Mean-Field Monte Carlo Method for Many-Body Ground States*

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ABSTRACT

A method is described for calculating the exact ground state energy of a many-body system, whether fermion or boson. The Hubbard-Stratonovich representation of the imaginary-time many-body propagator is used to express the ground-state energy as a ratio of two functional integrals. When discretized on a space-time mesh, the Monte-Carlo evaluation of this ratio is equivalent to many TDHF evolutions of the system in a random mean-field. The method is illustrated by application to a many-boson system in one dimension with a zero-range two-body interaction.

1. Introduction

Exact solutions of the many-body Schroedinger equation are of interest for several reasons. Among these are their uses as benchmarks against which to test approximation methods and as tests of a given Hamiltonian by comparison with experimental observables. To date, such solutions have been obtained for many-body ground-states using the Green's Function Monte-Carlo [1] (GFMC) or the related Path-Integral Monte-Carlo [2,3] (PIMC) approach. These methods have been applied with considerable success to liquid He [1], the electron gas [2], and three- and four-nucleon systems with state-independent potentials [3,4]. Although the GFMC and PIMC algorithms can provide a restricted description of fermion systems within the fixed-node approximation [1,2], the proper inclusion of the Pauli principle is a major difficulty in these methods and has, in fact, prevented their unrestricted application to nuclear systems with $A > 4$ or with state-dependent potentials. This is basically because the many-body wavefunction is described by a statistically evolving ensemble of configurations (specified by the coordinates of each nucleon). The Pauli principle, which enforces a spatially non-local relation between configurations which differ by the interchange

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of a pair of nucleons, is thus difficult to implement in the simple local algorithms used to evolve the ensemble.

In this note, we discuss an alternative algorithm for finding the exact ground state energy of a many-body system. It is based on a Monte-Carlo evaluation of the Hubbard-Stratonovich representation of the imaginary-time many-body propagator. Bosons and fermions are treated on the same footing. Instead of an ensemble of configurations, the many-body wavefunction is represented by a set of single-particle wavefunctions evolving in a randomly fluctuating one-body potential. As a result, anti-symmetrization for fermions can be enforced exactly.

2. Method

The basic idea behind our method is to use the imaginary-time evolution operator to filter a trial wavefunction to the exact ground state Ψ. Thus, we write the ground-state energy E_0 for a system of A particles as

$$E_0 = \lim_{T\to\infty} \frac{\langle H\Phi | e^{-HT} | \Phi\rangle}{\langle \Phi | e^{-HT} | \Phi\rangle} . \tag{2.1}$$

Here Φ is, in principle, any trial wavefunction not orthogonal to Ψ, although in practice our method is tractable only if Φ is a symmetrized product of single-particle orbitals for bosons or a Slater determinant for fermions. As in the GFMC and PIMC methods, the efficiency of MFMC calculations will be enhanced if Φ closely approximates Ψ. The many-body hamiltonian H is assumed to contain the kinetic energy and a local two-body potential:

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \tfrac{1}{2} \sum_{i\neq j=1}^{A} v(x_i - x_j). \tag{2.2}$$

(For simplicity, we write our equations assuming only one spatial dimension, x, and omit spin and isospin labels. We also put $\hbar$=1.)

Upon applying the Hubbard-Stratonovich transformation [5] to e^{-HT}, we can rewrite (2.1) as

$$E_0 = \lim_{T\to\infty} \frac{\int D[\sigma(x,t)]\, e^{\frac{1}{2}\int_0^T (\sigma, v\sigma) dt} \langle \Phi | U_\sigma | \Phi\rangle \dfrac{\langle H\Phi | U_\sigma | \Phi\rangle}{\langle \Phi | U_\sigma | \Phi\rangle}}{\int D[\sigma(x,t)] e^{\frac{1}{2}\int_0^T (\sigma, v\sigma) dt} \langle \Phi | U_\sigma | \Phi\rangle} . \tag{2.3}$$

Here, $\sigma(x,t)$ is a real field integration variable whose measure is defined in [5]. The symbol $(\sigma, v\sigma)$ denotes an inner product in which σ is thought of as a vector and v a matrix: $(\sigma, v\sigma) = \int dx\, dx' \sigma(x) v(x-x') \sigma(x')$. Finally, the evolution operator U_σ corresponds to evolution from $t=0$ to $t=T$ under the time-dependent

single-particle hamiltonian (in first-quantized notation) $h_\sigma = \frac{-1}{2m}\partial^2/\partial x^2 \pm \frac{1}{2}v(0) + \int dx' v(x-x')\sigma(x',t)$, where the -(+) refers to fermions (bosons). In essence, the Hubbard-Stratonovich transformation expresses the many-body propagator as the coherent superposition of an infinite number of one-body propagators, each involving a different one-body potential.

To evaluate (2.3) numerically, we bound space-time to a region $0 \le t \le T$, $|x| \le L/2$ and define an $(N+1)\times M$ mesh $t_i = (i-1)\Delta t$,$i=1, \cdots, N+1$ with $\Delta t = T/N$ and $x_j = (j-m/2-\frac{1}{2})\Delta x$, $j=1, \cdots, M$ with $\Delta x = L/M$ and M even. Of course, we suppose that Δx and Δt are sufficiently small. With the definition $\sigma_{ij} = \sigma(t_{i-\frac{1}{2}}, x_j)$, (2.3) can be discretized as:

$$E_0(T=N\Delta t) = \frac{\int D[\sigma_{ij}] e^{\frac{1}{2}\sum_{i=1}^{N}(\sigma,v\sigma)_i \Delta t} \langle\Phi|U_\sigma|\Phi\rangle \frac{\langle H\Phi|U_\sigma|\Phi\rangle}{\langle\Phi|U_\sigma|\Phi\rangle}}{\int D[\sigma_{ij}] e^{\frac{1}{2}\sum_{i=1}^{N}(\sigma,v\sigma)_i \Delta t} \langle\Phi|U_\sigma|\Phi\rangle}, \qquad (2.4)$$

where the measure can be taken as $D[\sigma_{ij}] = \prod_{i=1}^{N}\prod_{j=1}^{M} d\sigma_{ij}$ (any overall constants cancel in the ratio), the inner product is $(\sigma,v\sigma)_i = \sum_{j=1}^{M}\sum_{k=1}^{M} \sigma_{ij}\, v_{jk}\, \sigma_{ik} (\Delta x)^2$ with $v_{jk} = v(x_j - x_k)$, and $U_\sigma = \prod_{i=1}^{N} U_i$ with U_i effecting the one-body evolution from t_i to t_{i+1} under the single-particle hamiltonian $h_i(x_j) = -D^2/2m + \sum_{k=1}^{M} v_{jk}\, \sigma_{ik} (\Delta x)$ (D^2 is the usual 3-point discretization of the second-derivative). We may omit the self-energy term, $\pm\frac{1}{2}v(0)$ from h as this results in a constant shift of the energy scale for the time evolution which does not affect the right-hand side of (2.4).

As is clear from the standard derivation of the Hubbard-Stratonovich transformation by discretizing the time evolution [5], any approximation for U_i must be accurate through $O(\Delta t^2)$; we have used the Crank-Nicholson formula familiar from TDHF calculations, $U_i \sim (1-h_i\Delta t/2)(1 + h_i\Delta t/2)^{-1}$, whose effect on a single-particle wavefunction can be quickly evaluated by Gaussian elimination [6]. As is also clear from the usual derivation, the integrals over σ in (2.4) will not converge unless $(\sigma,v\sigma)_i$ is negative definite; i. e., the eigenvalues of v_{jk} are all less than zero. While this property is certainly not true in general, it can always be guaranteed to be so for a given v by adding an appropriate two-body interaction term to H. This makes the eigenvalues of the effective v_{jk} negative definite and shifts E_o in a trivial way [7].

Equation (2.4) is in a form suitable for Monte-Carlo evaluation. To make this explicit, we rewrite it as

$$E_0 = \frac{\int D[\sigma_{ij}]\, W[\sigma_{ij}] \dfrac{\langle H\Phi | U_\sigma | \Phi\rangle}{\langle \Phi | U_\sigma | \Phi\rangle}}{\int_N D[\sigma_{ij}]\, W[\sigma_{ij}]} ; \tag{2.5a}$$

$$W[\sigma] = e^{-\frac{1}{2}\sum_{i=1}^{N}(\sigma,v\sigma)_i \Delta t} \langle \Phi | U_\sigma | \Phi\rangle \ . \tag{2.5b}$$

Thus, E_0 is the average of $\langle H\Phi | U_\sigma | \Phi\rangle / \langle \Phi | U_\sigma | \Phi\rangle$ over all field configurations, weighted by $W[\sigma]$. To actually compute E_0, we use the well-known algorithm of Metropolis et al. [1] to generate an uncorrelated sequence of σ- fields distributed according to W and then simply average $\langle H\Phi | U_\sigma | \Phi\rangle / \langle \Phi | U_\sigma | \Phi\rangle$ over these configurations. Of course, this requires that $W[\sigma]$ be positive definite, which can be shown to always be the case for a symmetrized product trial boson state or for a spin and/or isospin symmetric deterimental trial state for fermions interacting through a spin-isospin independent potential. If $W[\sigma]$ is not positive definite, $|W|$ can be used as the weight and the sign $W/|W|$ appended to the energy contribution from each configuration. However, even here W must be predominantly of one sign for the denominator in (2.5a) to remain large and good statistical accuracy be achieved. While we have no guarantee that W be well-behaved in the general case, results for fermion systems treated by other methods offer some encouragement on this point [7].

Our general method is in some respects similar to one used in Monte-Carlo simulations of relativistic field theories [8]. There, the fermion degrees of freedom are "integrated out", leaving only a boson theory with an effective action (analogous to our $W[\sigma]$). However, the principal problem in such calculations is the evaluation of the enormous determinant (of dimension equal to the number of lattice sites) appearing in the effective action, essentially due to the presence of the filled Dirac sea. For the non-relativistic fermion systems we propose to treat (such as light nuclei), the dimensionality of the determinant required to compute $\langle \Phi | U_\sigma | \Phi\rangle$ is relatively small and its direct evaluation is possible. This also emphasizes the advantage of the MFMC method over the GFMC or PIMC methods in that positive and negative contributions to the norm are canceled exactly rather than statistically.

3. Model Calculation

For a first investigation of the MFMC method, we have chosen a system of A bosons of mass m in one-dimension interacting with each other through an

attractive zero-range potential: $v(x-x') = -V_0\delta(x-x')$. The hamiltonian is thus

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m} - \tfrac{1}{2}V_0 \sum_{i\neq j} \delta(x_i - x_j) + \tfrac{1}{2}mA\Omega^2(\sum_i x_i/A)^2, \qquad (3.1)$$

where we have confined the center-of-mass motion in an oscillator potential of frequency Ω. This additional term adds both one- and two-body parts to H, and it is easy to show that the effective $(\sigma,v\sigma)$ is negative definite provided $\Omega<\sqrt{6AV_0/mL^3}$ The oscillator frequency is also bounded from below by the requirement that the oscillator length, $\sqrt{1/mA\Omega}$, be smaller than the mesh size, L, so that the mesh boundaries have no affect on the solution. When this is satisfied, we are free to choose zero boundary conditions for the single-particle wavefunctions at $x = \pm L/2$.

The hamiltonian (3.1) is exactly soluble [9]; the eigenvalue of its only bound state is $E_0 = \tfrac{1}{2}\Omega - A(A-1)(A+1)V_0^2m/24$. It can also be solved in the Hartree approximation provided that the oscillator term (which gives only a very small contribution to the Hartree energy for the parameters we have used) is not treated self-consistently. In this latter case, the energy is found to be $E_H = \pi^2m\Omega^2b^2/24A - A(A-1)^2V_0^2m/24$ and the Hartree wavefunction is $\Phi(x_1,\cdots,x_A) = \prod_{i=1}^{A}\varphi(x_i)$ with $\varphi(x) = \sqrt{b/2}/\cosh bx$ and $b = mV_0(A-1)/2$. This is the trial function we used in our MFMC calculations. We also chose to work in physical units appropriate to nuclear systems, with $\hbar^2/m = 41.47MeV-fm^2$ and took $V_0 = 41.47MeV-fm$.

We have performed MFMC calculations of $E_0(T)$ for several different numbers of particles. The Metropolis et al. algorithm was implemented so that the entire σ -field over all space at one particular value of time was updated simultaneously; since only one single-particle wavefunction, $\varphi(x,t)$, is involved, an efficient algorithm could then be used for evaluating the change in W due to each update. Care was taken to ensure that the successive field configurations used for the energies $<H\Phi|U_\sigma|\Phi>/<\Phi|U_\sigma|\Phi>$ were sufficiently uncorrelated with each other so that the energies were statistically independent. (For an acceptance ratio of about 0.5, every 20'th Metropolis sweep of the mesh. The initial field configuration was taken to be the time-independent Hartree field; it was "thermalized" by some 1000 sweeps before the calculation of the energy began.) A mesh of 30 spatial points and up to 160 time points was used; we verified that our results do not depend significantly on either Δt or Δx when these parameters are small enough and that changes in Ω shift the large-T value of E_0 in the expected way. A typical calculation of some 60 time steps took 4 hours of CPU

time on a VAX 11/750 without floating point accelerator (about 5 minutes on a CDC 7600).

Results for the A=6, 10, and 20 systems are shown in Figures 1-3, where we plot $E_0(T)$. In all cases, Ω was 25 MeV. The energies shown are the results of averaging over some 200 field configurations. For A=6, we used $\Delta\tau$ = 0.15 fm, for A=10, $\Delta\tau$ was 0.10 fm, and for A = 20, $\Delta\tau$ was 0.04 fm. As can be seen from the figures, reasonable variations in the time step do not change our results. $E_0(T)$ shows an initial relaxation and asymptotically approaches a value which fluctuates around the expected result for each A. The convergence becomes more rapid with increasing A. This is due to the nature of the spectrum of excited states of our model, as can be seen from Figure 4, where we plot for A=10 the logarithm of the difference between $E_0(T)$ and its asymptotic value. Two different relaxation scales are clearly seen. The rapid initial relaxation corresponds to the energy gap between the intrinsic ground state and the excited continuum (at zero intrinsic energy); this is indicated by the dotted line. Note that this energy gap increases with increasing A. The slower relaxation is that associated with the center-of-mass motion in the harmonic oscillator potential.

4. Discussion

A number of considerations are important if more realistic systems are to be treated with the MFMC method. One of these is an adequate but tractable choice for the trial wavefunction since the method clearly becomes more efficient as the trial state approaches the true ground state. A strong repulsive core in the two-body potential (such as that between two He atoms or two nucleons) means that an independent-particle wavefunction is a poor approximation to the exact eigenstate, but our method is computationally feasible only for such trial wavefunctions; precisely how much of a penalty this implies remains to be investigated. Another important consideration is one of sheer computing power. Realistic systems require a spatial grid fine enough to resolve the details of the short-range few-body correlations in the wavefunction yet large enough to adequately enclose the system. Moreover, each single-particle wavefunction must be stored at every point in space time and determinants of moderate size must be evaluated often for fermion systems.

The results presented above are an encouraging demonstration that the MFMC method can be applied to describe the ground state energy of a simple

many-boson system; it is particularly noteworthy that the computational effort for such a boson system does not increase with the number of particles. The proper treatment of fermion systems, the primary motivation for studying the MFMC method, entails no foreseeable problems beyond those we have already faced and calculations along these lines for finite systems are in progress. Also of interest would be calculations of infinite systems, such as "nuclear matter", obtained by imposing periodic boundary conditions on a system confined within a fixed region of space.

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FIGURE 1: ENERGY PLOT A=6

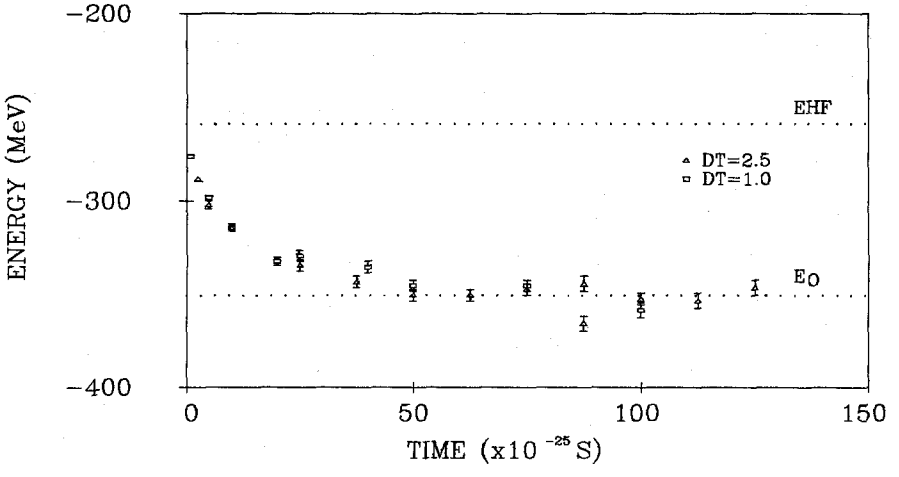

FIGURE 2: ENERGY PLOT A=10

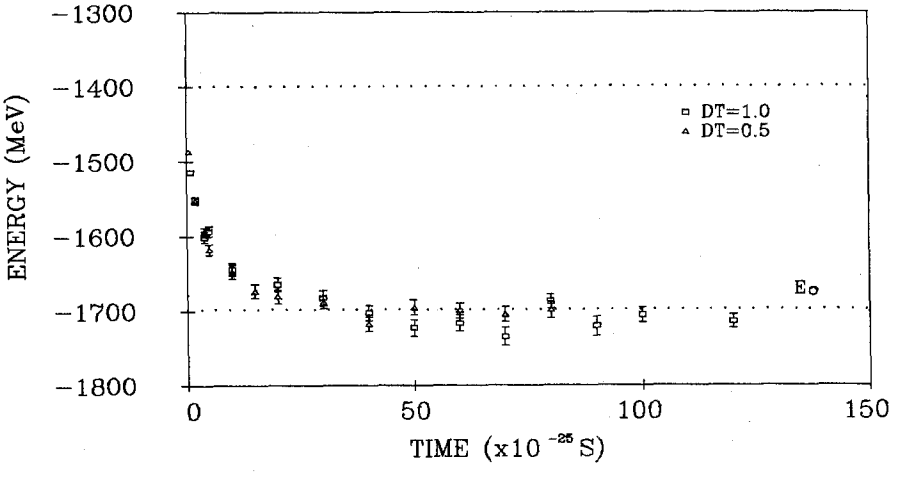

FIGURE 3: ENERGY PLOT A=20

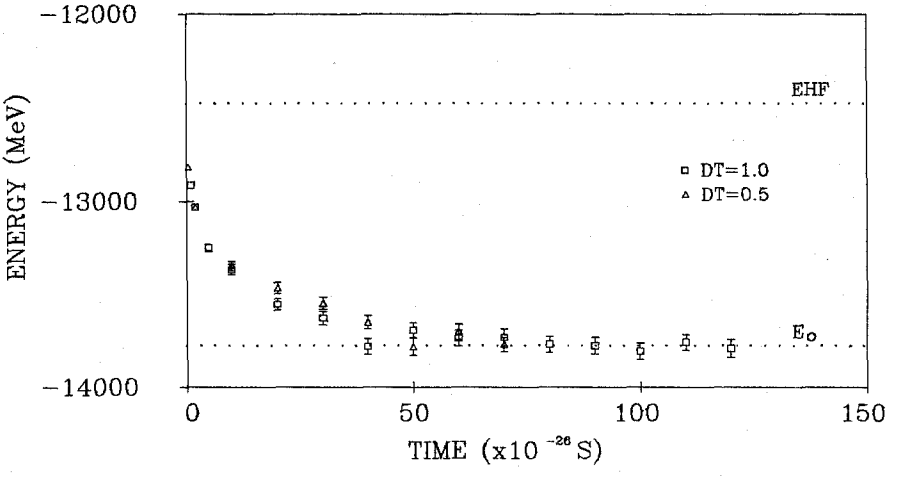

FIGURE 4: ENERGY GAP PLOT A=10