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Numerical renormalization group for finite Hubbard lattices

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We have developed a numerical renormalization-group approach for finite fermion systems, related to the approach used by Wilson for the Kondo problem. Results are similar to those of exact diagonalizations; however, larger systems can be studied and results are obtained for the ground state and many excited states simultaneously. Results for 4×4 Hubbard lattices are given.

There are two approaches currently in wide use for numerical studies of strongly interacting electrons systems, such as the two-dimensional Hubbard model: quantum Monte Carlo and exact diagonalization. The quantum Monte Carlo method, in its most widely used form,[1,2] can be used on Hubbard lattices as large as 16×16, but has difficulty in reaching low temperatures because of the sign problem.[3,4] Furthermore, while the imaginary-time Green's functions obtained from Monte Carlo techniques are very useful in calculating static properties,[2,5] information about excitations can only be obtained through a difficult analytic continuation to get dynamical correlation functions.[6-8]

Exact diagonalization,[9-11] usually using the Lanczos algorithm, gives ground-state static and dynamic correlation functions and energies, but is limited to small lattices. Only recently has it been possible to study a 4×4 lattice, and a 4×4 calculation is still extremely demanding computationally. Because the calculation time and memory required grow exponentially with the number of sites, a study of a 6×6 lattice is completely out of the question for the foreseeable future.

The renormalization-group method presented here is designed to give results similar to exact diagonalization but on larger, though still finite lattices. Results for the ground state and dozens of low-lying excited states on 4×4 lattices can be obtained in hours rather than weeks, with good accuracy. Most importantly, 6×6 and larger lattices are feasible: In addition to the 4×4 results we present here, we have obtained some preliminary results on 6×6 lattices. With foreseeable improvements to the algorithm, we believe 8×8 (or larger) lattices will be possible.

Our procedure is patterned after Wilson's treatment of the Kondo problem,[12] with some key differences. The first step in Wilson's treatment was a clever rewriting of the Hamiltonian which left it in nearly "tridiagonal" form: Matrix elements between states at widely separated iterations were very small. The existence of this transformation of the Hamiltonian is related to the radial nature of the Kondo problem, and is not available in the two-dimensional (2D) Hubbard model. We have found that one can still obtain good results for finite systems even when many of the off-diagonal matrix elements are not so small. The second step in Wilson's treatment was a numerical procedure which involved expanding the Hilbert space at each iteration by applying creation and annihilation operators involving an additional momentum, but then eliminating high-lying states to maintain a fixed number. This aspect of Wilson's treatment is the key ingredient in our approach. Finally, Wilson analyzed the results in terms of standard renormalization-group fixed-point analysis. Since our approach is intended only for finite systems, this step is not relevant: After the last iteration, one simply takes the final states as the ground and low-lying excited states of a finite lattice.

The Hubbard Hamiltonian in momentum space is

$$H=\sum_{p,\sigma}(\epsilon_p-\mu)c^\dagger_{p,\sigma}c_{p,\sigma}+\frac{U}{N}\sum_{k,p,q}c^\dagger_{p+q,\uparrow}c^\dagger_{k-q,\downarrow}c_{k,\downarrow}c_{p,\uparrow}\,, \tag{1}$$

where (in 2D) $\epsilon_p=-2t(\cos p_x+\cos p_y)$, σ is the spin, the lattice spacing is taken to be 1, and $N=N_x\times N_x$ is the number of sites. The allowed momenta are $p_{x,y}=0,2\pi/N_x,\ldots,2\pi(N_x-1)/N_x$. We start our procedure with a filled Fermi sea. The initial state is taken as

$$|0\rangle=\prod_{k<k_{F,\sigma}}c^\dagger_{k,\sigma}|\text{vac}\rangle\,. \tag{2}$$

We define creation operators $a^\dagger_{k,\sigma}$ as

$$a^\dagger_{k,\sigma}\equiv\begin{cases}c^\dagger_{k,\sigma}, & k>k_F\,,\\ c_{k,\sigma}, & k<k_F\,.\end{cases} \tag{3}$$

Before starting the procedure, we must *order* the N allowed momenta. The ordered list is used to specify at which iteration the degrees of freedom for a particular k are used to expand the Hilbert space. We order the list according to the following criteria: (1) the farther a k is in energy from k_F, the earlier it appears on the list (and the sooner it is used to create new states); and (2) k's which interact strongly, such as k and $-k$, or k and $k+Q$, where $Q=(\pi,\pi)$, are made adjacent in the list. These criteria are somewhat ambiguous; alternative orderings can be used to estimate errors in energy differences.

The basic algorithm is given in Table I. At each iteration i the number of states expands by a factor of 4, stemming from the four possible degrees of freedom associated with k_i. Clearly, if steps (2)–(5) in Table I were omitted, one would generate a complete basis for the 4^N-dimensional Hilbert space, and diagonalization within that basis would be exact. However, after diagonalization at each iteration the Hilbert space is truncated down to the lowest L states, where L ranges from 1000 to

TABLE I. Renormalization-group algorithm.

(0) Start with one state, $|\psi_1\rangle=\prod_{k<k_F,\sigma}c^\dagger_{k,\sigma}|0\rangle$. Calculate $\langle\psi_1|H|\psi_1\rangle$ and $\langle\psi_1|h_a|\psi_1\rangle$. Set $i=0$, $N_{\rm state}=1$.
(1) Set $i=i+1$. Replace each state $|\psi_j\rangle, j=1,\ldots,N_{\rm state}$ by four states: $|\psi_j\rangle$, $a^\dagger_{k_i,\uparrow}|\psi_j\rangle$, $a^\dagger_{k_i,\downarrow}|\psi_j\rangle$, and $a^\dagger_{k_i,\downarrow}a^\dagger_{k_i,\uparrow}|\psi_j\rangle$. Only a few numbers need be stored for each state, such as its quantum numbers and the index of its parent state. Set $N_{\rm state}=4N_{\rm state}$.
(2) Evaluate $\langle\psi_j|H|\psi_{j'}\rangle$ and $\langle\psi_j|h_a|\psi_{j'}\rangle$ for $j,j'=1,\ldots,N_{\rm state}$, using tabulated $\langle\psi_j|h_a|\psi_{j'}\rangle$ from previous iteration [see Eq. (4) in text].
(3) Diagonalize $N_{\rm state}\times N_{\rm state}$ matrix $\langle\psi_j|H|\psi_{j'}\rangle$. Eigenvectors form new set of $|\psi_j\rangle$.
(4) Change $\langle\psi_j|H|\psi_{j'}\rangle$ and $\langle\psi_j|h_a|\psi_{j'}\rangle$ to new eigenstate basis.
(5) Sort states in order of increasing energy. Set $N_{\rm state}=\min(N_{\rm state},L)$. Discard states $|\psi_j\rangle$ with $j>N_{\rm state}$.
(6) If $i<N$, go to step 1.

4000–5000. This truncation is the only approximation made. The states formed in the last iterations are the most important, involving k's at the Fermi surface. The states at earlier iterations consist of the original state $|\psi_1\rangle$ (partially dressed) plus high-lying excitations; the excitations serve to dress $|\psi_1\rangle$ and the low-lying states formed later.

No explicit representation of the states is kept in this procedure, only operator matrix elements between the states. The Hamiltonian is formed at iteration i using matrix elements of operators h_a, which we call *partial Hamiltonians,* between states from iteration $i-1$. For example, if $|\psi\rangle$ and $|\psi'\rangle$ are two of the L states which are kept at the end of iteration $i-1$, then two of the $4L$ states at iteration i are $|\psi\rangle$ and $c^\dagger_{k_i,\uparrow}|\psi'\rangle$ (assuming $k_i>k_F$). All states $|\psi\rangle$ from iteration $i-1$ have the property that $c_{k_i,\uparrow}|\psi\rangle=0$. The Hamiltonian matrix element between these two iteration-i states is thus trivially given in terms of a commutator and iteration $i-1$ states,

$$\langle\psi|H(c^\dagger_{k_i,\uparrow}|\psi'\rangle)=\langle\psi|[H,c^\dagger_{k_i,\uparrow}]|\psi'\rangle\,. \tag{4}$$

The h_a are the set of all operators which can be obtained by taking the commutator of H with $c^\dagger_{k,\sigma}$ or $c_{k,\sigma}$ one or more times (e.g., $[[H,c^\dagger_{k,\sigma}],c_{k',\sigma'}]$ but not $[[H,c^\dagger_{k,\sigma}],H]$). The complete list of the h_a is $\sum_p c^\dagger_{p,\sigma}$, $\sum_p c^\dagger_{p,\sigma}c_{p,\sigma}$, $\sum_{p,q}c^\dagger_{p,\sigma}c_{q,\sigma'}$, $\sum_{p,q}c^\dagger_{p,\uparrow}c^\dagger_{q,\downarrow}$, and $\sum_{k,p,q}c^\dagger_{k,\sigma}c^\dagger_{p,-\sigma}c_{q,-\sigma}$, plus all distinct Hermitian conjugates. The matrix elements of the h_a provide all the information needed to construct the matrix elements of H for the next iteration.

The states at each iteration can be classified by the number of up and down particles, $N_\uparrow$ and $N_\downarrow$, and the total momentum P. Because the corresponding operators commute with the Hamiltonian, the Hamiltonian matrix is block diagonal. Thus one needs to diagonalize only a small subset of the matrix at a time, allowing us to keep many more states than otherwise would be possible. The h_a are *not* block diagonal, so the change of basis for them is by far the most time-consuming part of the entire procedure.

One obtains as results the quantum numbers $N_\uparrow$, $N_\downarrow$, and P, and the kinetic and potential energies of L low-lying states. In addition, one gets the matrix elements of each of the partial Hamiltonians between each pair of states. In principle, we can obtain any static correlation function in the same way that we obtain the kinetic and potential energies.

The success of this approach hinges on whether one can keep enough states to include all those which interact *strongly* with the low-lying states of interest. Whether one state interacts strongly with another depends on the size of the interaction between them and on their energy difference. By diagonalizing the Hamiltonian at each iteration, we eliminate the couplings between each of the *current* low-lying states. However, as we add new states, new couplings are generated. In our momentum-space formulation, the size of the couplings generated is roughly U/N, independent of the iteration (as opposed to the Kondo problem, where the interaction scales with the energy-level spacings). Thus we would like to keep all low-lying states within a range of, say, 5 or 10 times U/N. In the early iterations, it is easy to keep enough states; in the later iterations, as momenta near k_F come in, more states are important. One is ultimately limited in what size lattice one can do by the growing number of excited states within a range of U/N of the ground state.

We do not expect this procedure to be especially accurate at total energies, but we do expect good results for *energy differences.* The main reason is that the vast majority of these truncated states involve excitations far from the Fermi surface, and these states, taken as a whole, affect all the low-lying states nearly equally. In particular, most of the low-lying final states have a recent common ancestor, and it is only in the last few iterations, after their last common ancestor, that two states could have had their energy difference affected by the truncated states. (Note that since the truncation of the Hilbert space is the only approximation used, results for total energies are variational.)

The total spin of each final state can be easily inferred: Since $c^\dagger_{k_i,\uparrow}$ and $c^\dagger_{k_i,\downarrow}$ are both used to create new states in the same iteration (before any truncation), the spin degeneracies are preserved exactly. Thus a sixteen-particle $S=1$ state appears as a degenerate triplet, with $N_\uparrow,N_\downarrow$ taking the values 7,9, 8,8, and 9,7. Exact degeneracies between different total momenta are not preserved, but can be used to estimate errors in energy differences.

Figure 1 summarizes the final results from a single 4×4 calculation, keeping $L=3000$ states, which took about 6 h on the University of California at Irvine Convex C240. The chemical potential was chosen to make the lowest-lying ten- through sixteen-particle states as close in energy as possible. Exact diagonalization results are available for a comparison of a few of these states. In general, we find excellent agreement with the available exact results, except that the renormalization-group procedure cannot

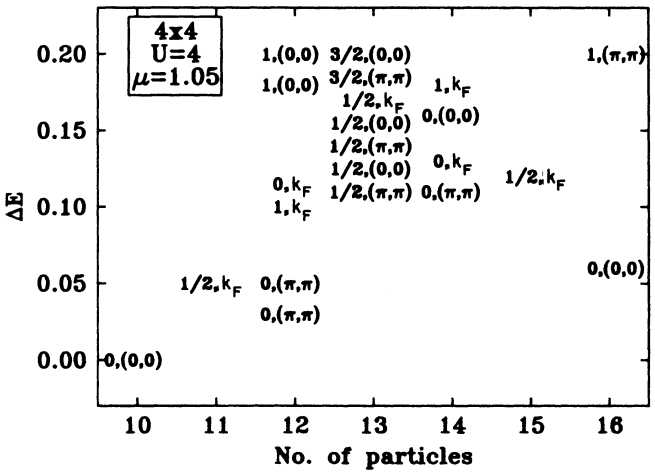

FIG. 1. Low-lying (final) states of the 4×4 Hubbard model with $U=4$, $t=1$ for various particle numbers. The first number for each state is the total spin, and the pair of numbers in parentheses is the total momentum. The vertical axis shows the difference in energy between the given state and the ten-particle ground-state energy of -29.041. The momenta labeled k_F represent the six states $(\pm\pi/2, \pm\pi/2)$, $(\pi,0)$, and $(0,\pi)$. Although the first four of these are not necessarily degenerate with the last two, the small energy splittings between these momenta could not be resolved accurately.

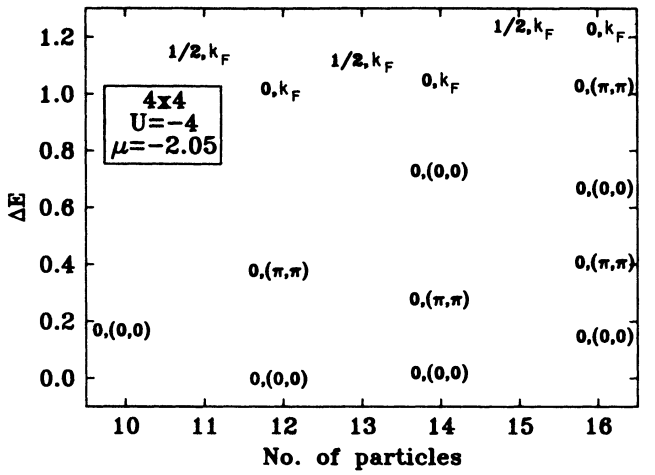

FIG. 2. Low-lying states with $U=-4$. The total energy for the twelve-particle ground state was -11.326.

resolve very close near degeneracies and gives poor results for total energies (as expected).

The lowest half-filled (sixteen-particle) state is the expected antiferromagnetic singlet. The next sixteen-particle state we interpret as having a spin wave with momentum (π,π), $S=1$, as one might have anticipated from the form of the spin-wave dispersion relation.[2] Its energy separation $E-E^0_{16}$ from the lowest sixteen-particle state is 0.14, in agreement with the exact-diagonalization result of 0.139.[13] The next state (not shown) has two (π,π) spin waves, for a total momentum of (0,0), $S=2$, with $E-E^0_{16}=0.44$. Parola *et al.*[10] have studied the fourteen-particle case with exact diagonalization, finding the lowest-lying $S=0$ state for each P. They found that the ground states for eight of the momenta were very nearly degenerate (with a splitting of 0.002). These eight states are represented by the three fourteen-particle $S=0$ levels shown in Fig. 1. The larger splittings of about 0.05 that we find are errors associated with only keeping 3000 states. They found a splitting of 0.99 from those eight states to the next lowest $S=0$ state $[P=(0,\pi/2)]$. We find a splitting of about 1.1. In general, we estimate an uncertainty of about 0.06 in energy splittings between low-lying states with the same particle number. Errors between states with different particle numbers are slightly larger. Total energies, as expected, are less accurate; they are off by about 1.

Figure 2 shows results for $U=-4$, again with $L=3000$. The superconducting nature of the ground state is evident: The ground states for different even particle numbers are nearly degenerate singlet states with total momentum 0. States with odd particle numbers have a single quasiparticle excitation, with a gap of about 1, and with the quasiparticle on the Fermi surface. We also find anomalously large matrix elements of $\Delta^\dagger=\sum_p c^\dagger_{p,\uparrow}c^\dagger_{-p,\downarrow}$ (obtained from one of the partial Hamiltonians) between the M and $M+2$ particle ground states, indicating superconducting order. We interpret the low-lying singlet states with momentum (π,π) as charge-density-wave states.

A rough estimate shows that the calculation time grows roughly as N^3 to N^4 with lattice size, assuming a fixed number of states are kept in each block containing low-lying states. We have tried out this procedure on a 6×6 lattice with $U=4$, keeping $L=3000$ states. The errors in energy differences, judging by the splitting of what should be degenerate total momenta, were about a factor of 3 worse than the corresponding 4×4 calculation keeping 3000 states. We believe the prospects for applying this technique to larger lattices are quite good.

The present procedure is still in a very early stage of development. We mention three promising directions for future improvement. First, one can work in other single-particle bases besides momentum space. A real-space basis would be much more appropriate in the large-U regime, and intermediate-coupling regimes would probably be best treated with a basis somewhat localized in both real and momentum space. Second, rather than keeping a state for each value of S_z and inferring spin quantum numbers, one should keep only one of the $2S+1$ degenerate states in each multiplet. This, plus a similar treatment of states related by lattice rational symmetry, might speed the calculation by an order of magnitude. Third, a Lanczos treatment of the final five or ten k_i's could easily be incorporated. In other words, the initial iterations would proceed as in the present procedure, but the final five or ten would be done all at once with no truncations, using the ability of the Lanczos procedure to handle large, sparse matrices. This would be possible because there is no need for the last iteration to keep track of all the partial Hamiltonian matrix elements.

Note added in proof. Recent exact diagonalization results[14] indicate that the ground state for twelve particles and $U=4$ has quantum numbers 0, (0,0), in disagreement with the result shown in Fig. 1.

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