Multilevel blocking approach to the fermion sign problem in path-integral Monte Carlo simulations

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A general algorithm toward the solution of the fermion sign problem in finite-temperature quantum Monte Carlo simulations has been formulated for discretized fermion path integrals with nearest-neighbor interactions in the Trotter direction. This multilevel approach systematically implements a simple blocking strategy in a recursive manner to synthesize the sign cancellations among different fermionic paths throughout the whole configuration space. The practical usefulness of the method is demonstrated for interacting electrons in a quantum dot.

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The quantum Monte Carlo (QMC) technique is one of the most powerful methods for the simulation of many-fermion systems. It is based on a path integral formulation of the fermion propagator and is one of the very few methods capable of delivering exact results for strongly correlated systems. Despite its potentials, applications of QMC have been severely handicapped by the notorious “fermion sign problem” [1,2]. As a consequence of exchange, fermionic density matrix elements are not positive-definite. The sign cancellations arising from sampling fermion paths then manifest themselves as a small signal-to-noise ratio that vanishes exponentially with either the system size or with decreasing temperature. Besides variational or approximate treatments such as the fixed-node approximation [3], the sign problem has remained unsolved.

In this Letter, we propose a simple and intuitive approach toward the general solution of the fermion sign problem. Our algorithm represents the systematic implementation of a blocking strategy [4]. The idea behind the blocking strategy is that by sampling groups of states, the sign problem can always be reduced compared to sampling single states. By suitably bunching states together into blocks, the sign cancellations among states within the same block can be accounted for non-stochastically. It can then be shown [4] that any such blocking will always reduce the sign problem — no blocking will ever make the sign problem more severe [5]. Any real progress on the sign problem will require an accurate treatment of the sign cancellations within suitably chosen subunits (blocks) of state space.

A systematic improvement of the sign problem can be achieved by formulating the blocking strategy in a recursive bottom-to-top fashion. Blocks of different sizes are defined on several levels, and after taking care of the sign cancellations within all blocks on a given (finer) level, the resulting sign problem can be transferred to the next (coarser) level. By doing this recursively, the sign problem on all the coarser levels can be handled in the same manner. It is then possible to proceed without numerical instabilities from the bottom up to the top level, where the last remaining cancellations pose no serious challenge.

In many ways, the algorithm we are proposing is related to the renormalization group approach. But instead of integrating out information on fine levels, the sign cancellations are “synthesized” within a given level and subsequently their effects are transferred to coarser levels. Our approach is actually closer in spirit to the multi-grid algorithm [6]. The method of Ref. [4] can be understood as a uni-level scheme which provides a partial solution to the sign problem. In contrast, given sufficient computer memory, the algorithm proposed here can provide a complete solution. Below we describe this multilevel blocking (MLB) algorithm and apply it to the simulation of correlated electrons in a quantum dot.

We consider a many-fermion system whose state is described by a set of quantum numbers \( r \) denoting, e.g., the positions and spins of all particles. For simplicity, we focus on calculating the expectation value of a diagonal operator \( \hat{A} \),

\[
\langle A \rangle = \frac{\sum_r A(r) \rho(r, r)}{\sum_r \rho(r, r)},
\]

where \( \sum_r \) represents either a summation for the case of a discrete system or an integration for a continuous system. Imaginary time is then discretized into \( P \) slices of length \( \epsilon = \beta/P \), where \( \beta = 1/k_B T \) and we require \( P = 2^L \). Inserting complete sets at each slice \( m = 1, \ldots, P \), and denoting the corresponding configuration on slice \( m \) by \( r_m \), the diagonal elements of the density matrix at \( r = r_P \) read

\[
\rho(P, P) = \sum_{1, \ldots, P-1} (1,2)_0(2,3)_0 \cdots (P,1)_0.
\]

As a shorthand notation, we use the slice index \( m \) for the quantum numbers \( r_m \). This equation also defines the level-0 bonds, which are simply the short-time propagators,
generating a MC trajectory containing configurations associated with the slices on level \( \ell \) using only configurations such as those arising from an integration over the fermions via the Hubbard-Stratonovich transformation \( L \), since they generally lead to long-ranged imaginary-time interactions.

\[
(m, m + 1)_0 = \langle r_{m+1} | e^{-\mathcal{H}} | r_m \rangle .
\]  

This formulation of the problem excludes effective actions such as those arising from an integration over the fermions via the Hubbard-Stratonovich transformation \( L \), since they generally lead to long-ranged imaginary-time interactions.

For instance, the slices of different levels \( m \), such that there are \( N = 2 \) bonds, are indicated by dashed and dotted lines.

\[ P_0 = |(1, 2)_0 (2, 3)_0 \cdots (P, 1)_0 | \]  

To describe the MLB strategy, we need to specify the different levels \( 0 \leq \ell \leq L \), where \( L \) defines the Trotter number \( P = 2^L \). Each slice \( m \) belongs to a unique level \( \ell \), such that \( m = (2j + 1)2^\ell \) and \( j \) is a nonnegative integer. For instance, the slices \( m = 1, 3, 5, \ldots, P - 1 \) belong to \( \ell = 0 \), \( m = 2, 6, 10, \ldots, P - 2 \) belong to \( \ell = 1 \), etc., such that there are \( N_\ell = 2^{-L+\ell+1} \) (but \( N_L = 1 \)) different slices on level \( \ell \), see Fig. 4. An elementary blocking is achieved by grouping together configurations that differ only at slice \( m \), so only \( r_m \) varies in that block while all \( r_{m \neq m} \) remain fixed. Sampling on level \( \ell \) therefore extends over configurations \( \{r_m\} \) living on the \( N_\ell \) different slices. In the MLB scheme, we move recursively from the finest (\( \ell = 0 \)) up to the coarsest level (\( \ell = L \)), and the measurement of the diagonal operator is done only at the top level using the configuration \( r_P \).

We now describe a practical implementation of the MLB scheme. A Monte Carlo sweep starts by changing only configurations associated with the slices on level \( \ell = 0 \) according to the weight

\[ P_0 = |(1, 2)_0 (2, 3)_0 \cdots (P, 1)_0 | , \]

generating a MC trajectory containing \( K \) samples for each slice on level \( \ell = 0 \). These \( N_0K \) samples are stored and they are used to generate additional coarser interactions among the higher-level slices.

\[
(m, m + 2)_1 = \langle \text{sgn} [(m, m + 1)_0 (m + 1, m + 2)_0] | r_0 | (m, m + 1)_1 \rangle P_0 | (m, m + 1)_0 \rangle \]  

where the summation \( \sum_{m+1} \) extends over the \( \mathcal{N}_0 K \) samples. As will be discussed in detail later on, for a complete solution of the sign problem, the sample number \( K \) should be chosen as large as possible. The level-1 bonds \( \mathcal{B} \) contain crucial information about the sign cancellations on the previous level \( \ell = 0 \). Using these bonds, the density matrix \( \mathcal{B} \) is rewritten as

\[
\rho(P, P) = \sum_{1, 2, \ldots, P-1} |(1, 2)_0 (2, 3)_0 \cdots (P, 1)_0 | \times (2, 1) \cdots (P - 2, P)_{P}(P, 2)_{P} , \]

Comparing this to Eq. \( \mathcal{B} \), we notice that the entire sign problem has been transferred to the next coarser level by using the level-1 bonds.

In the next step, the sampling is carried out on level \( \ell = 1 \) in order to generate the next-level bonds, i.e., only slices \( m = 2, 6, \ldots, P - 2 \) are updated, using the weight \( P_0 P_1 \) with

\[ P_1 = |(2, 4)_{P_1} (4, 1)_{P_1} \cdots (P, 2)_{P_1} | . \]

Moving the level-1 configurations modifies the level-0 bonds, which in turn requires that the level-1 bonds be updated. A direct re-calculation of these bonds according to Eq. \( \mathcal{B} \) would be too costly. Instead, we use the stored configurations on level \( \ell = 0 \) to perform an importance sampling of the new level-1 bonds. Under the test move \( m \rightarrow m' \) (i.e., \( r_m \rightarrow r'_m \)) on level \( \ell = 1 \), the bond \( \mathcal{B} \) can be obtained from

\[
(m', m + 2)_1 = \frac{\sum_{m+1} |(m', m + 1)_0 (m + 1, m + 2)_0 | \text{sgn} [(m', m + 1)_0 (m + 1, m + 2)_0]}{\sum_{m+1} |(m', m + 1)_0 (m + 1, m + 2)_0 |} .
\]

where \( \sum_{m+1} \) runs over the previously stored MC configurations \( r_{m+1} \). Note that for small values of \( K \), Eq. \( \mathcal{B} \) is only approximative, and thus a sufficiently large value of \( K \) should be chosen. With the aid of Eq. \( \mathcal{B} \), we obtain the updated level-1 bonds with only moderate computational effort. Generating a sequence of \( K \) samples for each slice on level \( \ell = 1 \), and storing these \( N_1 K \) samples, we then calculate the level-2 bonds in analogy to Eq. \( \mathcal{B} \),

\[
(m, m + 4)_2 = \langle \text{sgn} [(m, m + 2)_1 (m + 2, m + 4)_1] | r_1 | r_0 | (m, m + 2)_0 \rangle ,
\]

and iterate the process up to the top level \( \ell = L \) using the obvious recursive generalization of Eqs. \( \mathcal{B} \) and \( \mathcal{B} \) to define level-\( \ell \) bonds.

Thereby the diagonal elements of the density matrix are obtained as
\[
\rho(P, P) = \sum_{1, 2, \ldots, P-1} |(1, 2)_0(2, 3)_0 \cdots (P, 1)_0| 
\times |(2, 4)_1 \cdots (P - 2, P)_1(P, 2)_1| 
\cdots |(P/2, P)_{L-1}(P/2)_{L-1}|(P, P)_L.
\]  

By virtue of this algorithm, the sign problem is transferred step by step up to the coarsest level. The expectation value \(\langle A \rangle\) can thus be computed from

\[
\langle A \rangle = \frac{\langle A(P) \text{sgn}(P, P)_L \rangle_P}{\langle \text{sgn}(P, P)_L \rangle_P}.
\]  

The denominator in Eq. (11) gives the average sign

\[
\langle \text{sgn}(P, P)_L \rangle_P = \sum_{P, P/2} \delta(P, P/2)_{L-1}|(P, P)_L|.
\]  

The manifestly positive definite MC weight \(\mathcal{P}\) used for the averaging in Eq. (11) can be read off from Eq. (10),

\[
\mathcal{P} = |(1, 2)_0(2, 3)_0 \cdots (P, 1)_0| 
\times |(2, 4)_1 \cdots (P - 2, P)_1(P, 2)_1| 
\cdots |(P/2, P)_{L-1}(P/2)_{L-1}|(P, P)_L.
\]  

The denominator in Eq. (11) gives the average sign and indicates to what extent the sign problem has been solved. Under a naive application of the QMC technique, the average sign decays exponentially with \(\beta\) and is typically close to zero. This causes the numerical instabilities associated with the sign problem, i.e., to obtain statistically relevant results requires exponentially long CPU times. With the MLB algorithm, however, the sign problem can be completely eliminated. The average sign remains close to unity for any \(\beta\), with a CPU time requirement that increases only linearly. The price to pay for the stability of the algorithm is the increased memory requirement associated with having to store the sampled configurations on the fine levels, which scales at worst quadratically in \(K\). The example below demonstrates that modest memory requirements are sufficient to treat rather complex problems.

Next we address questions concerning the exactness of the MLB approach for a finite sample number \(K\). Clearly, \(K\) needs to be sufficiently large to produce a reliable estimate for the level-\(\ell\) bonds. If these bonds could be calculated exactly (corresponding to the limit \(K \to \infty\)), the manipulations leading to Eq. (11) yield the exact result. Hence for large enough \(K\), the MLB algorithm must (i) become exact and (ii) completely solve the sign problem. However, since the level-\(\ell\) bonds can only be computed for finite \(K\), the weight function \(\mathcal{P}\) amounts to using a noisy estimator, which in turn can introduce bias into the algorithm \(\mathcal{P}\). In principle, this problem could be avoided by using a linear acceptance criterion \(\mathcal{P}\) instead of the algorithmically simpler Metropolis choice \(\mathcal{P}\). But even with the Metropolis choice (which we used in the example below), the bias can be made arbitrarily small by increasing \(K\). Therefore, with sufficient computer memory, the MLB approach can be made to give numerically exact results. One might then worry about the actual value of \(K\) required to obtain stable and exact results. If this value were to scale exponentially with \(\beta\) and/or system size, the sign problem would be present in disguise again. Although we do not have a rigorous non-exponential bound on \(K\), our experience with the MLB algorithm indicates that this scaling is at worst algebraic.

We now illustrate the usefulness of the method for \(N\) interacting electrons confined in a quantum dot. Quantum dots are two-dimensional artificial atoms fabricated by means of suitable gates in semiconductor heterostructures. For simplicity, we consider only spinless electrons, zero magnetic field, and a parabolic confinement potential. We employ a symmetric Trotter breakup \(\mathcal{P}\) for \(H = H_1 + H_2\),

\[
H_1 = \sum_{j=1}^N \left( \frac{p_j^2}{2m^*} + \frac{\kappa e^2}{2|x_j|^2} \right), \quad H_2 = \sum_{i<j}^N \frac{\kappa e^2}{|x_i - x_j|},
\]  

where the positions (momenta) of the \(N\) electrons are \(x_j (p_j)\), the dielectric constant is \(\kappa\), and \(m^*\) is the effective mass. The short-time propagator \(\mathcal{P}\) under \(H_1\) is obtained by antisymmetrizing a product of \(N\) harmonic oscillator propagators, leading to a fermion determinant. Since the determinant can change sign, conventional QMC simulations run into the sign problem. The MC updating then employs randomly chosen single particle moves on the momentary level \(\ell\). This suffices for an efficient and ergodic sampling of configuration space. Here we present results for the energy \(E_N = \langle H \rangle\). Since the direct evaluation of the kinetic energy would involve a nonlocal operator, we have exploited the quantum virial theorem \(\mathcal{P}\) in order to sample \(E_N\). Simulations were done at \(\hbar = 0\) for two different interaction strengths, \(t_0/a = 2\) and 8. Here \(t_0 = (\hbar/m^*\omega_0)^1/2\) is a confinement lengthscale, and \(t_0/a = e^2/(\hbar\kappa e^2)\), with \(a\) being the effective Bohr radius. Trotter convergence was achieved at \(\ell = 3 (4)\) for \(t_0/a = 2 \) (8). The \(N = 2\) exact diagonalization results of Ref. \(\mathcal{P}\) have been accurately reproduced, which also serves as an independent check for our code. The simulations have been carried out on an IBM RISC6000/590 workstation.

| \(K\) | \(N\) | \(t_{CPU}\) | MB | \(\text{sgn}\) | \(E_N/\hbar\omega_0\) |
|---|---|---|---|---|---|
| 1 | 120 | 95 | 2 | 0.02 | 48.6(3) |
| 100 | 7 | 33 | 14 | 0.48 | 48.43(8) |
| 200 | 9 | 83 | 30 | 0.63 | 48.55(7) |
| 400 | 8 | 174 | 64 | 0.73 | 48.53(9) |
| 600 | 10 | 308 | 96 | 0.77 | 48.54(8) |
| 800 | 9 | 429 | 150 | 0.81 | 48.59(8) |

TABLE I. MLB results for \(N = 8\) and \(t_0/a = 2\). \(N\) is the number of samples (in 10\(^4\)), \(t_{CPU}\) the total CPU time (in hours), MB the required memory (in mega-bytes), and \(\langle \text{sgn} \rangle\) the average sign. Bracketed numbers are error estimates.
To elucidate how the MLB algorithm works in practice, in Table I we compare simulation results for \( N = 8 \) electrons at various values of \( K \). Compared to the naive approach (\( K = 1 \)), using a moderate \( K = 200 \) already increases the average sign from 0.02 to 0.63, making it possible to obtain more accurate results from much fewer samples. The data in Table also confirms that the bias can be systematically eliminated by increasing \( K \), so that the energy found at \( K \geq 200 \) essentially represents the exact result (within error bars). As expected, the CPU time per sample scales only linearly with \( K \), where the memory requirements grow at most quadratically with \( K \).

Results for \( E_N \) with \( N \leq 8 \) are shown in Figure 2. For \( N \leq 5 \), the fixed-node QMC and Jastrow wavefunction calculations of Ref. [12] are in fairly good agreement with our exact results. However, for larger \( N \), there are deviations, with the correct energies significantly lower than the values reported in Ref. [12], which represent variational upper bounds. Notably, there are no obvious cusps or breaks in the \( N \)-dependence of the energy. Such features would hint at the existence of magic numbers for which the artificial atom is exceptionally stable. Our data in Fig. 2 suggests that an explanation of the experimentally observed magic numbers [1] has to involve spin or magnetic field effects. Remarkably, the absence of pronounced cusps in \( E_N/N \) for strong correlations (\( l_0/a = 8 \)) is in accordance with a purely classical analysis [13].

To conclude, we have proposed a multilevel blocking approach to the fermion sign problem in finite-temperature QMC simulations. As presented, the method applies to the primitive path integral characterized by local imaginary-time interactions. Given sufficient computer memory, the MLB approach can provide a complete and exact solution of the sign problem. We believe that similar ideas may also lead to the resolution of the sign problem in other fermion or real-time QMC schemes.

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