMC, CPQMC and ED methods. The calculations were made on the $4 \times 4$ lattice and $\rho = 14/16$. Closed circles, crosses, and open squares denote ASQMC, ED, and CPQMC results, respectively.

FIG. 6. Errors of total energies per site as a function of $U/t$. The physical parameters and fillings are the same as Fig.5. Closed circles and open squares are errors of the ASQMC and the CPQMC results, respectively.
FIG. 7. The d-wave superconducting correlation function as a function of the distance $R$ calculated by the ASQMC and ED methods. The calculations were made on the $4 \times 4$ lattice. $U/t = 4$ and $\rho = 10/16$. Open circles and crosses are data obtained by the ASQMC and ED methods, respectively.