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THE STOCHASTIC SOLUTION OF THE MANY-BODY  
SCHROEDINGER EQUATION FOR FERMIONS

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This paper describes the basis of calculations we have made to compute the ground state properties of many-fermion systems. Elsewhere in this volume Kalos will discuss the Green's Function Monte Carlo (GFMC) approach to this problem. Earlier quantum calculations have been reviewed in ref. [1]. These GFMC methods of which the present method is a variant, are not to be confused with variational Monte Carlo, as first utilized by McMillan [2]. The latter give properties of model trial functions, whereas GFMC gives properties of the exact ground state.

We start by considering the Schroedinger equation for N particles written in imaginary time:

$$-\frac{\partial \phi(R,t)}{\partial t} = H\phi(R,t) = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(R) - V_0\right)\phi(R,t) \quad (1)$$

Here R is the 3N set of coordinates, V(R) is the potential energy function and V<sub>0</sub> an arbitrary constant. In order to make a many-body calculation feasible, importance sampling is introduced by multiplying this equation by a known trial function  $\Psi_T(R)$  and making the substitution:  $f(R,t) = \Psi_T(R)\phi(R,t)$ . With some algebra we arrive at the expression:

$$-\frac{\partial f}{\partial t} = \frac{\hbar^2}{2m} [-\nabla^2 f + \nabla(fF_Q(R))] + [E_L(R) - V_0]f \quad (2)$$

where  $F_Q(R)$  and  $E_L(R)$  are defined as:

$$F_Q(R) = \nabla \log \Psi_T^2 = \text{quantum trial "force"} \quad (3)$$

$$E_L(R) \equiv \Psi_T^{-1} H \Psi_T(R) = \text{local energy} \quad (4)$$

Equation (2) can be interpreted as a simple Markov process. Suppose we construct an ensemble of systems (points in 3N dimensional space) with the probability density  $f(R,0)$ . Usually the initial condition taken is  $f(R,0) = \Psi_T(R)^2$ . These systems then diffuse and branch such that their probability distribution is given by eq. (2). The three terms on the right hand side are interpreted respectively as random diffusion, drift and branching. By branching, it is meant that a particular system is either eliminated from the ensemble, if the local energy is less than V<sub>0</sub>, or duplicated in the ensemble, otherwise.

A steady state population requires that  $V_0$  be equal the lowest eigenvalue,  $E_0$ . It is easily shown that for large time  $f(R,t) = \Psi_T(R)\phi_0(R)$  where  $\phi_0$  is the exact ground state eigenfunction. The eigenvalue then can be estimated as:

$$E_0 = \frac{\int \Psi_T H \phi_0}{\int \Psi_T \phi_0} = \frac{\int \phi_0 H \Psi_T}{\int \Psi_T \phi_0} = \langle E_L(R) \rangle \quad (5)$$

where  $\langle \dots \rangle$  means the average over the distribution  $f(R,t)$  for large enough  $t$ . By the usual statistical formulas the variance of the energy estimate is given by:

$$\text{var}(E_0) = \langle (E_L(R) - E_0)^2 \rangle / M \quad (6)$$

where  $M$  is the number of independent sample points. As usual with Monte Carlo methods the error bar on  $E_0$  is proportional to the inverse square root of computer time. However by choosing a good trial function  $\Psi_T$ , we can reduce the coefficient dramatically. In the limit as  $\Psi_T$  approaches  $\phi_0$  the variance vanishes. In practice by using Slater-Jastrow trial functions we can eliminate many of the singularities in  $E_L(R)$ . The importance sampling by  $\Psi_T$  is also essential in controlling fluctuations and instabilities in the branching process.

Our algorithm for this process essentially uses a short time approximation to the exact Green's function. This approximation has been described for a classical polymer system in ref. [3]. Equation (2) is identical to the classical Smoluckowski equation except for the presence of the local energy term. In this approximation if a system has diffused from  $R_0$  to  $R$  within a time  $t$ , then the expected number of copies at time  $t$  will be:

$$\exp [-t(E_L(R) + E_L(R_0) - 2V_0)/2]$$

This method is much simpler than the exact GFMC method of Kalos (9), but only exact in the limit as  $t \rightarrow 0$ .

The above method is easily implemented to calculate the ground state properties of boson systems. But for fermion systems, there are serious and, as yet, not resolved difficulties. The crux of the problem is that unless  $\phi_F$  (the exact fermion eigenfunction) and  $\Psi_T$  have the same sign everywhere, then  $f = \phi_F \Psi_T$  cannot be interpreted as a probability density. Hence the nodes of  $\phi_F$  are required. Except for one dimensional or few particle problems exact specification of the nodal locations is an extremely tough problem. However important progress has been made in circumventing this difficulty for several systems.

### The Fixed-Node Method

A simple, though approximate, method of accounting for antisymmetry is simply to let the nodes of a trial function act as an absorbing barrier to the diffusion.

Suppose  $\Psi_T(R)$  is an antisymmetric trial function. The nodes of  $\Psi_T$  divide the configuration space into connected volumes. Using the above Monte Carlo method we can so obtain the eigenfunctions ( $\phi_k$ ) and eigenvalues ( $e_k$ ) inside each nodal volume ( $V_k$ ) and which vanish outside that volume:

$$\begin{aligned} H\phi_k &= e_k \phi_k \\ \phi_k(R) &= 0 \quad R \notin V_k \end{aligned} \quad (7)$$

Each of the eigenvalues  $e_k$  is an upper bound to the fermion energy,  $E_F$ , since the antisymmetric function:

$$\hat{\phi}_k(R) = \sum_P (-)^P \phi_k(PR) \quad (8)$$

has a variational energy  $e_k$ , where  $P$  is a permutation.

$$e_k = \frac{\int \hat{\phi}_k H \hat{\phi}_k}{\int \hat{\phi}_k^2} \geq E_F \quad (9)$$

It is easily shown that  $\phi_k$  is non-zero, since at each point, only permutations of the same sign can contribute to the sum in eq. (8). Otherwise the volume  $V_k$  would contain both positive and negative regions of  $\Psi_T(R)$ . This variational argument can be easily generalized to include spin.

In practice the fixed-node method is carried out in the following way. The initial ensemble is chosen as before, to be  $f(R,0) = \Psi_T(R)$ . If the population is large enough, all the different nodal regions will be populated. The diffusion and branching process precedes as in the boson case, except that whenever a system crosses a node of  $\Psi_T$  that system is eliminated from the ensemble. It is easily seen that the  $V_0$  necessary to maintain a stationary population in the ensemble is given by  $e_{FN} \equiv \min_k \{e_k\}$ . Thus if  $e_k$  depends on the nodal volume, the diffusion process will select out those with the lowest  $e_k$ .

In practice this method achieves a good upper bound to  $E_F$  because all of the correct many-particle boson correlations are in  $\hat{\phi}_k$ . Because the shape of the volume  $V_k$  is in general incorrect,  $\hat{\phi}_k$  is a solution of the Schroedinger equation everywhere except at the nodes of  $\Psi_T$  where it has a discontinuous gradient. (The discontinuity will not contribute to the integral in eq. (9) since  $\hat{\phi}_k$  is zero there.) By the usual arguments ( $e_k - E_F$ ) must vanish quadratically as the nodes of  $\Psi_T$  approach those of  $\phi_F$ . In principle one could vary the nodal locations to obtain the best upper bound but the highly dimensional nodal surfaces are difficult to parameterize in a systematic fashion.

## Nodal Relaxation

If the nodes of  $\Psi_T$  are sufficiently close to those of  $\phi_F$ , an improvement in the fixed-node procedure will give the exact fermion eigenfunction. The basic idea is that, if the diffusion process begins in an antisymmetric state (i.e., with configurations carrying  $\pm$  signs depending on the sign of  $\Psi_T$ ) the diffusion process, including allowing diffusion across the nodes, will maintain the antisymmetry and must converge to the antisymmetric ground state. This procedure is however unstable since a fluctuation of the boson ground state will grow and dominate at large times.

We can represent the diffusion process, with the importance function  $\Psi_T$ , in terms of its Greens function as:

$$f(R, t) = \int dR_0 \Psi_T(R) e^{-(H - V_0)t} \Psi_T^{-1}(R_0) f_A(R_0, 0) \quad (10)$$

where  $e^{-(H - V_0)t}$  is the Green's function for eq. (1). If  $f_A(R, 0)$  is symmetric and  $\Psi_T(R)$  is antisymmetric then:

$$\lim_{t \rightarrow \infty} f_A(R, t) \propto \Psi_T(R) \phi_F(R) e^{-(E_F - V_0)t} \quad (11)$$

But the diffusion process can only have positive importance functions--otherwise one is lead to negative probabilities; the sign of  $\Psi_T$  must be taken out as a weight. Let  $\sigma(R) = \text{sign}(\Psi_T(R)) = \pm 1$ . Then we can rewrite eq. (10) as

$$f_A(R, t) = \int dR_0 \sigma(R) \sigma(R_0) |\Psi_T(R)| e^{-(H - V_0)t} |\Psi_T(R_0)|^{-1} f_A(R_0, 0) \quad (12)$$

Since the time for which this algorithm is stable is short, it is desirable to take the initial distribution as close as possible to the limiting distribution in eq. (11). A convenient choice is the fixnode distribution,  $f_A(R, 0) = \Psi_T(R) \phi(R)$ .

The integral in eq. (12) can be performed by a very simple extension of the fixed-node diffusion process. Suppose we wish to calculate the fermion eigenvalue Define:

$$E_A(t) = \frac{\int \Psi_T^H \Psi_T^{-1} f_A(R, t)}{\int f_A(R, t)} = \frac{\langle \sigma(R) \sigma(R_0) E_L(R) \rangle}{\langle \sigma(R) \sigma(R_0) \rangle} \quad (13)$$

Now from our initial conditions  $E_A(0) = e_{FN}$  and from eq. (11)  $E_A(\infty) = E_F$ .  $E_A(t)$  will relax from the fixed-node energy to the fermion energy. Each system is now assigned a new clock, denoted  $s$ . Until a system diffuses across a node for

the first time,  $s = 0$ , but as soon as a system crosses a node of  $\Psi_T$  then  $s$  begins counting. If a system branches the clock is reproduced in all copies. When  $s$  reaches some maximum value  $s_M$ , the system is eliminated from the ensemble. The collection of all systems at all times for which  $s = 0$  is simply the fixed-node distribution,  $f_A(R,0)$ . The collection of all systems at all times for which  $s \leq t$  with the weight  $\sigma(s)\sigma(0)$  has the distribution  $f_A(R,t)$ , since this collection represents all the systems which evolved from the fixed node distribution in time  $t$ . Then to calculate  $E_A(t)$  one merely performs the averages in eq. (13) over all configurations for which  $s \leq t$ . This will give  $E_A(t)$  for  $0 \leq t \leq s_M$ . Since  $|\Psi_T|$  contains nodes, care must be taken in constructing the short time Green's function so that systems can tunnel through the nodes properly.

Because of the the instability referred to earlier, the number of configurations needed in order to determine  $E_A(s_M)$  grows with  $s_M$  like  $\exp(s_M(E_F - E_0))$ . Hence an upper limit to  $s_M$ , assuming a reasonable computer run, is determined by the difference between the boson and fermion energies, in other words, the node crossing frequency. Thus we are limited, by this algorithm, to problems for which the nodes of  $\Psi_T$  can be repaired in a time small compared with  $(E_F - E_0)^{-1}$ . The available evidence on jellium suggests that we have met this criterion; the potential is soft enough so that the Hartree-Fock nodes are rather good. The situation on  $^3\text{He}$ , at this moment, does not appear as promising; more sophisticated algorithms or methods may be needed.

## Applications

The applications, to date, have been to jellium in two and three dimensions, liquid  $^3\text{He}$  and hydrogen (as a two component system of protons and electrons). I will not discuss the latter two systems as our calculations are still incomplete. The electron gas has been discussed in refs. [4,5]. The following phases were studied: the boson fluid, the normal paramagnetic fluid, the spin-polarized or ferromagnetic fluid and the Wigner crystal. The ground state energies as obtained by the nodal relaxation method are given in Table I with the error bars in parentheses. Because of importance sampling, the errors are much smaller than usual with Monte Carlo. Table II contains the energy differences in going from variational Monte Carlo with a Jastrow-Slater trial function to the fixed-node energy and then to the exact energy. At low density, we find, that the normal electron gas undergoes a phase transition at  $r_s = 75$  to a ferromagnetic fluid and at  $r_s = 100$  to a Wigner crystal. The boson system undergoes Wigner crystallization at  $r_s = 160$  ( $r_s$  is the Wigner sphere radius in units of Bohr radii).

Table I

$r_s$	$E_{PMF}$	$E_{FMF}$	$E_{BF}$	$E_{BCC}$
1.0	1.174(1)	-----	-----	-----
2.0	0.0041(4)	0.2517(6)	-0.4531(1)	-----
5.0	-0.1512(1)	-0.1214(2)	-0.21663(6)	-----
10.0	-0.10675(5)	-0.1013(1)	-0.12150(3)	-----
20.0	-0.06329(3)	-0.06251(3)	-0.06666(2)	-----
50.0	-0.02884(1)	-0.02878(2)	-0.02927(1)	-0.02876(1)
100.0	-0.015321(5)	-0.015340(5)	-0.015427(4)	-0.015339(3)
130.0	-----	-----	-0.012072(4)	-0.012037(2)
200.0	-----	-----	-0.008007(3)	-0.008035(1)

The ground state energy of the charged Fermi and Bose systems. The density parameter,  $r_s$ , is the Wigner sphere radius in units of Bohr radii. The energies are Rydbergs and the digits in parenthesis represent the error bar in the last decimal place. The four phases are: paramagnetic or unpolarized Fermi fluid (PMF); the ferromagnetic or polarized Fermi fluid (FMF); the Bose fluid (BF); and the Bose crystal with a BCC lattice.

Table II

$r_s$	$\delta_{PMF}$	$\gamma_{PMF}$	$\delta_{FMF}$	$\gamma_{FMF}$	$\delta_{BF}$	$\delta_{BCC}$
2	40	9	11.0	---	12.0	-----
5	17	2	7.2	---	6.8	-----
10	11	1	6.5	1.8	5.1	-----
20	6.7	0.7	3.0	1.0	3.3	-----
50	2.9	0.31	1.6	0.25	1.7	2.0
100	1.7	----	1.2	----	1.2	0.41
130	----	----	---	----	1.1	0.30

The error in the variational approximation in  $10^{-4}$  Rydbergs for four different phases.  $\delta = E_V - E_0$  (the difference between the Jastrow trial function and the exact ground state energy).  $\gamma = E_{FN} - E_0$  (the difference between the 'fixed-node' energy with plane wave nodes and the exact ground state energy).

## Errors

Finally, I would like to close with a discussion of the type of errors which limit the accuracy of a GFMC calculation. They are ranked in order of increasing importance in the one system we have studied most extensively, the three dimensional electron gas.

- 1) Numerical errors. (Truncation errors or the use of a short time Green's function, round-off errors, use of pseudo-random numbers, etc.) These errors with a sufficient amount of programming effort can be made very small. For the diffusion model the exact Kalos algorithm [1] can be used.
- 2) Convergence of  $f(R,t)$  to  $\Psi_T \phi_0$ . With homogeneous quantum systems and good trial functions the convergence is very rapid, indicating only local diffusion processes are needed to convert  $\Psi_T$  into  $\phi_0$ .
- 3) Statistical errors. As demonstrated above these errors depend on the fluctuations in the local trial energy and on the number of independent systems that can be generated. For the electron gas, the Jastrow-Slater trial function is good enough so that this error is quite small, compared with the accuracy of other types of calculations, and small enough to determine the phase transitions. But for more complicated systems the trial functions will be more difficult to construct.
- 4) The fermion problem. Our experience with the electron gas at many different densities suggests that the Hartree-Fock nodes are good enough for the present method to converge to the exact ground state. But clearly this error is not under control. We need both better algorithms and more experience.
- 5) Finite system effects. With present supercomputers we have been able to simulate up to 250 fermions. For the electron gas, even with periodic boundary conditions, this is far from the thermodynamic limit. Our simulations show that the correction to the kinetic energy behaves like  $N^{-2/3}$  and to the potential energy as  $N^{-1}$ . To extrapolate to the limit of large  $N$ , we have taken some simple model, for example Hartree-Fock, with some adjustable parameters and have analytically calculated the finite system effects. Then using simulations at a variety of values of  $N$ , we have both fixed the adjustable parameters, and tested the model. The model is satisfactory for the electron gas although the range of  $N$  is rather limited. Faster computers and algorithms will help, both of which are in the offing.

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