Efficient Monte Carlo Procedure for Systems with Fermions

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A new Monte Carlo approach applicable to systems with fermion and boson degrees of freedom is proposed. The main advantage of the method is its speed: For systems in one space and one time dimension (1 + 1) the calculation reduces to doing Monte Carlo computations on a two-dimensional classical system with local interactions. Here the potential of the method is illustrated by application to various (1 + 1)-dimensional systems.

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There has recently been considerable interest in the application of Monte Carlo techniques to the study of systems with coupled boson and fermion degrees of freedom.[1-6] The most common approach has been to integrate out the fermion variables and evaluate the resulting fermion determinant exactly or approximately in as efficient a manner as possible. This approach leads to computer calculations which are considerably more time consuming than for pure boson theories.

In this paper we propose a new Monte Carlo technique which has proven to be very efficient for (1+1)-dimensional systems, and which we believe can be extended to higher numbers of dimensions. Because we work with the canonical ensemble for the fermions rather than the grand canonical ensemble, we avoid the time-consuming process of evaluating a fermion determinant. Our work is closest in spirit to the method of Suzuki, Miyashita, and Kuroda[7] for the study of quantum spin systems by Monte Carlo techniques. A modification of that procedure has also recently been introduced by Raedt and Lagendijk to study a fermion model.[8]

For simplicity we will first discuss a pure fermion theory. The partition function for N fermions can be written in the form

$$Z_N = \mathrm{Tr}_N e^{-\beta H} = \sum_{i_1 \cdots i_L} \langle i_1 | e^{-\Delta\tau H} | i_2 \rangle \langle i_2 | e^{-\Delta\tau H} | i_3 \rangle \cdots \langle i_L | e^{-\Delta\tau H} | i_1 \rangle . \tag{1}$$

Here we have written $\Delta\tau = \beta/L$ and introduced a complete set of states at each time slice. The next step is to find a simple prescription for evaluating the matrix elements of $e^{-\Delta\tau H}$. To this end we write the Hamiltonian in the form $H = H_1 + H_2$ and note that $\exp(-\Delta\tau H) \simeq \exp(-\frac{1}{2}\Delta\tau H_1)\exp(-\Delta\tau H_2)\exp(-\frac{1}{2}\Delta\tau H_1)$ with an error of order $(\Delta\tau)^3$. Then inserting additional intermediate states we can write

$$Z_N = \sum_{i_1 \cdots i_{2L}} \langle i_1 | e^{-\Delta\tau H_1} | i_2 \rangle \langle i_2 | e^{-\Delta\tau H_2} | i_3 \rangle \langle i_3 | e^{-\Delta\tau H_1} | i_4 \rangle \cdots \langle i_{2L} | e^{-\Delta\tau H_2} | i_1 \rangle . \tag{2}$$

What distinguishes our approach from others[7,8] is the choice of a breakup of H which provides for a simple evaluation of matrix elements, no sign problems in 1 + 1 dimensions, and an efficient implementation of the conservation laws contained in H. Since a large number of possible changes in the fermion configuration are forbidden by such conservation laws, it is essential to build them in from the start in order to have an efficient Monte Carlo algorithm. We propose a real-space breakup for H such that H_1 and H_2 are composed of sums of *nonoverlapping* cell Hamiltonians. Explicitly, for a system in 1 + 1 dimensions with short-range interactions we take

$$\begin{aligned} H_1 &= \textstyle\sum_p H(2pn, 2pn+1, \ldots, 2pn+n) \\ H_2 &= \textstyle\sum_p H(2pn+n, 2pn+n+1, \ldots, 2(p+1)n), \end{aligned} \tag{3}$$

where $H(i, i+1, \ldots, i+n)$ contains only operators at sites $i, i+1, \ldots, i+n$. Note that for a Hamiltonian with interactions of range less than or equal to n, H_1 and H_2 are composed of sums of pieces that commute between themselves. Thus, the evaluation of the matrix elements in Eq. (2) reduces to solving an n-site problem. Ordinarily

it is only possible to express the matrix elements that appear in Eq. (1) as a sum of terms with alternating signs corresponding to the number of crossings of the world lines for the fermions. However, the simpler matrix elements of Eq. (2) can be evaluated in closed form and in the $(1+1)$-dimensional models that we have studied to date are positive definite. Here we will consider only nearest-neighbor Hamiltonians where it suffices to take $n=1$.

In Fig. 1 we show a typical $(1+1)$-dimensional lattice. The shaded regions indicate sites which are connected by the time evolution operator. The sum over intermediate states in Eq. (2), which is to be performed by importance sampling, corresponds to a sum over all possible arrangements of the fermions at each time slice. In performing these sums we must take into account fermion number conservation. To this end we draw world lines for each fermion as shown in Fig. 1. Because fermion number is conserved within each shaded box, a world line can only be moved at a given time interval if it is running along a vertical edge of a shaded box. In that case it can be moved across the adjacent unshaded box. The Boltzmann factor for such a move depends only on the occupation of four neighboring sites, so that the process is comparable to a Monte Carlo calculation on a two-dimensional classical nearest-neighbor Ising model.

The updating algorithm described above samples all possible states in a system with free-end boundary conditions, but in the case of periodic boundary conditions it neglects states for which the nth fermion arrives at the initial position of the $(n\pm1)$st fermion after $L=\beta/\Delta\tau$ time steps.

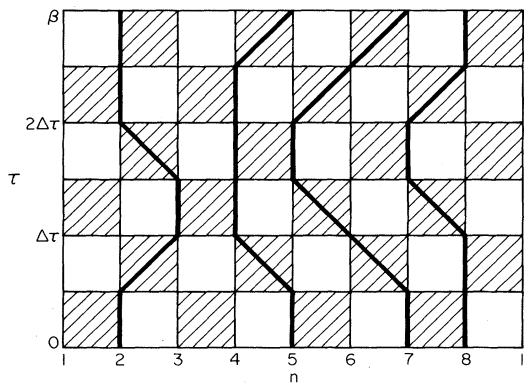

FIG. 1. The $n-\tau$ checkerboard lattice for a ring of eight spatial sites and three time slices $3\Delta\tau=\beta$. World lines for $N=4$ fermions are shown.

TABLE I. Internal energy per site for 20 noninteracting electrons ($t=1$, $U=0$) on a 40-site periodic lattice at various temperatures. $E_{(\text{exact})}$ and E_{CB} give results obtained from numerically evaluating the canonical and checkerboard partition functions, respectively. E_{MC} lists the Monte Carlo results obtained from 10 000 measurements each separated by 5 lattice sweeps. For E_{CB} and E_{MC}, $\Delta\tau=0.1$.

T	$E_{(\text{exact})}$	E_{CB}	E_{MC}
0.5	−0.5659	−0.5668	−0.5668 ± 0.0032
1.0	−0.4141	−0.4148	−0.4162 ± 0.0030
2.5	−0.1971	−0.1975	−0.1979 ± 0.0023

However, it can be shown that the error in omitting such states is negligible for large systems. This is confirmed by our numerical results.

As a first example we apply this formalism to a one-dimensional spinless fermion model with nearest-neighbor interactions:

$$H=-t\sum_i[c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i]+U\sum_i n_i n_{i+1}. \quad (4)$$

This model is equivalent, via a Jordan-Wigner transformation, to the spin-$\frac{1}{2}$ XXZ model.[9] We consider only the half-filled-band case here for definiteness and treat a periodic ring of M sites. For $U\leq 2$ the infinite system has algebraic order and has no gap, while for $U>2$ a charge-density wave develops and a gap in the spectrum opens up.

In Table I we show the internal energy for the free-fermion case ($U=0$). We also list E_{CB} in Table I which is the exact result for the trace over

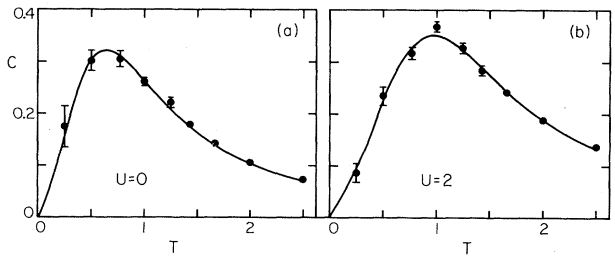

FIG. 2. (a) The specific heat per site for a 40-site periodic lattice containing 20 noninteracting electrons ($t=1$, $U=0$). The solid line is a numerical calculation of specific heat in a canonical ensemble. The points are the results of a Monte Carlo calculation of 10 000 averages with 5 lattice sweeps between each average. (b) The specific heat per site for 20 electrons on a 40-site periodic lattice with $t=1$ and $U=2$ corresponding to the isotropic Heisenberg antiferromagnet. The solid line is the finite-cell extrapolation of Bonner and Fisher (Ref. 10).

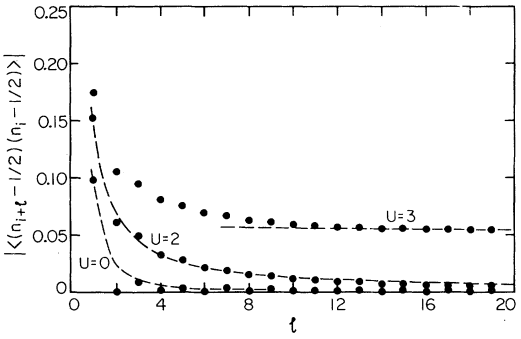

FIG. 3. The magnitude of the particle-particle correlation function $|\langle(n_{i+l}-\frac{1}{2})(n_i-\frac{1}{2})\rangle|$ for 20 electrons on a 40-site lattice for $U=0$, 2, and 3. The errors fall within the dots. The dashed lines give the asymptotic behavior for the different cases: l^{-2} for $U=0$, l^{-1} for $U=2$, and the $M\to\infty$ extrapolation Ref. 10.

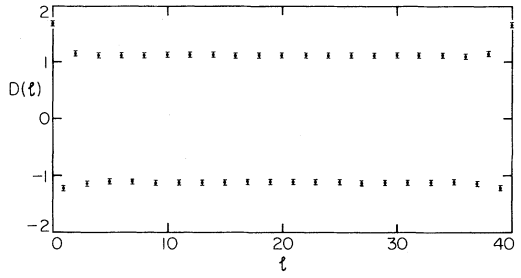

FIG. 4. The equal-time lattice displacement-displacement correlation function $D(l)=\langle\varphi_0\varphi_l\rangle$ showing the dimerization structure for a 40-site lattice.

all states using the breakup of Eq. (3) with $n=1$. As can be seen, these and the Monte Carlo results agree with the exact result for a 40-site lattice remarkably well. In Fig. 2 we show the specific heat for the cases $U=0$ and $U=2$, compared, respectively, with exact results for the canonical ensemble and with extrapolation from finite-cell calculations by Bonner and Fisher.[10]

In Fig. 3 we show the low-temperature ($\beta=4$) spatial decay of the magnitude of the density-density correlation function $|\langle(n_{i+l}-\frac{1}{2})(n_i-\frac{1}{2})\rangle|$ for the cases $U=0$, $U=2$, and $U=3$. The exact results for $U=0$ on a 40-site lattice with 20 electrons fall within the dots. The dashed lines show the asymptotic zero-temperature envelopes for an infinite lattice. For $U=0$ and $U=2$ this varies as l^{-2} and l^{-1}, respectively. For $U=0$ and l even the correlation function vanishes. This result is reproduced by the Monte Carlo calculations. For $U=3$ one is in the ordered region and the correlation function decays exponentially to a finite value. The dashed line labeled $U=3$ corresponds to the $M\to\infty$ extrapolation by Bonner and Fisher.[10]

Finally, we consider an example of a coupled boson-fermion system with a partition function[2]

$$Z_N=\int D\varphi(\tau)\exp\{-\int_0^\beta d\tau\sum_i[\tfrac{1}{2}\dot{\varphi}_i^2(\tau)+\tfrac{1}{2}\Omega^2\varphi_i^2(\tau)]\}\times \mathrm{Tr}_N\Big(T_\tau\exp\{-\int_0^\beta d\tau[\sum_i\lambda\varphi_i(\tau)(c_i^\dagger c_i-\tfrac{1}{2})-t\sum_i(c_i^\dagger c_{i+1}+\mathrm{H.c.})]\}\Big). \quad (5)$$

Here the boson field φ is functionally integrated over in the usual way while the fermion part is left as a trace over τ-ordered operators. We then decompose the trace over the fermion degrees of freedom in the form described above and do a Monte Carlo calculation over both the bosons and fermions simultaneously. As an illustrative example, we show in Fig. 4 the equal-time correlation function for the boson field,

$$D(l)=\langle\varphi_0\varphi_l\rangle, \quad (6)$$

for the case of a 40-site lattice with $\beta=4$, $\Omega=0.5$, $\lambda=1.4$, and $t=1$. The time slices are taken to be $\Delta\tau=0.5$. These parameters have been chosen so that the ground state exhibits a well-developed Peierls distortion which is clearly seen in Fig. 4.

The main advantage of our method over previous methods is its speed. For systems in $1+1$ dimensions, the number of operations it takes to update a site in the lattice is of order 1, that is $L\times M$ operations per Monte Carlo sweep. By comparison, the most naive evaluation of the fermion determinant would involve $(L\times M)^4$ operations per sweep. A more sophisticated approach[2] which made use of the local nature of the coupling required $L\times M^3$. To evaluate the fermion determinant by another Monte Carlo procedure involves $L\times M\times n$ steps per sweep with n possibly a large number and introduces additional approximations.[1] It should also be emphasized that our approach does not require the fermion Hamiltonian to be bilinear. This is an important advantage since it avoids the necessity of introducing auxiliary boson fields to treat fermion-fermion interactions. Finally, although we have shown equal-time correlation functions it is just as simple to calculate correlations on different τ slices. As discussed in Ref. 2, this provides dy-

namic information.

We are currently investigating the application of the present method to higher-dimensionality systems. The minus signs and resulting cancellations ordinarily associated with Fermi statistics do arise for two or more space dimensions. However, a major part of the cancellation will automatically be taken into account by our breakup method, so that we expect our approach to be applicable. Our Monte Carlo algorithm will remain local in more dimensions so that the time required for the calculation will be comparable to that for a boson Monte Carlo calculation. In 1+1 dimensions, there are many interesting models in condensed-matter physics involving electron-electron and electron-phonon interactions, as well as in high-energy physics with fermion and gauge field degrees of freedom, some of which are presently under investigation.

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Vibrational Overtone Absorption in Solid Hydrogen

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The first measurements of the second-overtone absorption spectrum of solid n-H_2 are reported. The observed frequencies and line strengths are not predicted from the known high-pressure gas data, but the trend is consistent with similar data for the fundamental band. The observation of this very weak optical absorption provides important data for reexamination and extension of theoretical treatment of this important molecular solid.

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Overtone spectra of fundamental vibrational modes in condensed phases of large molecules such as benzene,[1,2] methane,[3,4] and ethylene[5] have been extensively studied. The strength of overtone absorption in these molecules arises from the single-molecule properties and the effects of collisions (or pressure) are seen only as the modification of band positions and bandwidths. Hydrogen, on the other hand, whose forbidden fundamental vibrational frequency lies in the 4150-cm^{-1} region, shows only very weak overtone spectra in the low-pressure region.[6] McKellar and Welsh[7] have summarized the high-pressure gas data for the second and third harmonics of H_2 and have shown that in the pressure region of ~30–40 amagat and at $T \approx 80$ K a description based on binary collisions reasonably explains the observed absorption strengths. Further, the single- (isolated) molecule frequencies accurately describe their spectra.

We report a study of second and third harmonics of solid H_2 in the 8000- and 12 000-cm^{-1} regions, respectively. Solid H_2 is a molecular solid in which the rotational quantum number, J, remains a good quantum number for the H_2 molecules.[8] Further, because of the small mass of H_2, molecular solid H_2 exhibits large zero-point motion. Dipole moments induced in pairs of neighboring H_2 molecules by intermolecular forces lead to infrared absorption on vibrational overtones of H_2

