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Computer renormalization-group technique applied to the Hubbard model

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We present a computer renormalization-group technique of value in solving Hamiltonians which may be expressed in site-interactive forms of short range. The technique delivers the eigenfunctions and eigenvalues in a finite energy range about the highest occupied energy level for a finite chain or cluster. With the method, the Hubbard Hamiltonian is solved up to 16 sites, and the thermodynamical quantities and $2k_F$ density autocorrelation function are computed.

The purpose of this paper is to introduce a new computational technique of value in solving a variety of Hamiltonians which may be expressed as terms which transfer particles a short distance from site to site on a lattice. The technique is a computer renormalization-group (CRG) treatment which delivers an inexact but controlled approximate solution to the eigenfunctions and eigenvalues, and therefore to all properties, of the Hamiltonian. To illustrate the technique, we present solutions to the one-dimensional (1-D) Hubbard model.[1] Solutions of this model are themselves of interest in connection with the role of Coulomb interactions in quasi-1-D systems. In particular, the elucidation of such properties as magnetic susceptibility and the $2k_F$ and $4k_F$ anomalies (k_F is the Fermi wave vector) may require a complete understanding of the Hubbard model.

The Hubbard model in one dimension has been the subject of many theoretical papers. The model is simply stated:

$$H_N = \sum_{\substack{i=1 \\ \sigma}}^{N} (t a_{i\sigma}^{\dagger} a_{i+1,\sigma} + H.C.) + \sum_{i=1}^{N} U n_{i\uparrow} n_{i\downarrow} , \qquad (1)$$

where $n_{i\sigma} a \equiv a_{i\sigma}^{\dagger} a_{i\sigma}$, $a_{i\sigma}^{\dagger}(a_{i\sigma})$ is the creation (destruction) operator for an electron on site i with spin σ, t is the nearest-neighbor transfer energy, and U is the on-site Coulomb energy. The chain consists of N sites with uniform spacing d. The Hubbard model is usually regarded as the $N \to \infty$ limit. The model has two parameters: the ratio U/t and the average number of electrons per site ρ.

A very large number of calculations have been performed on this model. The ground state has been found exactly by Lieb and Wu,[2] and the spectrum of excited states can be calculated from the work of Shiba,[3] Ovchinikov,[4] and Cole.[5] Further calculations that give good results for particular cases have been performed by Brinkman and Rice[6] and Economou and White.[7] However, there has so far been no calculation by which the low-lying eigenfunctions of (1) for arbitrary ρ can be obtained within a controlled approximation; i.e., the spectral densities are not known. The elimination of this roadblock and the subsequent realization of a complete, quantitative solution of the Hubbard model are possible within our CRG calculation.

Various computer solutions of the Hubbard model on finite chains or rings have been produced.[8,9] Generally, the number of sites N in such calculations must be less than six because otherwise the size of the matrices to be diagonalized becomes too great—the number of possible eigenstates goes roughly as 2^{2N}. A number of properties which one would like to calculate for the infinite chain cannot be extracted from treatments of such small chains. In addition, the properties of longer chains are interesting in themselves in the study of polymers and in finite-chain models of quasi-1-D systems. Our method allows treatment of chains with $N \gg 6$.

Our CRG method is an iterative technique in which each step, or stage, begins with the solution (eighfunctions and eigenvalues) of the Hamiltonian H_N. We then double the chain length and solve H_{2N} by reexpressing (renormalizing) H_{2N} in terms of the eigenstates of H_N (Fig. 1). This

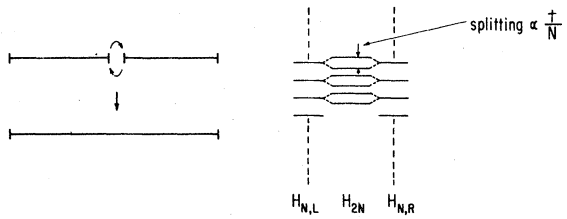

FIG. 1. Left and right chains of length Nd interact at their end points, and their energy levels split as shown.

process continues until the chain length is as long as required.

In more detail, consider

$$H_{2N}=H_{NL}+H_{NR}+H_I\ ,$$

where

$$\begin{aligned} H_{NL} &= t\sum_{\substack{i=1\\ \sigma}}^{N}(a_{i\sigma}^{\dagger}a_{i+1\sigma}+H.C.) \\ &\quad +U\sum_{i=1}^{N}n_{i_\uparrow}n_{i_\downarrow}\ , \\ H_{NR} &= t\sum_{\substack{i=N+1\\ \sigma}}^{2N}(a_{i\sigma}^{\dagger}a_{i+1\sigma}+H.C.) \\ &\quad +U\sum_{i=N+1}^{2N}n_{i_\uparrow}n_{i_\downarrow}\ , \\ H_I &= t\sum_{\sigma}(a_{N\sigma}^{\dagger}a_{N+1,\sigma}+H.C.)\ . \end{aligned} \tag{2}$$

We begin by solving H_2 exactly. The eigeninformation for H_{2N} is then computed by iterating scheme (2) $(\ln N)/(\ln 2)$ times. In any given step, the eigenfunctions of H_{2N} are those of H_N perturbed by H_I (Fig. 1). The eigenfunctions of H_N have $\sim N^{-1/2}$ of their weight at the ends of the chain, and so if we renormalize H_{2N} in terms of the eigenfunctions of H_N (H_{NL} and H_{NR}), the off-diagonal matrix elements (i.e., the strength of the perturbation from H_I) will be of order t/N. Since the number of eigenstates of H_N goes as $\sim 2^{2N}$, only a limited number may be retained at each iteration step after H_4. Thus we discard all eigenstates outside of some energy interval about the highest occupied eigenstate (E_F), which is the energy level of interest and is determined by ρ. To retain accuracy, the width of this energy interval should be much greater than the strength of H_I, e.g., $10t/N$. Therefore, at each iteration stage the energy interval within which states must be retained is decreased correspondingly as the total number of states increases such that the size of the computation remains unaltered with each iteration. As N increases, the eigenstates are computed to increasingly greater accuracy (relative to an infinite chain), but in an increasingly smaller interval about E_F.

We shall reserve fine details of the CRG to a later paper. Briefly, the process is expedited by using the quantum numbers of (1). We note that states of (1) may be simultaneously eigenstates of total charge, total spin, z component of total spin, and parity. We can thus enhance computational capability by working with one particular charge-spin-parity(CSP) manifold at a time in the above described iterative process. The eigenfunctions for H_{2N} are obtained by forming all possible product states of retained eigenfunctions of H_N ($\psi_{2N}=\psi_{NR}\psi_{NL}$), which are then diagonalized separately for each CSP. We retained around 600 product states in each of 30 CSP for a total of 18 000 states/iteration. About 150 of these 600 states which are closest to E_F were diagonalized directly and the rest by second-order perturbation theory. The lowest 10 (relative to E_F) diagonalized eigenvalues were retained in each CSP. These numbers for states calculated and retained in a CSP, while given in principle by the size of the t/N interval about E_F, were determined empirically by calculating a known case ($U/t=0$)(Ref.10) and adjusting until an accuracy of ~5% was obtained for the eigenvalues in the fourth stage. We note that for $U/t\neq 0$, the error should be smaller because a finite U pushes a number of eigenstates to higher energy (relative to E_F). Each of the higher stages of iteration requires ~15-min processor time and $\sim 81\times 10^3$ word random access memory (based on a Univac 1108).

Using the eigenvalues produced at each of several stages M (number of sites $N=2^M$), we have calculated the standard thermodynamical quantities versus temperature T. In Fig. 2 we show the entropy (S), specific heat (C), and magnetic susceptibility (χ) for the $U/t=2$, $\rho=1$ case. Note that three curves are shown for stages 2–4 (4, 8, and 16 sites). For stage 2, all states are retained, and the curves agree with the calculations of Shiba and Pinus.[9] For 8 and 16 sites, states are discarded away from E_F as previously described. Therefore, each of these curves gives accurate results only when $k_BT\ll E_M$, where E_M is the maximum energy of the retained states relative to E_F; i.e., k_BT must be small enough that the contribution of the discarded states to sums over $\exp(-E_i/k_BT)$ are negligible. By comparison to exact calculations for $U/t=0$, we have found that for $k_BT\leq 1.6\ t/2^{M-1}$ ($M\geq 3$, M is the stage), the error is less than $\sim 3.75\ (2^{M-1})\%$, which is three times the maximum absolute error of the eigenvalues in this calculation.

Another question is under what conditions these finite chain curves approximate the infinite chain. Two criteria must be met: the width of the total energy spectrum E_B for the finite chain should closely approximate the infinite chain (i.e., $E_B=4t+U$), and $\Delta E_M\lesssim k_BT$, where ΔE_M is the average level spacing among retained energies of state M. Calculations for $U=0$ indicate that the first condition is fulfilled to within 19%, 6%, and 2% at states 2, 3, and 4, respectively. Inspection of the energy levels shows $\Delta E_M\simeq t/2^{M-1}$. Thus this second criterion agrees with a further condition based on the fact that finite chains have a boundary energy of order $t/2^M$; viz., $k_BT\gtrsim t/2^{M-1}$, so that the boundary energy is not domi-

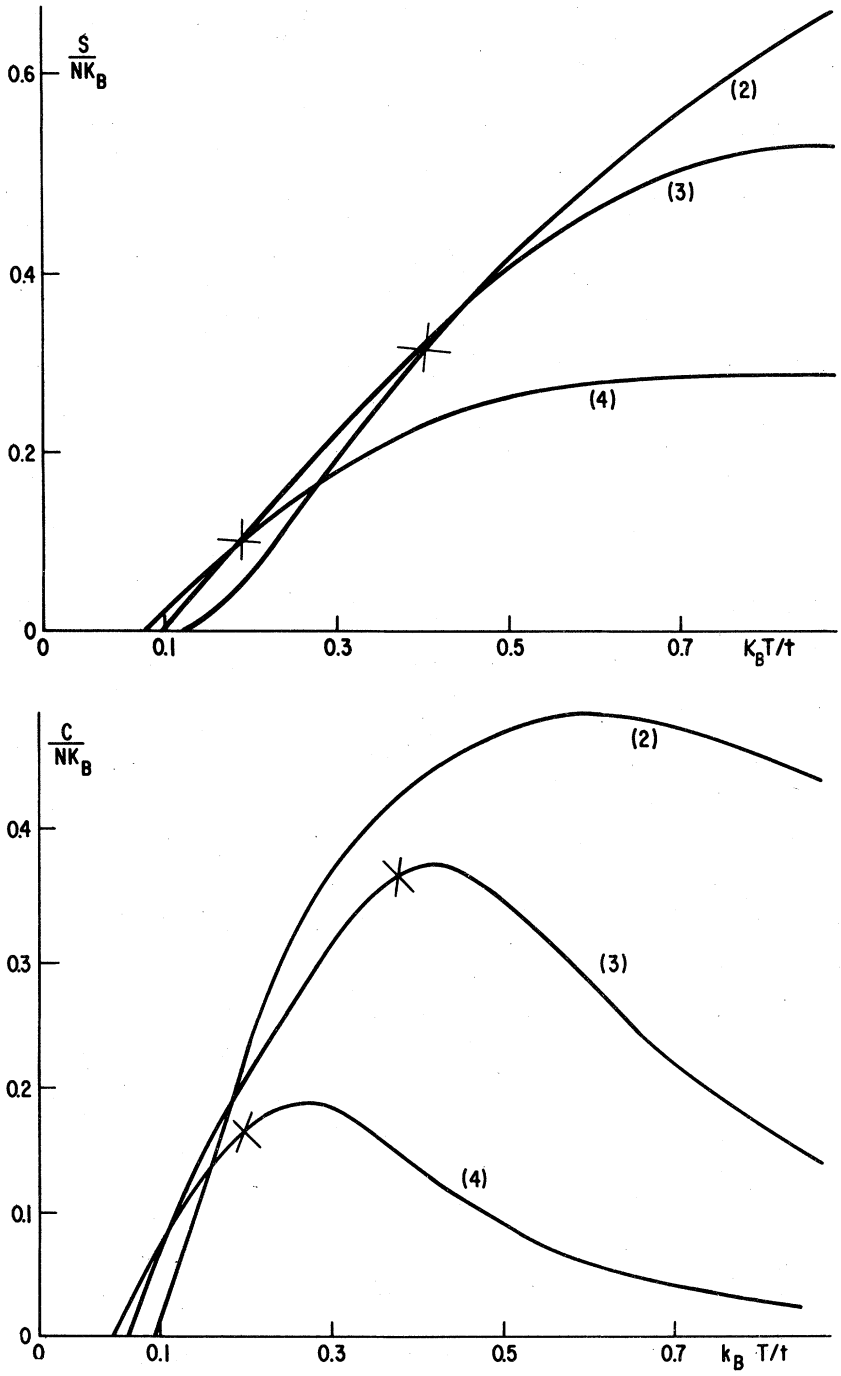

FIG. 2. Entropy S, specific heat C, and magnetic susceptibility χ for $U/t = 2$, $\rho = 1$. The numbers on the curves are the stage. An $\times$ denotes the upper limit of accuracy. (μ_B is equivalent to the Bohr magneton; $g = 2$.)

nant. Therefore, the envelope of the curves in Fig. 2 approximates the infinite chain above $T = \Delta E_4/k_B$ with an accuracy of at least 19%.

We have also calculated the $2k_F$ retarded density autocorrelation function at finite temperature. This function is given by

$$D^R(2k_F,\omega) = Z^{-1} \sum_{m,L} (2\pi e^{-\beta E_m} |\langle m|d'_{2k_F}|L\rangle|^2 \times [1 - e^{-\beta(E_L - E_m)}] [\omega - (E_L - E_m) + i\eta]^{-1}); \quad (3)$$

where

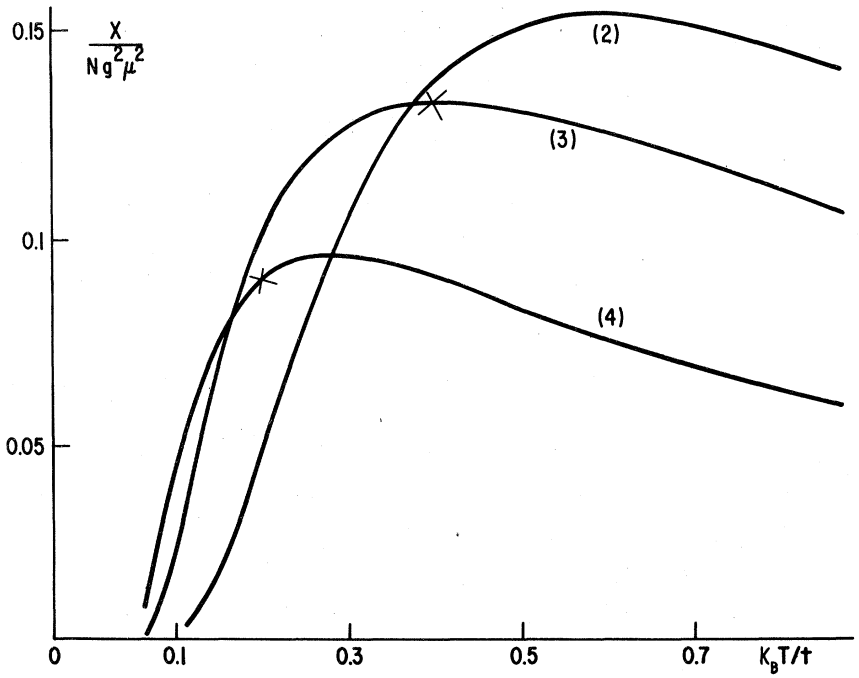

Fig. 2. (*Continued*)

$$Z \equiv \mathrm{Tr}(e^{-\beta H_N}),$$

$$d'_{2k_F} \equiv d_{2k_F} - \langle d_{2k_F} \rangle, d_{2k_F} \equiv \sum_{\substack{j=1 \\ \sigma}}^{N} e^{i2k_F j a} a^\dagger_{j\sigma} a_{j\sigma} .$$

Note that, in contrast to the thermodynamic quantities, the calculated eigenfunctions $|L\rangle$ are also used in this calculation. Figure 3 shows results for $U/t = 2$, $\rho = 1$. The validity range in temperature is more complicated for a correlation function because the matrix elements include transitions from the ground to excited states which are less than exponentially damped. If there is no gap in the energy spectrum, low-lying states are most important and the CRG results should be good within the limits given for C. A gap decreases the accuracy. In general, varying the number of states retained at each stage is the best way to obtain information on this matter. In Fig. 3, there is a gap since the $T = 0$ value of the real part does not diverge as $N \to \infty$, and the accuracy is 40%. ($M \geq 3$) to the indicated temperatures. The imaginary part for stage 4 only is shown because the imaginary parts for stages 3 and 2 were much smaller and qualitatively similar. We note that the $4k_F$ autocorrelation function is zero for $\rho = 1$.

Our CRG technique is similar to some other recent computer calculations. Drell *et al.*[11] have suggested a similar method for the φ^4 model of spinless fermions in one dimension and carried out a free-field case. Jullien *et al.*[12] have treated a 1-D chain of spins with a closely related technique but retained few states at each iterative stage. Wilson[13] has provided a valuable solution to the Kondo problem using a CRG technique. In this calculation, Wilson employed a simplified Kondo Hamiltonian of the form $H = |k| a^\dagger_k a_k$ with the Fermi surface at $k = 0$ (giving particle-hole symmetry). He considered only one electronic state for each order of k; i.e., he picked a constant $\Lambda > 1$ and considered only those states for which $|k| = \Lambda^{-N}$ for integers N. We have not performed this "logarithmic discretization" of Wilson but instead have treated the full Hamiltonian (1) in order to take the band structure and band filling

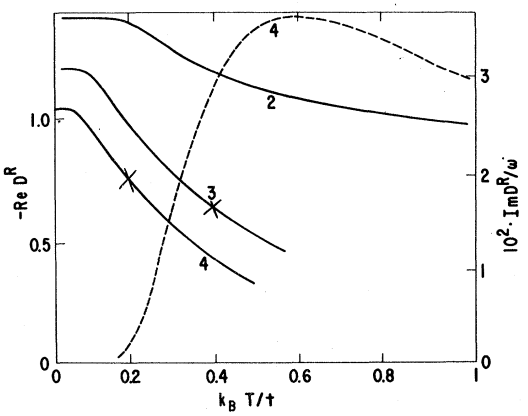

FIG. 3. Real (solid curve) and imaginary (dashed curve) parts of $D^R(2k_F, 0)$. $\mathrm{Im}(D^R/\omega)$ is for $\omega \to 0$. The numbers label the stage M. The curves are multiplied by 2^M for display. An $\times$ denotes the upper limit of accuracy.

fully into account. Therefore, the only source of error in the eigeninformation of our CRG is the elimination of the high-lying states at each stage.

In summary, we emphasize that this CRG technique[14] should have wide applicability to 1-D Hamiltonians which can be expressed in site-interactive forms with finite ranges. In addition, the method is intrinsically capable of being generalized to higher dimensions by treating 3-D clusters in an analogous manner. By such a generalization one can, for instance, include interchain coupling in the Hubbard model, a facet of the problem which appears necessary to obtain realistic descriptions of real quasi-1-D systems. Since our CRG is rather more complicated than most analytical approximations but since it delivers a controlled approximate solution, it can compliment other approximations by serving as a reference for their accuracy. We intend to calculate and report elsewhere more extensive solutions to the Hubbard model for other values of U/t and $\rho \neq 1$.

ACKNOWLEDGMENT

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