Reptation Quantum Monte Carlo: A Method for Unbiased Ground-State Averages and Imaginary-Time Correlations

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We introduce a new stochastic method for calculating ground-state properties of quantum systems. Segments of a Langevin random walk guided by a trial wave function are subject to a Metropolis rejection test performed on the time integral of the local energy. The algorithm—which is as simple as variational Monte Carlo—for bosons provides *exact* expectation values of local observables, as well as their static and dynamic (in imaginary time) response functions, without mixed-estimate nor population-control biases. Our method is demonstrated with a few case applications to ^{4}He. [S0031-9007(99)09325-4]

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The analogies existing between the classical diffusion equation and the quantum imaginary-time Schrödinger equation constitute the basis of a simulation method—known as *diffusion Monte Carlo* (DMC)—which has been successfully applied to the study of interacting bosons and fermions at zero temperature [1,2]. The DMC crucially relies on *importance sampling*, i.e., on letting the diffusing walkers be guided by our prior knowledge of some approximate wave function, Φ_0, for the system under study. The resulting stochastic process consists of a (biased) diffusion term plus a *branching* term which determine the variation of the local number of random walkers. Sampling the asymptotic distribution of the random walk allows one to calculate the ground-state energy exactly within statistical noise (at least for bosons). However, the calculation of observables which do not commute with the Hamiltonian requires the so-called *mixed estimate* [2]—a procedure which is biased by the trial function. One can remove this bias and obtain information on imaginary-time correlations by the *forward walking* technique [3] which, however, substantially increases the statistical noise. The control of the walker population introduces a further systematic error [1,2] whose elimination [2] leads to additional fluctuations.

In this paper we propose a new method, named *reptation quantum Monte Carlo* (RQMC) [4], which avoids the above difficulties by exploiting the *dynamical properties* of the classical diffusion process—rather than retaining the asymptotic distribution alone—and mapping them onto the (imaginary-time) dynamical properties of the quantum system of interest. In the following we first discuss the formalism starting from classical diffusion as described by the Langevin equation; we then outline an algorithm suitable for practical implementations, and, finally, we present results for superfluid ^{4}He which are meant to be representative of the potential of the method.

The time-discretized Langevin equation,

$$x(\tau + \epsilon) = x(\tau) + f(x(\tau))\epsilon + \xi(\tau), \qquad (1)$$

describes the motion in configuration space under a deterministic force $f(x)$ and a white noise ξ [$\langle\xi(\tau)\rangle = 0$, $\langle\xi(\tau)\xi(\tau')\rangle = 2\epsilon\delta_{\tau\tau'}$]. For notational simplicity, in Eq. (1) and in the following, we consider a one-dimensional system, the generalization to many dimensions being straightforward. The process described by Eq. (1) is readily simulated by a pseudorandom walk with transition probability $\mathcal{W}_\epsilon(x\,|\,y) \propto \exp\{-[x - y - f(y)\epsilon]^2/4\epsilon\}$. The associated Fokker-Planck equation for the probability distribution, $P(x,\tau)$, in the continuous limit reads

$$\frac{\partial P(x,\tau)}{\partial \tau} = \frac{\partial^2 P(x,\tau)}{\partial x^2} - \frac{\partial}{\partial x}\left[f(x)P(x,\tau)\right]. \qquad (2)$$

With the identifications $f(x) = 2\partial[\log\Phi_0(x)]/\partial x$ and $P(x,\tau) = \Phi(x,\tau)\Phi_0(x)$, Eq. (2) is formally equivalent to a Schrödinger equation in imaginary time, $-\partial\Phi(x,\tau)/\partial\tau = \mathcal{H}\Phi(x,\tau)$, for the wave function Φ, with a *fictitious* Hamiltonian $\mathcal{H} = -\partial^2/\partial x^2 + \Phi_0^{-1}(\partial^2\Phi_0/\partial x^2)$ (here and in the following we set $\hbar^2/2m = 1$). It can be verified by inspection that (i) the *trial function* Φ_0 is the ground-state of $\mathcal{H}$ with eigenvalue 0; (ii) the asymptotic solution of Eq. (2) is $P(x, \tau \to \infty) = \Phi_0^2(x)$; and (iii) the transition probability $\mathcal{W}_\epsilon$ of the random walk is a short-time approximation for the importance-sampled propagator of $\mathcal{H}$, namely, $\mathcal{W}_\epsilon(x\,|\,y) = \Phi_0(x)\langle x|e^{-\epsilon\mathcal{H}}|y\rangle\Phi_0(y)^{-1} + \mathcal{O}(\epsilon^2)$. Because of property (ii), Eq. (1) can be used in the so-called variational monte carlo (VMC) method to sample Φ_0^2; in addition, because of (iii), the Langevin equation (1) describes the imaginary-time dynamics generated by the fictitious Hamiltonian $\mathcal{H}$, for $\epsilon \to 0$.

The difference between the true Hamiltonian H and $\mathcal{H}$ is the *local energy* associated with the trial function, $\mathcal{E}(x) = \Phi_0(x)^{-1}H\Phi_0(x)$. In order to recover from the Langevin dynamics the correct imaginary-time evolution generated by the true Hamiltonian H, we invoke a generalization of the Feynman-Kac formula [5]:

$$\langle\Phi_0|e^{-\tau H}|\Phi_0\rangle = \int e^{-S[X]}\mathcal{P}[X]\mathcal{D}[X] + \mathcal{O}(\epsilon), \qquad (3)$$

where $X \equiv \{x_0, x_1, \ldots, x_N\}$ indicates a time-discretized path generated by the random walk, $N = \tau/\epsilon$, $\mathcal{P}[X] \equiv \mathcal{W}_\epsilon(x_N, x_{N-1}) \times \cdots \times \mathcal{W}_\epsilon(x_1, x_0)\Phi_0(x_0)^2$ is the corresponding joint probability distribution, $S[X] = \epsilon[\frac{1}{2}\mathcal{E}(x_0) + \mathcal{E}(x_1) + \cdots + \mathcal{E}(x_{N-1}) + \frac{1}{2}\mathcal{E}(x_N)]$ is the (discretized) integral of the local energy along the path, and the integral $\int \mathcal{D}[X]$ is calculated over all of the paths generated by the random walk.

The ground-state energy E_0, the expectation values of local operators $O(x)$, and the corresponding generalized susceptibilities can be obtained by differentiation from the *pseudo-partition-function* $\mathcal{Z}_0 = \langle\Phi_0|e^{-H\tau}|\Phi_0\rangle$. For example, one has

$$E_0 = -\lim_{\tau\to\infty}\frac{d}{d\tau}\log\mathcal{Z}_0 = \lim_{\tau\to\infty}\frac{\langle\mathcal{E}(\tau)e^{-S[X]}\rangle}{\langle e^{-S[X]}\rangle}, \quad (4)$$

where $\langle\cdots\rangle$ denotes the average over the probability distribution $\mathcal{P}[X]$.

This formalism (worked out in more detail elsewhere [4]) is the basis for the pure diffusion Monte Carlo method (PDMC) [6], in which weighted averages such as Eq. (4) are directly accumulated. Since the local energy is an extensive quantity, the fluctuations of the weights grow exponentially with the system size, and PDMC simulations are bound to fail but for the smallest systems.

The RQMC offers a cure for the fluctuating weight problem, *without* losing information on the dynamics of classical diffusion. This is achieved using a generalized Metropolis rejection method [7] to sample the *product* $P[X] \equiv \mathcal{P}[X]e^{-S[X]}$, rather than $\mathcal{P}[X]$ alone. The basic variable of our algorithm is a *path*, $X = \{x_0, x_1, \ldots, x_N\}$, whose length in imaginary time, $N = \tau/\epsilon$, is chosen so large that the limit $\tau \to \infty$ in Eqs. (6) and (7) is reached within the desired accuracy. We refer to this object as a *reptile* [8]. Given a reptile, X, we generate a new one, Y, by chopping off from its tail a piece of length $\delta = M\epsilon$ ($M < N$), and by sticking on its head a piece of equal length, built up of M steps of the Langevin dynamics (1). The action by which the new reptile Y is generated from X is called *reptation* [8], and we indicate the corresponding transition probability by $W^0[Y, X]$. Iterating the reptation move, the resulting asymptotic distribution for the reptile is, by construction, $\mathcal{P}[X]$. One can sample $\mathcal{P}[X]e^{-S[X]}$ instead, interpreting W^0 as a *proposal* for a move, and letting the proposal pass an acceptance test, so as to impose detailed balance with respect to $P[X]$. The resulting acceptance probability is [7]

$$A[Y, X] = \min\{1, W^0[X, Y]P[Y]/(W^0[Y, X]P[X])\} = \min\{1, e^{-S[Y]}/e^{-S[X]}\}. \quad (5)$$

By explicitly including the acceptance test in the dynamics of the random walk, the weights $e^{-S[X]}$ drop out of the averages. For example, the expression for the ground-state energy, Eq. (4), becomes

$$E = \lim_{\tau\to\infty}\langle[\mathcal{E}(0) + \mathcal{E}(\tau)]\rangle/2, \quad (6)$$

where the average $\langle\cdots\rangle$ is now over the *reptile* random walk whose dynamics is given by reptation supplemented with the Metropolis acceptance test described above (and a time-symmetrized form of the estimator has been used). Analogously, expectation values of local operators $O(x)$ and their imaginary-time correlations $C_{12}(\tau) = \langle O_1(\tau)O_2(0)\rangle$ can be cast in the form

$$\langle O\rangle = \lim_{\tau\to\infty}\left\langle\int_\sigma^{\tau-\sigma}\frac{O(\tau')\,d\tau'}{\tau - 2\sigma}\right\rangle$$
$$\langle C_{12}(\tau)\rangle = \lim_{\tau'\to\infty}\left\langle\int_\sigma^{\tau'-\tau-\sigma}\frac{O_1(\tau'' + \tau)O_2(\tau'')\,d\tau''}{\tau' - \tau - 2\sigma}\right\rangle. \quad (7)$$

The average of $O(x)$ taken at one end of the path, $\langle\Phi_0|Oe^{-H\tau}|\Phi_0\rangle/\mathcal{Z}_0$, is the mixed estimate [2]. In the time integrals of Eq. (7), the exclusion of two portions of length σ from the head and tail of the reptile makes the convergence to the unbiased estimates faster.

The implementation of the algorithm is very simple, at the level of a VMC simulation. The initial configuration of the reptile is just a segment of a random walk generated with the Langevin equation, and the simulation proceeds as follows: (1) Select a "direction of time" (*forward* or *backward*) with equal probability. If the choice is *backward*, set $X \leftarrow \bar{X} = \{x_N, x_{N-1}, \ldots, x_0\}$. This step is introduced to enforce detailed balance at each reptation move. (2) Using the Langevin equation, generate a new segment of the reptile corresponding to the time interval $[\tau, \tau + \delta]$ to get $Y = \{x_M, x_{M+1}, \ldots, x_{M+N}\}$. The value of δ is sampled from a uniform deviate in the interval $[0, \Delta]$ whose width is chosen so as to minimize the autocorrelation times of the measured quantities. (3) Evaluate $A[Y, X]$ according to Eq. (5) and set $X \leftarrow Y$ with probability A. (4) Accumulate the ground-state energy and other observables using Eqs. (6) and (7); go to (1).

The efficiency of the algorithm obviously depends on the quality of the trial function. The relaxation time of the reptile is proportional to $\tau^2/\langle\delta\rangle$, where $\langle\delta\rangle$ is the average length of the reptation moves. In the limit of perfect importance sampling the local energy is constant, so that moves of arbitrary length will be accepted with probability one and the algorithm achieves an optimal efficiency with $\langle\delta\rangle = \tau$. With a necessarily approximate trial function, the acceptance rate for a fixed length of the reptation move δ will decrease with an increasing number of particles N_P. Therefore, for large N_P, one is forced to decrease δ, thus deteriorating the efficiency of the algorithm. However, even the branching algorithm suffers from the same pathology, and the issue is whether simulations are feasible for system sizes of *practical* interest. Among various conceptually similar techniques [6,9,10], the variational path integral (VPI) method has a better asymptotic scaling with N_P, because it does not suffer from uncontrolled fluctuations of the local energy [9]. However for systems of $\sim$100 ^{4}He atoms, for which it has been tested, VPI is far less efficient than RQMC [11].

A preliminary test of the RQMC algorithm has been performed for the hydrogen atom with an approximate

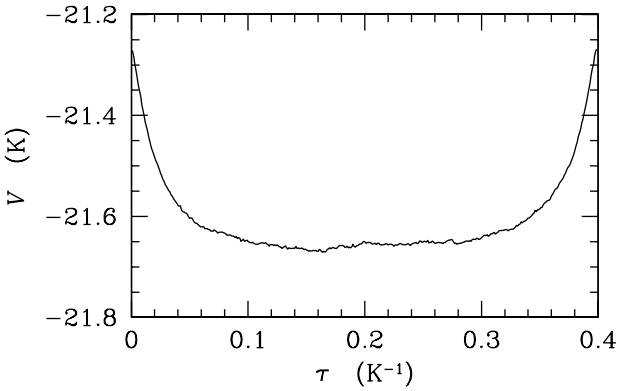

FIG. 1. Average of the potential energy in ^{4}He, calculated on individual time slices along the path. The statistical error on the central slices is ≃0.03 K. This result was obtained using a trial function with pair correlations only: Note that V converges to the same value given in Table I, obtained using a trial function with pair and triplet correlations.

trial function, reproducing exact results for several moments of electron-nucleus distance. As a demonstration, we now present the calculation of several properties of superfluid ^{4}He, showing that the method can be successfully applied to systems of actual physical interest.

We simulate $N_P = 64$ ^{4}He atoms in a cubic box with periodic boundary conditions at the equilibrium density, $\rho = 0.02186$ Å^{-3}. The particles interact with a realistic pair potential obtained from first-principles calculations [12]. Most of the simulations use a trial function Φ_0 with pair and nearly optimal three-body correlations [13]. We compute E_0, the potential energy V, the diffusion coefficient of the center of mass motion $D(\tau) = \langle[\mathbf{r}_{\rm CM}(\tau) - \mathbf{r}_{\rm CM}(0)]^2\rangle N_P/(6\tau)$, and the imaginary-time correlations of the density fluctuation operator $F(q,\tau) = \langle\rho_q(\tau)\rho_{-q}(0)\rangle/N_P$, where $\rho_q = \sum_i \exp(-i\mathbf{q}\cdot\mathbf{r}_i)$.

The time step is $\epsilon = 0.001$ K^{-1}, which gives a systematic bias of the order of 10^{-2} K on the total energy. E_0 and V are well converged for $\tau = 0.4$ K^{-1}, corresponding to $N = 400$ time slices. For the calculation of $F(q,\tau)$ a longer path with $N = 700$ is used. The number of time slices of each reptation move is uniformly sampled between 0 and 20, yielding an acceptance ratio of ≈80%. In the averages (7) for V and $F(q,\tau)$, we exclude the contributions from 150 time slices on each side of the path. The convergence of V from the mixed estimate at slice 0 or N to the unbiased estimate is shown in Fig. 1.

Our results for E_0 and V are listed in Table I, together with the corresponding data obtained from a branching DMC calculation using the same time step and trial function. Here the branching evaluation of V is complemented with forward walking, implemented in the "backward storing" mode [10]. From the estimated statistical error we infer that reptation is roughly 3 times slower than branching for the calculation of E_0, but twice as fast for V. This comparison, far from being a conclusive statement of relative efficiency, still suggests that, whenever explicit information on imaginary-time correlations is used, RQMC is likely to be competitive or better.

TABLE I. Ground-state energy, E_0, and potential energy, V, in ^{4}He, computed from RQMC and branching DMC runs of 3×10^6 Monte Carlo steps with $\epsilon = 0.001$ K^{-1}. The length of the path in the RQMC calculation is $\tau = 0.4$ K^{-1}, and the length of the forward walk for V in the diffusion Monte Carlo calculation is 0.2 K^{-1}. The extrapolation of E_0 to $\epsilon \to 0$ yields −7.3789(15) for RQMC and −7.3812(14) for DMC. The overestimate of the experimental binding energy, −7.17 K, is due to neglect of three-body forces, mostly triple-dipole repulsion, in the interparticle potential adopted [12].

	E_0 (K)	V (K)
RQMC	−7.4066(27)	−21.644(15)
DMC	−7.3902(15)	−21.674(21)

From the density-density correlation function $F(q,\tau)$ we obtain the static structure factor $S(q) = F(q,0)$ and the static linear response function $\chi(q) = -2\int_0^\infty F(q,\tau)\,d\tau$, both shown in Fig. 2. In particular, the present calculation of the response for a Bose system is remarkably simple and efficient in comparison with the standard route utilized so far with branching algorithms [14] (note that at virtually no additional cost more q vectors could have been included in the calculation). The agreement with the measured $S(q)$ and $\chi(q)$ [15] is excellent. The

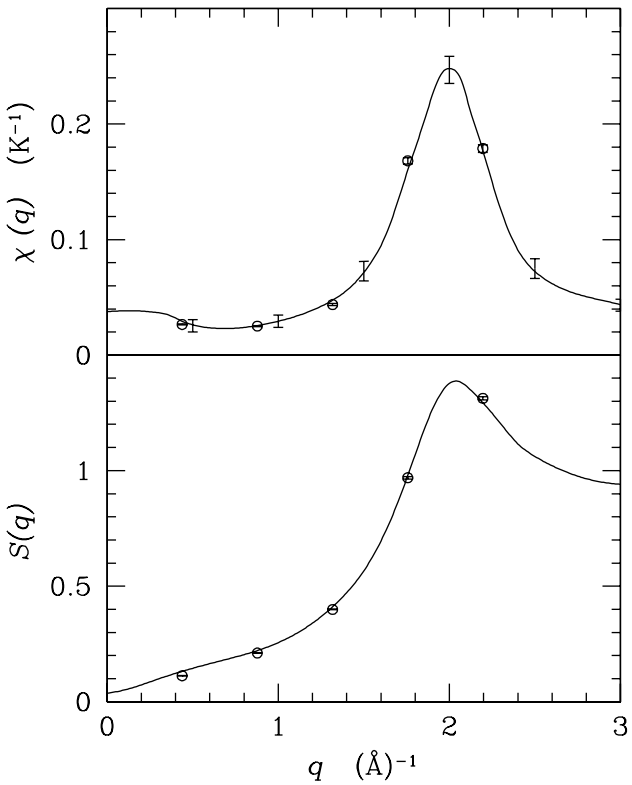

FIG. 2. Computed (open circles) and measured[15] (solid lines) static structure factor (upper panel) and static linear response function (lower panel). The discrepancy in $S(q)$ at the smallest value of q is due to the finite temperature of the experimental setup.

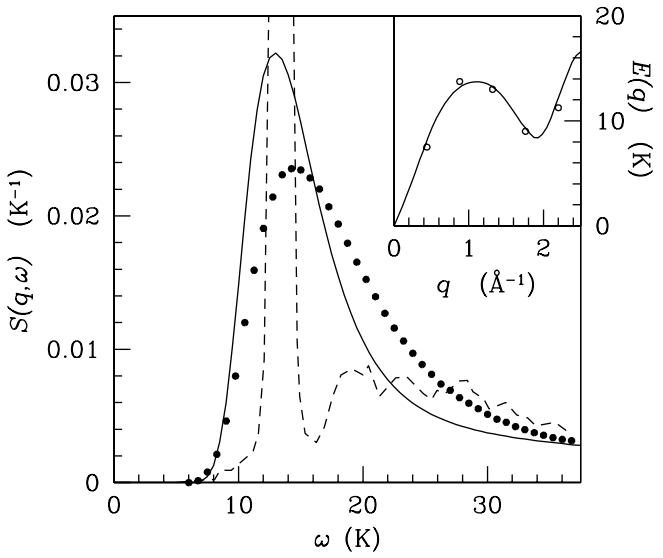

FIG. 3. The ME reconstruction of the dynamical structure factor of ^{4}He at $q = 1.32$ Å^{-1} (solid line). The dotted line is the result of a path integral Monte Carlo calculation [17], and the dashed line is the measured $S(q, \omega)$. The inset compares the positions of the ME peaks at various wave vectors (open circles) with the experimental excitation spectrum.

f-sum rule, $\partial F(q,t)/\partial\tau|_{\tau=0} = q^2$, is also fulfilled with high precision.

Inferring the dynamical structure factor $S(q, \omega)$ requires an inverse Laplace transform, $F(q,\tau) = \int_0^\infty S(q,\omega)\exp(-\omega\tau)\,d\omega$. We perform a maximum entropy (ME) analysis [16] of our data, with results similar to those obtained in Ref. [17]. The ME reconstruction of $S(q, \omega)$, shown in Fig. 3, is too smooth and does not reproduce the sharp features exhibited by the experimental structure factor in the superfluid phase. Some known properties of the spectrum are recovered: The presence of a gap in the excitation spectrum is clearly revealed, and the position of the peak of the reconstructed dynamical response closely follows the measured dispersion of the elementary excitations [4,17]. However, the general reliability of the ME analysis as a *predictive* tool, with the statistical accuracy of the data typically achieved from the simulation of continuum systems, is hard to assess.

We finally outline the calculation of the superfluid density ρ_s. The superfluid transition is of interest even at zero temperature, for instance, in the presence of an external disordered potential $V_{\rm ext}$. We can compute ρ_s from the diffusion coefficient of the center of mass motion, $\rho_s/\rho = \lim_{\tau\to\infty} D(\tau)$, which is the zero temperature limit of the winding number estimator used in path integral simulations [9]. We consider a model system of static impurities in ^{4}He represented by attractive Gaussians placed at random sites and we observe that the computed ρ_s, which is correctly one for the pure system, is indeed reduced in the presence of the impurities [4].

Based on our limited experience, the RQMC method features distinct advantages over standard branching DMC. Clusters, films, and superfluids in restricted geometries are natural candidates for further applications. For Fermion problems, the fixed-node approximation [1,2] can be used to cope with the sign problem. The dynamical information contained in the path is, in this case, incorrect [6], but the algorithm is still free from the mixed estimate and the population control biases. Furthermore, because it samples an explicit expression for the imaginary time evolution, RQMC gives access to quantities obtained by differentiation, for instance, a low-variance estimator of electronic forces [18].

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