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Auxiliary-Field Monte Carlo Methods

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I discuss Monte Carlo algorithms for quantum many-body systems that employ an auxiliary field to linearize a two-body interaction. These reduce the evaluation of the partition function to sampling many one-body evolutions in a fluctuating field. Fermions and bosons are treated on an equal footing. Applications to potential models and to quantum spin systems are discussed.

KEY WORDS: Monte Carlo methods; Hubbard–Stratanovich transformation; quantum spin systems.

The notion of independent particles moving in a common potential underlies our intuition for many quantum many-body systems and also provides the foundation for more sophisticated analytical and numerical treatements. It is therefore natural to ask whether we can develop methods that take the mean-field solution as a starting point and then use Monte Carlo techniques to refine this to an exact description. In this paper, I discuss the progress we have made along these lines during the last few years, describing first the general method[1] and then its application to one-dimensional potential systems[2] and quantum spin systems.[3]

METHOD

Suppose that we are faced with describing a system of A particles of mass m (fermion or boson) interacting through a two-body potential v, so that the Hamiltonian is

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

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where the $\{x_i\}$ are the coordinates and the $\{p_i\}$ the conjugate momenta. In particular, suppose that we are interested in Ψ, the lowest eigenstate of H (energy E_0). This state can be generated from any trial state Φ (with $\langle \Phi/\Psi \rangle \neq 0$) by "filtering" with the imaginary-time evolution operator. A specific expression for the exact ground state is

$$E_0 = \lim_{T \to \infty} \frac{\langle H\Phi \,|e^{-HT}|\, \Phi \rangle}{\langle \Phi \,|e^{-HT}|\, \Phi \rangle} \tag{2}$$

and the expectation of any observable A is similarly

$$\langle \Psi \,|A|\, \Psi \rangle = \lim_{T \to \infty} \frac{\langle \Phi \,|e^{-HT/2} A e^{-HT/2}|\, \Phi \rangle}{\langle \Phi \,|e^{-HT}|\, \Phi \rangle} \tag{3}$$

Although the many-body evolutions involved in (2 and 3) makes them of dubious practical value, considerable simplification is achieved if Φ is taken to be a symmetrized (antisymmetrized) product of single-particle orbitals for bosons (fermions) and if we use the Hubbard–Stratanovich representation of the evolution operator

$$e^{-HT} = \int D[\sigma(x, t)]\, e^{1/2 \int_0^T (\sigma, v\sigma) dt} U_\sigma(T, 0) \tag{4}$$

Here, the integral is over all c number fields $\sigma(x, t)$ and U_σ is a one-body evolution operator for a Hamiltonian linear in σ

$$\frac{\partial U_\sigma(t, 0)}{\partial t} = -h_\sigma(t)\, U_\sigma(t, 0) \tag{5a}$$

$$h_\sigma = \frac{p^2}{2m} \pm \frac{1}{2} v(0) + (\sigma, v\rho) \tag{5b}$$

In (4 and 5), we have employed the inner-product notation

$$(A, vB) = \int dx \int dx'\, A(x)\, v(x - x')\, B(x')$$

$\rho(x)$ is the one-body density operator, and the $+(-)$ sign (5b) is for bosons (fermions).

With the representation (4), the energy (2) can be written as the ratio of two functional integrals

$$E_0 = \lim_{T \to \infty} \frac{\int D[\sigma]\, e^{1/2 \int_0^T (\sigma, v\sigma) dt} \langle \Phi \,|U_\sigma|\, \Phi \rangle (\langle H\Phi \,|U_\sigma|\, \Phi \rangle / \langle \Phi \,|U_\sigma|\, \Phi \rangle)}{\int D[\sigma]\, e^{1/2 \int_0^T (\sigma, v\sigma) dt} \langle \Phi \,|U_\sigma|\, \Phi \rangle} \tag{6}$$

In this way, E_0 is expressed as a coherent superposition of the results of (infinitely) many one-body evolutions, each of which is parametrized by auxiliary field σ and weighted by the Gaussian factor appearing in (4).

If the integrals in (6) are evaluated through a saddle-point approximation, the usual nonlinear Hartree approximation is recovered. (Hartree–Fock can be obtained by a slightly different linearization of the two-body Hamiltonian [ ]). To the extent that this is a good approximation, corrections associated with the (possibly anharmonic) fluctuations of σ about its mean value can be evaluated by Monte Carlo techniques.

The practical numerical evaluation of (6) for suitably large but finite T (or a similar expression for $\langle \Phi | A | \Phi \rangle$), procedes by a standard Metropolis algorithm following discretization on a uniform Cartesian space-time lattice. In setting up the calculation,[2] it is important to have a temporal discretization of U_σ accurate to second-order (as follows from the derivation of the Hubbard–Stratanovich representation) and to have an efficient way of evaluating changes in the Monte Carlo weight (integrand of the denominator in (6)) associated with trial steps in the auxiliary field at each time slice. It should be noted that convergence of the integrals requires $(\sigma, v\sigma) < 0$ for all σ, which implies that the momentum-space representation of v is negative-definite. If this is not the case, it can be made so by a suitable shift in the one-body Hamiltonian. Furthermore, the weight is guaranteed to be positive for a boson system or for a fermion system with an internal symmetry (e.g., spin or isospin). For other cases (such as the spin systems below), the weight can be negative and the sign must be accounted for.

Overall, the method is similar to the "integrating out" of the fermion variables in a lattice field theory. However, in those relativistic situations the filled Dirac sea implies as many fermions in the vacuum as there are lattice sites, with correspondingly large determinants to evaluate. In the nonrelativistic systems of interest here there are only a few fermions, and anti-symmetry can be guaranteed by evaluating the associated determinants explicitly.

ONE-DIMENSIONAL POTENTIAL SYSTEMS

As a testing ground for these ideas, we considered fermion and boson systems interacting in one dimension.[2] For the boson case, an attractive zero-range potential, $v(x) = -V_0 \delta(x)$, was assumed. This Schrödinger problem can be solved exactly, and also in the Hartree approximation. In the auxiliary field calculations, some 30 space and up to 160 time points were used and an external one-body harmonic oscillator potential coupled

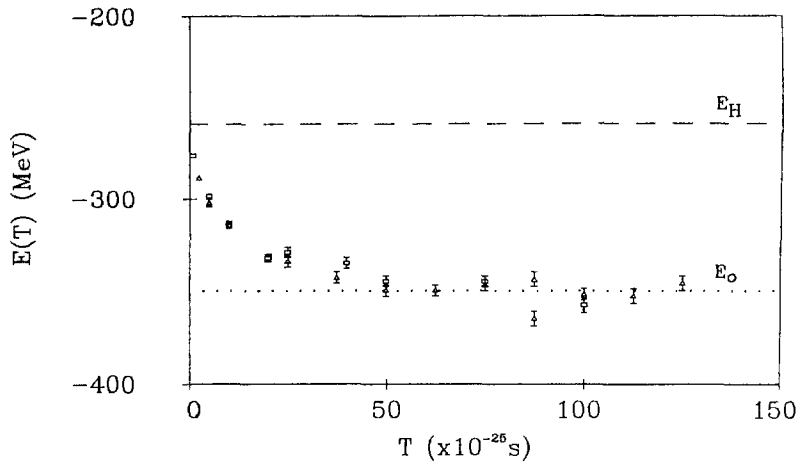

Fig. 1. Relaxation of the $E(T)$ for a system of six bosons in one dimension. E_H is the Hartree energy and E_0 the exact energy. Different symbols correspond to different time steps.

to the center-of-mass coordinate localized the system. The trial state was the Hartree solution. In general, we found the method to work well for these boson systems, as shown in Fig. 1.

For a model fermion system to test the method, we assumed a four-fold internal symmetry and used the two-body potential of Ref. 4, a superposition of attractive and repulsive exponential that mimics a nuclear force. The trial wave function was a determinant of harmonic oscillator wave functions, with the oscillator length chosen to minimize the variational

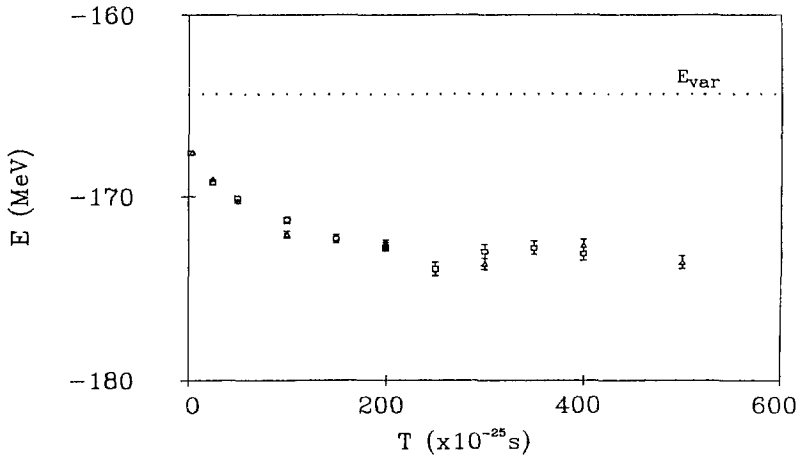

Fig. 2. Relaxation of the ground-state energy of a 12-fermion system in one dimension.

energy. Relaxation of the energy of the $A = 12$ system (three single-particle wave functions) from the variational value to a value consistent with that of other exact Monte Carlo methods is shown in Fig. 2.

These studies have indicated several advantages and drawbacks of the auxiliary field Monte Carlo method as applied to potential problems. On the positive side, fermions and bosons are treated with equal ease and an extension to describe light nuclei as nucleons interacting via meson exchange does not appear impractical. On the negative side, only determinental trial states are tractable (because of the one-body evolution), making pair correlations difficult to include. Moreover, the spatial grid must be fine enough to describe two-body correlations, yet large enough to contain the whole system.

APPLICATION TO SPIN SYSTEMS

We have also attempted to apply the auxiliary field method to simulate quantum spin systems at finite temperature.[3] Consider, for example, the nearest-neighbor one-dimensional Heisenberg model, with A spins whose Hamilton is

$$H = -v \sum_{i=1}^{A} \vec{\sigma}_i \cdot \vec{\sigma}_{i+1} \tag{7}$$

Here $v > 0 (< 0)$ for a ferromagnetic (antiferromagnetic) system. We are generally interested in thermodynamic averages at a temperature β^{-1}, characterized by the density operator $U(\beta) = \exp - \beta h$.

Our strategy is to express U as a product of many evolutions, each associated with a "bond"

$$U(\beta) = \lim_{N \to \infty} \left\{ \prod_{i=1}^{A} (1 + \varepsilon v \vec{\sigma}_i \cdot \vec{\sigma}_{i+1}) \right\}^N \tag{8}$$

where $\varepsilon \equiv \beta / N$ is the "time" step. A Hubbard–Stratonovich linearization can then be applied to each bond evolution by introducing an auxiliary vector field $\vec{\lambda}_i$ at each bond

$$1 + \varepsilon v \vec{\sigma}_i \cdot \vec{\sigma}_{i+1} \sim \int d\vec{\lambda}_i e^{-\varepsilon |v| \lambda_i^2 / 2} (1 + \varepsilon v \vec{\lambda}_i \cdot \vec{\sigma}_i)(1 + \varepsilon |v| \vec{\lambda}_i \cdot \vec{\sigma}_{i+1}) \tag{9}$$

so that each spin evolves for each time step under the sum of the fields associated with the bonds to which it belongs

$$(1 + \varepsilon v \vec{\lambda}_i \cdot \vec{\sigma}_i)(1 + \varepsilon |v| \vec{\lambda}_{i-1} \vec{\sigma}_i) \approx 1 + \varepsilon (v \vec{\lambda}_i + |v| \vec{\lambda}_{i-1}) \cdot \vec{\sigma}_i \tag{10}$$

These expressions are, of course, accurate only to lowest order in ε.

By compounding many steps of the term (eq. 9 and 10) together in (8), the problem can be reduced to that of many single-spin evolutions in fluctuating, but correlated, auxiliary fields. These fields can be sampled via a Metropolis algorithm, the required spin evolutions for each update being carried out easily using the algebra of the Pauli matrices. Note that (9) shows that λ scales as $\varepsilon^{-1/2}$, so that fluctuations become larger as ε decreases. Note also that both $v > 0$ and $v < 0$ are treated on equal footing.

As analytical mean-field approximation can give some insight into this formulation. The functional integral for the partition function is found to have a saddle-point at $\vec{\lambda} = 0$ if $\beta |v| < \frac{1}{4}$ and at $\vec{\lambda} = \lambda_0 \hat{n}$ if $\beta |v| > \frac{1}{4}$, where $\hat{n}$ is an arbitrary unit vector and λ_0 satisfies $\lambda_0 = 2 \tan h(2\beta |v| \lambda_0)$. This is to be contrasted with the usual treatment that predicts a nonvanishing mean field for $\beta |v| > \frac{1}{2}$. The difference is connected with how we have written the functional integral. Fluctuation of $\vec{\lambda}$ about its mean value, which we evaluate by Monte Carlo, and then correct the saddle-point approximation to the exact solution.

We have explored the Monte Carlo simulation of the auxiliary-field functional integral for ferromagnetic and antiferromagnetic Heisenberg systems in one and two dimensions. For both small systems (which can be solved analytically) and large systems (up to 8×8 in two dimensions) we find good convergence for the energy and specific heat at high temperatures, but there is a marked deterioration in the precision for values of β large enough to have a nonvanishing saddle-point field. The precise reason for this failure, and possible reformations of the functional integral to avoid it, are currently being investigated.

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