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The Determinant Method and Quantum Simulations of Many-Body Effects in a Single Impurity Anderson Model

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We present a short description of a quantum Monte Carlo technique that has proved useful for simulating many-body effects in systems of interacting fermions at finite temperatures. We then report our preliminary results using this technique on a single impurity Anderson model. Examples of such many-body effects as local moment formation, Kondo behavior, and mixed valence phenomena found in the simulations are shown.

KEY WORDS: Quantum Monte Carlo; single impurity Anderson model; Kondo effect; mixed valence phenomena.

1. INTRODUCTION

Using a Hubbard–Stratonovich type of transformation, certain interacting fermion problems can be expressed in terms of noninteracting fermions coupled to a space-time dependent classical field which is functionally integrated over. When the fermion degrees of freedom are integrated out, one is left with a problem of integrating over configurations of the Hubbard–Stratonovich field. This latter problem can, in principle, be approached using Monte Carlo techniques.[1] Here, in the context of the single impurity Anderson model,[3] we give a brief description of one method[2] that has been used to carry out such Monte Carlo simulations and present preliminary results.

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The Hamiltonian for this model has the form

$$H = -t \sum_{\langle ij \rangle s} (c_{is}^{+} c_{js} + c_{js}^{+} c_{is}) + V \sum_{s} (c_{os}^{+} d_s + d_s^{+} c_{os}) + E_d(n_{d\uparrow} + n_{d\downarrow}) + U n_{d\uparrow} n_{d\downarrow} \tag{1}$$

Here c_{is}^{+} is the fermion creation operator for an electron in an "s orbital" on site i with spin s, d_s^{+} is the corresponding operator asociated with a local "d orbital" on impurity site o, which has energy E_d. The s and d orbitals are hybridized by an overlap V, and if two electrons occupy the d orbital, there is a Coulomb interaction U. A nearest-neighbor pair of lattice sites is denoted by $\langle ij \rangle$. The goal of our simulations is to provide further insight into the physics of the local moment, Kondo, and valence fluctuation regimes known to exist for this model, and we will show results of our efforts to simulate these regimes.

2. BASIC IDEA

What we want to evaluate are thermodynamic averages of different physical quantities. Such an average for a typical quantity A is defined by

$$\langle A \rangle = \operatorname{tr} A e^{-\beta H}/Z \tag{2}$$

where the partition function Z is

$$Z = \operatorname{tr} e^{-\beta H} \tag{3}$$

The problem is in general the inability not only to exponentiate the quantum Hamiltonian but also to perform the required trace. To mitigate these problems, we make an approximation that introduces additional degrees of freedom and an extra (finite) dimension into the problem. The approximation is controlled in the sense that the error in principle can be made as small as we like. For each configuration of these new variables the approximation corresponds to replacing the original Hamiltonian by an effective one for which we can perform the trace over the original (i.e., the fermion) degrees of freedom. Symbolically, we have

$$\langle A \rangle \simeq \frac{\operatorname{tr}_\sigma \operatorname{tr} A e^{-\beta h[\sigma]}}{\operatorname{tr}_\sigma \operatorname{tr} e^{-\beta h[\sigma]}} \tag{4}$$

$$= \frac{\operatorname{tr}_\sigma z[\sigma](z[\sigma]^{-1} \operatorname{tr} A e^{-\beta h[\sigma]})}{\operatorname{tr}_\sigma z[\sigma]}$$

$$= \frac{\operatorname{tr}_\sigma A(\sigma)\, z[\sigma]}{\operatorname{tr}_\sigma z[\sigma]} \tag{5}$$

where σ represents a configuration of the new degrees of freedom and

$$z[\sigma] = \text{tr}\, e^{-\beta h[\sigma]} \tag{6}$$

is the partition function of the configuration-dependent effective Hamiltonian. It is the average represented by (5) that is done by the Monte Carlo methods; however, instead of using the standard statistical probability density $e^{-\beta h}/Z$ we now must use $z[\sigma]/Z$. It is in $z[\sigma]$ where the quantum mechanical details are embodied.

3. SOME DETAILS

3.1. The Trotter Approximation

To add the details of the method, we focus on the calculation of the partition function. The first step is to introduce a small parameter τ into the problem. Because the Hamiltonian commutes with itself, we can write

$$\begin{aligned} Z &= \text{tr}\, e^{-\beta H} \\ &= \text{tr}\, e^{-\tau H} e^{-\tau H} \cdots e^{-\tau H} \end{aligned} \tag{7}$$

with $\tau = \beta/L$ where L, the number of $e^{-\tau H}$ factors, is the argument of the trace. We now approximate $e^{-\tau H}$. To do this we note that

$$H = H_0 + H_I$$

where H_0 is the noninteracting part of the Hamiltonian, which is quadratic in the fermion degrees of freedom, and H_I is the interacting part, which for the models we consider is quartic in the fermion degrees of freedom. Since H_0 and H_I do not commute we use the Trotter approximation[4] to write

$$e^{-\tau H} \simeq e^{-\tau H_0} e^{-\tau H_I} + O(\tau^2) \tag{8}$$

Hence, in principle, we can make this a very good approximation by making τ small. Having done this, we have a piece $\exp(-\tau H_0)$, which generally is easily evaluated, but are still faced with exponentiating H_I, which is in general difficult to evaluate. Fortunately, this task is easily accomplished for certain models by using a form of the Hubbard–Stratanovich transformation.[5]

3.2. The Hubbard–Stratanovich Transformation

This transformation is best illustrated by an example for which we chose the single impurity Anderson model Hamiltonian (1). For this model

$$H_I = U n_{d\uparrow} n_{d\downarrow} \tag{9}$$

The transformation uses the following identity[6]

$$e^{-\tau U n_{d\uparrow} n_{d\downarrow}} = \frac{1}{2} \sum_{\sigma = \pm 1} e^{-\tau J \sigma (n_{d\uparrow} - n_{d\downarrow}) - \tau U (n_{d\uparrow} + n_{d\downarrow})/2} \tag{10}$$

with $\cosh \tau J = e^{\tau U/2}$, which is applied to each site in (9) and to each factor in (7). For the single impurity problem there is only one lattice site to which the transformation is applied. If there were a sum over such sites and the sites were arranged in a two-dimensional lattice, then at each site we have an Ising spin at L sites in a third dimension. From more formal approaches to the problem this third dimension corresponds to an imaginary time axis obtained by the change of variable $it = (kT)^{-1}$. Additional factors in (7) then correspond to different time steps of the problem. For convenience in the following we will use this "time" terminology.

From (10) we see that the term in (8) that is quartic in the creation and destruction operators has been replaced by one that is quadratic: The orginal H in the lth factor of (7) has been replaced by an $H(l)$ that is non-interacting, and hence its exponential form is treatable by standard means. In particular we define

$$H(l) \equiv \sum_{ijs} c_{is}^{+} h_{ij}^{s}(l) c_{js}$$

We can now rewrite (7) as

$$Z = \mathrm{tr}_\sigma \, \mathrm{tr} \, e^{-\tau H(L)} e^{-\tau H(L-1)} \cdots e^{-\tau H(1)}$$

and because of the quadratic form of $H(l)$ we can trace out the fermion degrees of freedom to obtain

$$\begin{aligned} Z &= \mathrm{tr}_\sigma \det(I + B_L B_{L-1} \cdots B_1) \\ &= \mathrm{tr}_\sigma \det(I + B_{L-1} \cdots B_1 B_L) \qquad \text{etc.} \\ &= \mathrm{tr}_\sigma \, z[\sigma] \end{aligned}$$

where

$$B_l = e^{-\tau h(l)}$$

and

$$z[\sigma] = \det(I + B_l \cdots B_1 B_L \cdots B_{l+1}) \tag{11}$$

is the partition function associated with a given configuration of the Ising-like variables.

3.3. The Green's Function

For every time step l, the Monte Carlo procedure consists of deciding whether to accept or reject a spin flip at each site to which the Hubbard–

Stratanovich transformation was applied. The decision is generally based on the Metropolis[3] or heat bath algorithms; however, in contrast to classical statistical mechanics where one examines the ratio

$$e^{-\beta H[\sigma']}/e^{-\beta H[\sigma]}$$

we must examine

$$z[\sigma']/z[\sigma]$$

The evaluation of $z[\sigma]$ generally involves LN^3 multiplications where N is the number of degrees of freedom in the original problem. To reduce the computation time, the following alternatives have been devised[1]: The cyclic properties of the products of the Bs presented in (11) are used so that at the lth time step

$$z[\sigma] = \det(I + B_{l+1} \cdots B_1 B_L \cdots B_l) \tag{12}$$

Then, for a new configuration we write the new B_l as $B_l \Delta_l$. Hence

$$\frac{z[\sigma']}{z[\sigma]} = \frac{\det(I + B_{l+1} \cdots B_1 B_L \cdots B_l \Delta_l)}{\det(I + B_{l+1} \cdots B_1 B_L \cdots B_l)}$$

Defining

$$g_l = (I + B_{l+1} \cdots B_1 B_L \cdots B_l)^{-1} \tag{13}$$

we can reexpress the ratio by

$$\det[I - (g_l - I)(\Delta_l - I)] \tag{14}$$

When the interactions are short-ranged, $\Delta_l - I$ is a sparse matrix and (14) can be directly evaluated for the single impurity Anderson model in terms of the local matrix elements of g_l with operations of order 1.

On the surface, g_l requires as many operations $O(N^3)$ to compute as the original determinant. However, there are several useful relations[2] which allow the operation count to be reduced. The first generates a new g'_l from the old g_l whenever the configuration changes. Starting with

$$g'_l = (I + B_{l+1} \cdots B_1 B_L \cdots B_l \Delta_l)^{-1}$$

one can show[2]

$$g'_l = g_l - (I - g_l)(\Delta_l - I)\, g'_l \tag{15}$$

Because of the sparseness of $(\Delta_l - I)$ the equation can usually be solved for g'_l in $O(N^2)$ operations.

We also have a procedure[2] to go from one time to another more efficiently than by constructing the appropriate g from (13). It is

$$g_{l+1} = B_l\, g_l B_l^{-1} \tag{16}$$

The main point is, after having made g_1 via (13) at the very start of the simulation, we in principle can generate all other g_ls in considerably fewer operations via (15) and (16) than by (13). In practice, errors buildup and so, to maintain an acceptable level of precision, (13) is used, from time to time, to control these errors.

The functions g_l instead of $z[\sigma]$ are the principal quantities needed and computed in the simulations. This in some sense is a fortunate circumstance, for one can show[2-4] that

$$[g_l]_{ij} = \langle c_i(l)\, c_j^+(l) \rangle$$

and

$$\langle n_i(l) \rangle = 1 - [g_l]_{ii}$$

One can also find specific expressions[1,7] for the unequal time Green's functions in terms of products of the B_ls.

3.4. Computed Quantities

The Green's function is the principal result obtained from our simulation. With it and the use of Wick's theorem, we are able to compute relevant thermodynamic and many-body correlation functions. Quantities computed by this method include: the energy, specific heat, magnetic susceptibility, etc. To illustrate the procedure, we will now sketch the computation of the average energy for the single impurity Anderson Hamiltonian,

$$E = \langle H \rangle$$

From (8) we see that averages like $\langle c_{is}^+ c_{js} \rangle$ and $\langle n_{d\uparrow} n_{d\downarrow} \rangle$ are needed. Since in (8) $i \neq j$, $\langle c_{is}^+ c_{js} \rangle = -\langle c_{is} c_{js}^+ \rangle$, which is just g_{ij}^s. To do the other type of average, we use Wick's theorem[8]:

$$\begin{aligned} \langle n_{d\uparrow} n_{d\downarrow} \rangle &= \langle d_{d\uparrow}^+ d_{d\uparrow} d_{d\downarrow}^+ d_{d\downarrow} \rangle \\ &= \langle d_{d\uparrow}^+ d_{d\uparrow} \rangle \langle d_{d\downarrow}^+ d_{d\downarrow} \rangle - \langle d_{d\downarrow} d_{d\uparrow}^+ \rangle \langle d_{d\uparrow} d_{d\downarrow}^+ \rangle \end{aligned}$$

The averages in the first term on the right-hand side are just $\langle n_{is} \rangle = 1 - g_{ii}^s$. Those in the last term are zero! The Hubbard–Stratanovich transformation took the term with explicit interactions between opposite spins and replaced it with one that produces an effective Hamiltonian block diagonal in s. For purposes of computing $\langle d_{d\uparrow} d_{d\downarrow}^+ \rangle$ etc. there are no correlations between spins, and so such averages are zero. The spin correlations remain only implicitly: the spins interact through the Ising spin field which may be regarded as an imaginary-time dependent, external field that is summed over all possible configurations.

4. RESULTS

To date our simulations of the single impurity Anderson model have been for a one-dimensional chain appropriate to a quasi one-dimensional material. In this case the band energies resulting from the hopping term in the Hamiltonian are $\varepsilon_k = -2t \cos k$. The same simulation code gives results for two- and three-dimensional systems when ε_k is suitably altered. For example, a 16-site chain has 16 ε_k states and its running time is equivalent to a 4×4 two-dimensional lattice. A $4 \times 4 \times 4$ three-dimensional lattice has a running time equivalent to a 64-site, one-dimensional chain.

For the model we have computed a variety of physical quantities, including energy, specific heat, and d-orbital susceptibility

$$\chi_d = \int_0^\beta d\tau \langle [n_{d\uparrow}(\tau) - n_{d\downarrow}(\tau)][n_{d\uparrow}(0) - n_{d\downarrow}(0)] \rangle \tag{17}$$

the magnitude of the d-orbital magnetization

$$M_d = \langle |n_{d\uparrow} - n_{d\downarrow}| \rangle$$

and the d orbital occupation

$$N_d = \langle n_{d\uparrow} + n_{d\downarrow} \rangle$$

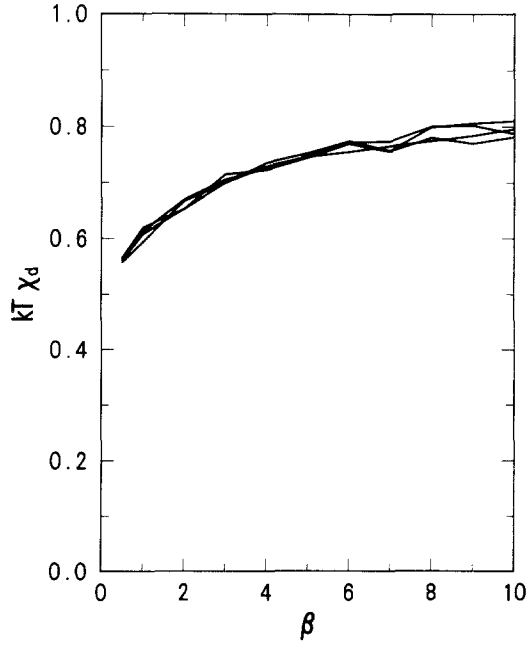

Fig. 1. The impurity susceptibility $kT\chi_d$ for the symmetric model as a function of β. $E_d = -U/2$, $V = 1$, and the different curves are for $N = 4$, 8, 12, and 16.

We also have calculated the spatial spin correlation function

$$C(i) = \langle (n_{i\uparrow} - n_{i\downarrow})(n_{d\downarrow} - n_{d\uparrow}) \rangle \tag{18}$$

and the charge density correlations

$$D(i) = \langle (n_{i\uparrow} + n_{i\downarrow})(n_{d\uparrow} + n_{d\downarrow}) \rangle \tag{19}$$

These latter quantities are extremely difficult to compute by renormalization group[9] and Bethe-ansatz[10] approaches to the related problems.

In Figs. 1–3 we know $kT\chi_d$ as a function of β where χ_d is in units of the Bohr magneton squared and kT in units of the halfband width $2t$. Figure 1 is for a symmetric model where $U = -E_d/2 = 1$. Such models have particle-hole symmetry and can exhibit local moment formation and Kondo peaks in $kT\chi_d$. For our choice of parameters and range of β we clearly see the growth in $kT\chi_d$ associated with local moment development. Our $kT\chi_d$ results are consistent with local moment development implied by our M_d calculations. Mixed valence behavior is illustrated in Fig. 2 by $kT\chi_d$ obtaining a low temperature values of $\frac{2}{3}$. Again M_d, as well as N_d, calculation also implies mixed valence behavior. The Kondo peak in the

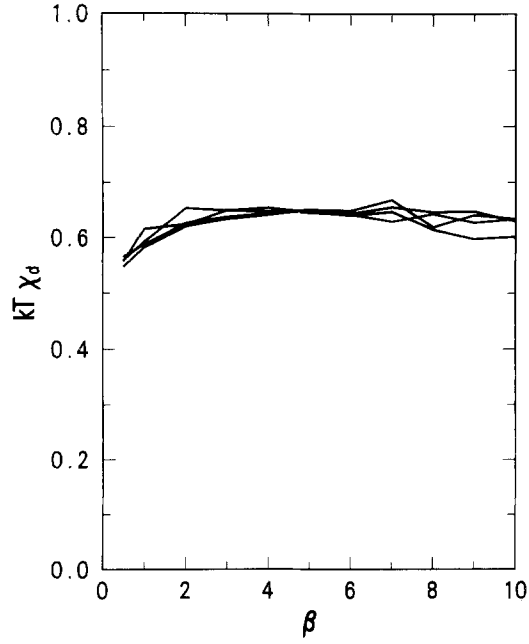

Fig. 2. The impurity susceptibility $kT\chi_d$ for a function of β. $U = 1$, $E_d = 0$, $V = 1$, and the different curves are for $N = 4$, 8, 12, and 16.

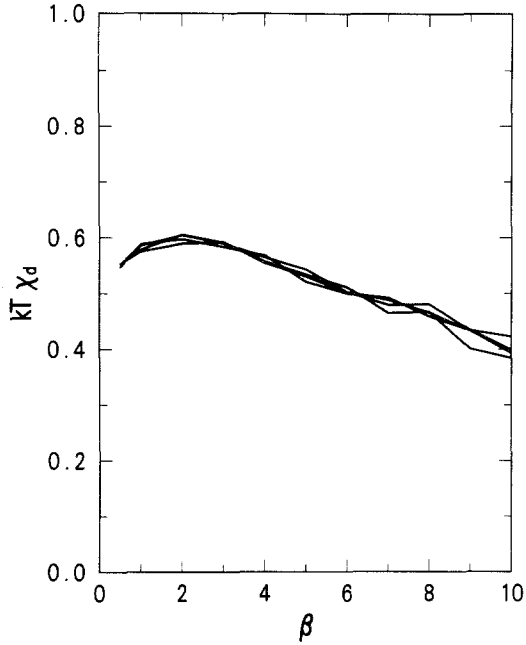

Fig. 3. The impurity susceptibility $kT\chi_d$ for an asymmetric model as a function of β. $U=1$, $E_d=0.1$, $V=1$, and the different curves are for $N=4$, 8, 12, and 16.

susceptibility is shown in Fig. 3. Besides the peak, the freezing out of the local moment, indicated by $kT\chi_d$ tending to zero as β is increased, is also seen. Similar behavior might occur for the case shown in Fig. 1; however, we are unable to carry the simulation to β large enough so see this decease.

We also observed RKKY and Friedel-like oscillations in the spatial spin (18) and charge density (19) correlation functions. For the spatial spins a negative correlation between the spin at the impurity site and at site 0 exists. For both correlation functions the amplitude increases as the temperature decreases, decreases as the distance from the impurity increases, and alternates in sign from site to site. For a value of $U=1$, we observed that as V increases the spatial spin correlations become stronger even though the measured magnetic moments become smaller. These trends were more pronounced for an asymmetric model ($E_d=0$) than for the symmetric model ($E_d=-0.5$). The charge density correlation function showed the same trends with V, but the size of the effect was approximately the same for both the symmetric and asymmetric cases. To a good approximation, the charge at the impurity site is uncorrelated with the charge at the lattice sites.

5. SUMMARY

We presented a brief description of the determinant method and reported our initial findings on using the method to simulate many-body effects in a single impurity Anderson model. We have successfully simulated local moment formation, Kondo peaking in the susceptibility, and mixed valence behavior and have presented calculations of the impurity susceptibility that illustrate these effects. We have also observed RKKY and Friedel-like oscillations in the spatial spin and charge density correlation functions. Our full results will be reported elsewhere.

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