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# Exact Monte Carlo Method for Continuum Fermion Systems

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We offer a new proposal for the Monte Carlo treatment of many-fermion systems in continuous space. It is based upon diffusion Monte Carlo with significant modifications: correlated pairs of random walkers that carry opposite signs, different functions "guide" walkers of different signs, the Gaussians used for members of a pair are correlated, and walkers can cancel so as to conserve their expected future contributions. We report results for free-fermion systems and a fermion fluid with 14 $^3$He atoms, where it proves stable and correct. Its computational complexity grows with particle number, but slowly enough to make interesting physics within the reach of contemporary computers.

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Monte Carlo methods provide powerful tools for quantum many-body physics [1,2]. They include Green's function Monte Carlo [3], diffusion Monte Carlo (DMC) [4], or path integral Monte Carlo [5] that give, at least for moderate size bosonic systems, answers with no uncontrolled approximations. Such accurate treatment of fermionic systems has been made difficult by a "sign problem." Progress in the application of quantum Monte Carlo to condensed matter physics, to electronic structure, and to nuclear physics has been impeded for years by the lack of exact and efficient methods for dealing with fermions.

We offer a new proposal for solving many-fermion systems by an extension of DMC. In the systems we have studied, the signal-to-noise ratio of the Monte Carlo estimates is constant at long imaginary times, by contrast to the behavior of ordinary DMC where they decay exponentially [2]. Except for the use of a short-time Green's function, no approximations—physical, mathematical, or numerical—are made. The effect of a finite imaginary time step is easily controlled.

It is no surprise that Monte Carlo methods can solve the Schrödinger equation for bosonic systems. Let $\vec{R}$ denote all coordinates of an $N$-body system and $V(\vec{R})$ be the potential at $\vec{R}$.

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{R})\right]\psi(\vec{R},\tau) + \hbar\frac{\partial\psi(\vec{R},\tau)}{\partial\tau} = 0. \quad (1)$$

This equation also describes the diffusion of a random walker in a $3N$ dimension space in which the potential $V(\vec{R})$ serves as a generalized absorption rate. The potential in physical problems can be unbounded so that a direct simulation of that diffusion will be inefficient. Some form of importance sampling has been highly useful. In the standard DMC [3,4], this is a technical device for accelerating the convergence; in our new method it becomes an essential feature.

DMC uses an "importance" or "guiding" function $\psi_G(\vec{R})$ and a trial eigenvalue $E_T$ to construct a random walk. A simple version is as follows: Set $\hbar^2/m = 1$. Using a fixed step in imaginary time, $\delta\tau$, a walker at $\vec{R}$ is (a) moved to $\vec{R} + \delta\tau\vec{\nabla}\ln\psi_G(\vec{R})$; (b) then each coordinate is incremented by an element of a vector $\vec{U}$, a Gaussian with mean zero and variance $\delta\tau$; finally, (c) each walker is turned into $M$ walkers with $\langle M\rangle = \exp\{\delta\tau[E_T - \hat{H}\psi_G(\vec{R})/\psi_G(\vec{R})]\}$, where $\hat{H}$ is the Hamiltonian.

The resulting random walk has expected density

$$f(\vec{R},\tau) = \psi_G(\vec{R})\sum_k a_k \exp[(E_T - E_k)\tau]\phi_k(\vec{R}), \quad (2)$$

where $\phi_k(\vec{R})$ are eigenfunctions of $\hat{H}$ with eigenvalues $E_k$, and $a_k$ are expansion coefficients. At large $\tau$, $f(\vec{R},\tau)$ is dominated by that $\phi_0$ having the lowest eigenvalue $E_0$.

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We alter DMC in the following ways: (i) To represent an antisymmetric wave function that is positive and negative, we use walkers, $(\vec{R}_m^+, \vec{R}_m^-)$, that add or subtract their contributions to expectations. The computation now involves ensembles of pairs of walkers carrying opposite signs. (ii) Two distinct functions, $\psi_G^{\pm}(\vec{R})$ are used to guide the $\pm$ walkers. (iii) The Gaussians $\vec{U}^{\pm}$ for the paired walkers are correlated; $\vec{U}^-$ is obtained by reflecting $\vec{U}^+$ in the perpendicular bisector of the vector $\vec{R}^+ - \vec{R}^-$. (iv) The overlapping distributions that determine the new $\vec{R}^{\pm}$ are added allowing positive and negative walkers to cancel, but preserving expected values.

In a Monte Carlo calculation, we "project" quantities by calculating integrals weighted with some trial function, say $\psi_T(R)$. In DMC the energy eigenvalue, $E_0$, can be determined from

$$E_0 = \frac{\int \hat{H}\psi_T(\vec{R})\phi_0(\vec{R})\,d\vec{R}}{\int \psi_T(\vec{R})\phi_0(\vec{R})\,d\vec{R}} = \frac{\sum_m \dfrac{\hat{H}\psi_T(\vec{R}_m)}{\psi_G(\vec{R}_m)}}{\sum_m \dfrac{\psi_T(\vec{R}_m)}{\psi_G(\vec{R}_m)}}, \qquad (3)$$

replacing integrals by sums over positions of the random walk.

In our modified dynamics, Eq. (3) becomes

$$E_0 = \frac{\sum_m \left[ \dfrac{\hat{H}\psi_T(\vec{R}_m^+)}{\psi_G^+(\vec{R}_m^+)} - \dfrac{\hat{H}\psi_T(\vec{R}_m^-)}{\psi_G^-(\vec{R}_m^-)} \right]}{\sum_m \left[ \dfrac{\psi_T(\vec{R}_m^+)}{\psi_G^+(\vec{R}_m^+)} - \dfrac{\psi_T(\vec{R}_m^-)}{\psi_G^-(\vec{R}_m^-)} \right]}. \qquad (4)$$

If $\{\vec{R}_m^+\}$ and $\{\vec{R}_m^-\}$ follow the same dynamics, then because the fermion and boson energies satisfy $E_A > E_S$, the values of the numerator and the denominator of Eq. (4) decay exponentially at large $\tau$. Some correlation among walkers is essential. This observation is reinforced by noting that the requirement that fermion wave functions be antisymmetric is a global condition that cannot be satisfied by independent walkers. It will be necessary to have dynamics that distinguish between walkers of different signs. These motivate aspects (ii) and (iii) of our method above.

The density that one obtains naturally from a random walk is the symmetric ground state. In order for Eq. (4) to have an asymptotically bounded signal-to-noise ratio, walkers of opposite signs must be able efficiently to cancel. This justifies modification (iv) given above. The need for cancellation has been a theme of research starting with the work of Arnow *et al.* [6]. The need for distinct dynamics for positive and negative walkers was stressed in [7]. That these two aims could be accomplished by appropriate correlation among walkers was pointed out by Liu, Zhang, and Kalos [8]. The use of distinct guiding functions is new; it connects the different algorithmic ideas to permit the treatment of general potentials.

Stable results can be obtained using correlated pairs only. Unbiased results are ensured because the actual histories—apart from cancellation—follow ordinary diffusion Monte Carlo with particular choices of guiding functions. Thus "projections"—i.e., averages over the walks such as appear in Eq. (4), are unbiased. Because such averaging is linear in the density of the walks, they are unchanged by the use of pairs of correlated walkers. Finally, as we shall discuss, cancellation can be carried out so that averages weighted by antisymmetric functions are unchanged.

Let $\varphi_A(\vec{R})$ and $\varphi_S(\vec{R})$ be trial functions for the fermionic and symmetric ground states of the Hamiltonian. These can be any of the functions used in variational studies of these systems [9]. Define

$$\psi_G^{\pm}(\vec{R}) = \sqrt{\varphi_S^2(\vec{R}) + c^2\varphi_A^2(\vec{R})} \pm c\,\varphi_A(\vec{R}). \qquad (5)$$

The following properties of these two functions are significant: (a) they are positive; (b) when $c$ is small, they are dominated by $\varphi_S$, so that opposite walkers behave similarly; (c) $\psi_G^+$ transforms under an odd permutation $\mathcal{P}$ as $\psi_G^+(\mathcal{P}\vec{R}) = \psi_G^-(\vec{R})$. As mentioned above we modify simple DMC in several ways. The "drift" is applied in the usual way to walkers assumed to be at $\vec{R}_0^{\pm}$, using the two guiding functions:

$$\begin{aligned} \vec{R}^+ &= \vec{R}_0^+ + \delta\tau\vec{\nabla}\ln\psi_G^+(\vec{R}^+), \\ \vec{R}^- &= \vec{R}_0^- + \delta\tau\vec{\nabla}\ln\psi_G^-(\vec{R}^-). \end{aligned} \qquad (6)$$

Diffusion of the walkers, however, is carried out in a correlated way: let $\vec{U}^+$ be a vector of $3N$ Gaussian random variables each of mean zero and variance $\delta\tau$. New trial positions $\vec{R}_n^{\pm}$ are now given by

$$\vec{R}_n^+ = \vec{R}^+ + \vec{U}^+; \qquad \vec{R}_n^- = \vec{R}^- + \vec{U}^-, \qquad (7)$$

where the random vector $U^-$ is obtained by reflection in the perpendicular bisector of the vector $\vec{R}^+ - \vec{R}^-$. This choice of correlated dynamics is motivated by its success in solving fermionic harmonic oscillator problems [10] and because it guarantees that two diffusing walkers meet in any number of dimensions, providing efficient cancellation in many-body systems.

Walker cancellation is achieved by subtracting weighted estimates of their arrival at a possible common point, say $\vec{R}_n^+$. Now

$$G(\vec{R}' - \vec{R}) = \frac{\exp[-(\vec{R}' - \vec{R})^2/(2\delta\tau)]}{(2\pi\delta\tau)^{3N/2}} \qquad (8)$$

is the Gaussian density used in DMC.

To assess the degree of cancellation, we now subtract $G(\vec{R}_n^+ - \vec{R}^-)$ from $G(\vec{R}_n^+ - \vec{R}^+)$ weighted, respectively, with the inverse of the importance functions, and with the expected total future contribution to any projected quantity. The analysis of "forward walking" [1,11,12] allows one to determine ratios of future contributions. In order for cancellation to have no net change in the expected value

of projections, a positive walker at $\vec{R}_n^+$ must survive to the next time step with probability

$$P^+(\vec{R}_n^+;\vec{R}^+,\vec{R}^-) = \max\left[0, 1 - \frac{B^-(\vec{R}_n^+ \mid \vec{R}^-)G(\vec{R}_n^+ - \vec{R}^-)\psi_G^+(\vec{R}_n^+)}{B^+(\vec{R}_n^+ \mid \vec{R}^+)G(\vec{R}_n^+ - \vec{R}^+)\psi_G^-(\vec{R}_n^+)}\right]. \quad (9)$$

In the particular form of DMC described above, the branching factors, $B^+(\vec{R} \mid \vec{R}^+)$ and $B^-(\vec{R} \mid \vec{R}^-)$, depend only on the coordinates after diffusion:

$$B^\pm(\vec{R} \mid \vec{R}^\pm) = \exp\left\{\delta\tau\left[E_T - \frac{H\psi_G^\pm(\vec{R})}{\psi_G^\pm(\vec{R})}\right]\right\}. \quad (10)$$

An analogous expression is used for negative walkers.

An isolated walker may appear as a result of different branching factors at $\{\vec{R}_m^+\}$ and $\{\vec{R}_m^-\}$; if, with probability one-half, one generates a walker of opposite sign by interchanging the coordinates of two like-spin particles, then a pair is reconstituted that preserves future expectations.

To determine the energy, we use the estimator of Eq. (4). A sharp indication of the stability of the calculation is the behavior of its denominator

$$\mathcal{D} = \left[\frac{\psi_T(\vec{R}_m^+)}{\psi_G^+(\vec{R}_m^+)} - \frac{\psi_T(\vec{R}_m^-)}{\psi_G^-(\vec{R}_m^-)}\right]. \quad (11)$$

In a naive calculation, $\mathcal{D}$ decays to zero in an imaginary time of order $\tau_c = 1/(E_A - E_S)$. A stable method will show $\mathcal{D}$ asymptotically constant.

Although a system of free fermions in a periodic box is analytically trivial, it presents an exigent test of this method. For this system, the lowest symmetric state is constant, and the exact fermionic wave function is a determinant of plane waves. We use $\rho = 0.5$ and set

$$\psi_G^\pm(\vec{R}) = \sqrt{1 + c^2\varphi_A^2(\vec{R})} \pm c\varphi_A(\vec{R}), \quad (12)$$

where $\varphi_A$ is a Slater determinant of orbitals $\chi_{\vec{r}_i}^{\vec{k}}$; $\eta$ is the standard backflow function [13].

$$\chi_{\vec{r}_i}^{\vec{k}} = \exp\left[i\vec{k} \cdot \left(\vec{r}_i + \lambda_B \sum_{j\neq i} \eta(r_{ij})\vec{r}_{ij}\right)\right]. \quad (13)$$

The parameter $\lambda_B$ controls the departure of the nodal structure of this function from the exact shape. The fact that these functions are modulated only a little from a constant by $\varphi_A$ means that the polarization of the population of plus and minus walkers is small.

In Table I we report the results obtained for periodic systems of 7, 19, and 27 free fermions. The results agree with the analytic eigenvalues within the Monte Carlo estimates of the standard error. It has been conjectured that the computational complexity of fermion Monte Carlo calculations will grow as $N!$, where $N$ is the number of particles in the system. Since $(27!/7!) = 2.16 \times 10^{24}$, a calculation with 27 or even 19 bodies would be impossible were that conjecture to be true.

TABLE I. Energies and errors for a periodic system of $N$ free fermions. The analytic result is $E_{\text{ex}}$.

| $N$ | $E$ | $E_{\text{ex}}$ |
|---|---|---|
| 7 | 2.912 85(49) | 2.912 712 |
| 19 | 2.760(25) | 2.757 454 |
| 27 | 2.796(30) | 2.763 316 |

We have also tested this algorithm with a strongly interacting system, using 14 $^3$He atoms in a periodic box at equilibrium density, $\rho = 0.0216$ Å$^{-3}$. Energies are expressed in degrees Kelvin, and lengths in Å.

With interatomic potentials that have a hard core, we may use the same function $\varphi_A$ as for free fermions, but we now also need a Jastrow product. With $\varphi_S = \varphi_S(\vec{R}) = \prod_{i<j} \exp[-(b/r_{ij})^5]$, the guiding functions now have the form

$$\psi_G^\pm(\vec{R}) = \varphi_S(\vec{R})[\sqrt{1 + c^2\varphi_A^2(\vec{R})} \pm c\varphi_A(\vec{R})]. \quad (14)$$

In Fig. 1 we plot the *cumulative* denominator as a function of imaginary time for a typical run. A stable calculation will exhibit linear growth; the fundamental stability of the method is well demonstrated. Figure 2 shows the decay of the same denominator, plotting the *differential* values when the method is made unstable by setting $c = 0$.

Table II exhibits the eigenvalues of various runs with our method applied to the periodic system with 14 $^3$He atoms. They are all consistent and yield a weighted average of $-2.2558(39)$. The run marked (b) is a continuation of the run labeled (a) separated by a long run with a longer time step. As a whole, including such continuations, the longest aggregate sequence comprises a total imaginary time of 1830 K$^{-1}$. Using a total system energy difference of 20 K (as we have measured), that corresponds to $3.6 \times 10^4$ fermion decay times. An alternative measure of the length of the run, suggested by Ceperley [14], is the ratio

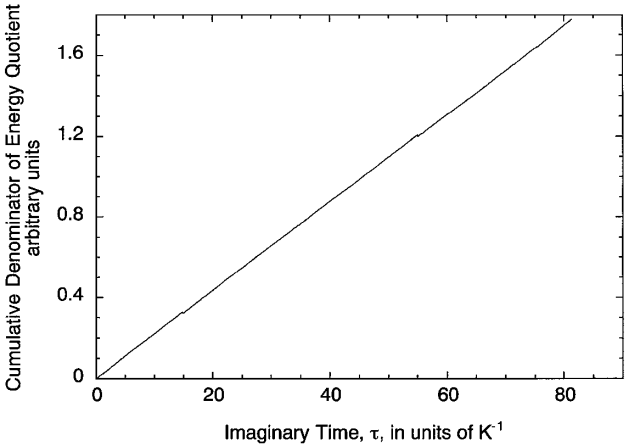


FIG. 1. Cumulative denominator of energy quotient: a stable calculation. Imaginary time in inverse degrees Kelvin.

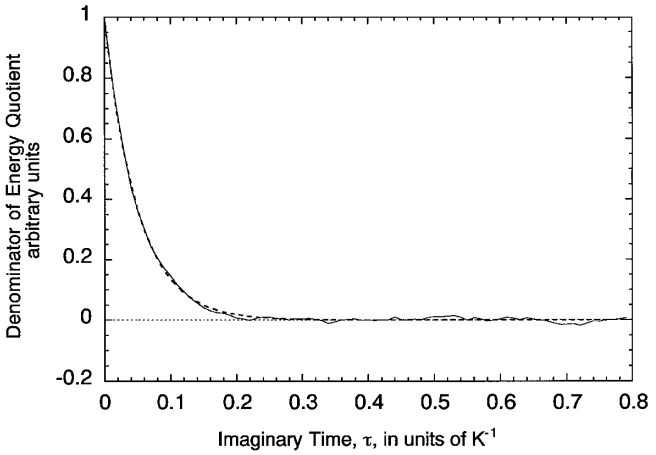


FIG. 2. Denominator of energy quotient: an unstable calculation. The smooth curve is $\exp(-20.08\tau)$, a fit to the data. Imaginary time in inverse degrees Kelvin.

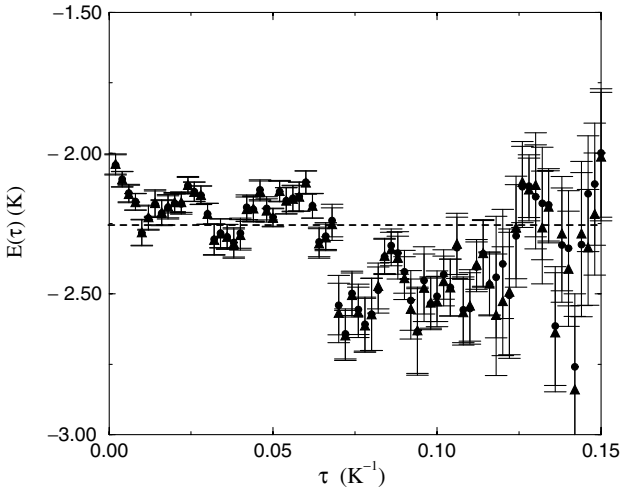


FIG. 3. Relaxation of eigenvalue from fixed node: a transient calculation. The dashed line shows the mean obtained by our fermion Monte Carlo, −2.256. Imaginary time in inverse degrees Kelvin.

of the rms diffusion length of a particle to the mean spacing between particles. For this sequence of runs, that ratio is 19. Thus the observation of stable values of the sums in Eq. (4) is significant.

Space limitations preclude a complete description of the other checks that we have made that the results for $^3$He are correct: they include a fixed node calculation of exactly the same model problem, which yielded an eigenvalue of −2.08(1) K. A transient estimate (cf. Fig. 3), relaxing from the fixed node, is consistent with our result (shown as the dashed line). Analysis of the results in Fig. 2 leads to a fermion-boson energy difference of 1.434(35) K per particle. When combined with the fermion result above, this agrees well with a direct calculation of the energy of a 14-body mass-3 boson system that gave −3.68(1) K. Finally, we may mention that the method has proved stable and correct in treating some simple atomic [15] and molecular [16] systems.

By construction, the method proposed here introduces no approximations other than that of the short imaginary-time Green's function. In other words, if the results are stable, then they are correct. Although we have have not yet proved the stability of the method (i.e., that the long-term average of the denominator of the eigenvalue quotient is not zero), we believe that we have convincingly demonstrated the stability. Perhaps the most important conclusion that we may draw is that the sign problem of fermion Monte Carlo for continuous systems is not intractable; the search for elegant computational methods in this and related applications is justified.

TABLE II. Energies and errors for a periodic system of 14 $^3$He atoms.

| $b$, Å | $c$ | $\lambda_B$ | $E, K$ |
|---|---|---|---|
| 2.939 | 0.025 | 0 | −2.251(08)[a] |
| 2.927 | 0.025 | 0 | −2.258(17) |
| 2.901 | 0.025 | 0 | −2.257(10) |
| 2.939 | 0.016 | 0 | −2.246(20) |
| 2.939 | 0.010 | 0 | −2.250(19) |
| 2.939 | 0.025 | 0 | −2.2559(84)[b] |
| 2.939 | 0.025 | −0.05 | −2.249(12) |
| 2.9395 | 0.025 | 0.05 | −2.268(10) |

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