Real-space renormalization-group study of the Hubbard model: A modified scheme

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The real-space renormalization-group technique is applied to the Hubbard model on a linear chain with a half-filled band; a recently proposed modified scheme is used for the renormalization of the parameters. The result for the ground-state energy is quite improved with respect to the earlier results of the existing scheme. Both the energy and its derivative with respect to the on-site repulsion term agree reasonably well with the exact solution. However, it is indicated that the calculation of the correlation function and energy gap requires further refinement of this scheme. [S0163-1829(98)01616-6]

The development of suitable approximate techniques for solving an interacting many-fermion system remains a challenging task at present. There are few exact solutions and standard approximations such as the mean-field technique or the perturbative approaches often turn out to be inadequate for systems with strong fluctuations and intermediate coupling. These lead one to develop or improve upon a nonperturbative scheme such as the renormalization group (RG) that is particularly capable of handling the fluctuations. A real-space version of the RG[1–3] seemed to be very promising for studying the correlated electron systems such as the Hubbard model,[4] especially in low dimensions. Several modifications and extensions of this technique were worked out[5–7] for different types of short-ranged electronic correlations in such systems. In spite of its success in bringing out the essential physics,[1,5–7] this method suffered from a lack of quantitative precision. The reason behind this problem has recently been addressed[8,9] and consequently an approach known as the density-matrix RG has emerged. Inspired by similar ideas for removing the ''end effects'' and the effects of ''basis truncation'' in the finite-sized blocks used in the existing RG scheme,[1–7] we employed a different prescription[10] for renormalization of coupling parameters for a many-fermion system. In a preliminary calculation for the noninteracting fermions this showed a marked improvement over the existing RG results as far as the ground-state energy is concerned.[10] In this paper we attempt an application of this scheme to calculate the ground-state properties of the Hubbard model in one dimension for a half-filled band.

We start with a generalized Hubbard Hamiltonian on a linear chain:

$$H=t_1\sum_{\langle ij\rangle,\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}(1-n_{i-\sigma}-n_{j-\sigma})^2 + t_2\sum_{\langle ij\rangle,\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}[n_{i-\sigma}(1-n_{j-\sigma})+n_{j-\sigma}(1-n_{i-\sigma})] + U\sum_i n_{i\uparrow}n_{i\downarrow}-\mu\sum_{i,\sigma} n_{i\sigma}, \tag{1}$$

where $c_{i\sigma}^{\dagger}(c_{i\sigma})$ creates (annihilates) an electron with spin σ at the Wannier orbital at site i. t_1 and t_2 are hopping integrals between the nearest-neighbor sites i and j. U is the on-site correlation, while μ is the chemical potential. The case $t_1=t_2$ corresponds to the usual Hubbard model.[4] We start with $t_1=t_2=t$. $\mu=U/2$ for a half-filled band, which is particle-hole symmetric on a bipartite lattice. So we proceed with the effective Hamiltonian

$$H=t_1\sum_{\langle ij\rangle,\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}(1-n_{i-\sigma}-n_{j-\sigma})^2 + t_2\sum_{\langle ij\rangle,\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}[n_{i-\sigma}(1-n_{j-\sigma})+n_{j-\sigma}(1-n_{i-\sigma})] - \frac{U}{2}\sum_i (n_{i\uparrow}-n_{i\downarrow})^2 + C\sum_i \mathbf{1}_i. \tag{2}$$

We have added a constant term C ($\mathbf{1}_i$ corresponds to the identity operator at site i), which is zero to start with and accounts for the renormalization of the ground-state energy. We then divide our lattice into identical three-site blocks. The block Hamiltonian is diagonalized to retain the four low-lying states of the block Hamiltonian in the subspaces $\{S_z=0,\ \nu=2\}$, $\{S_z=\frac{1}{2},\ \nu=3\}$, $\{S_z=-\frac{1}{2},\ \nu=3\}$, and $\{S_z=0,\ \nu=4\}$. These are identified with the renormalized $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow\downarrow\rangle$ states, respectively. Here S_z and ν are two conserved quantities of the block Hamiltonian, namely, the z component of the total spin and the total number of particles, respectively. Out of the retained states the first and the fourth are connected by the particle-hole symmetry, while the second and the third are connected by the spin-reversal symmetry. The parameters of the Hamiltonian are then renormalized within this truncated basis to yield the RG recursion relations.

Now to renormalize the on-site terms such as U and C we use the same prescription as used in the earlier works,[1,2,5–7] e.g.,

$$U^{(n+1)}=E_2^{(n)}-E_3^{(n)},\qquad C^{(n+1)}=3C^{(n)}+E_2^{(n)}, \tag{3}$$

where E_2 and E_3 are the lowest-energy states in the subspaces $\{S_z=0,\ \nu=2\}$ and $\{S_z=\frac{1}{2},\ \nu=3\}$, respectively. The

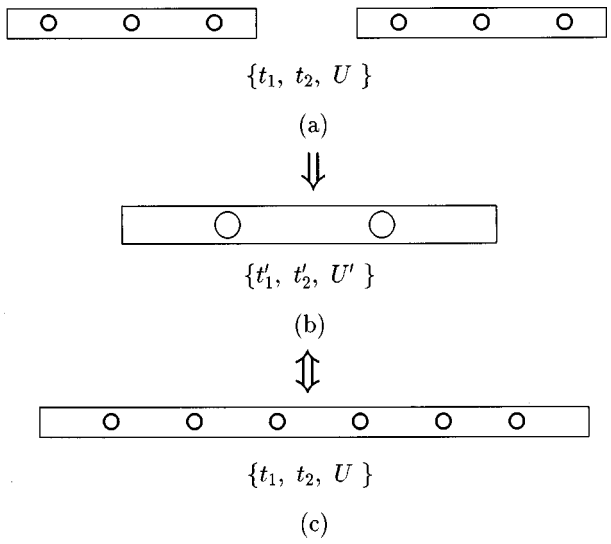

FIG. 1. Schematic diagram for the prescription of renormalizing the intersite parameters t_1 and t_2 using a superblock of six sites: (a) two adjacent blocks with three sites each before renormalization (with parameters t_1,t_2,U) and (b) the renormalized version (with parameters t_1',t_2',U') of those two blocks, i.e., a block of two renormalized ''sites,'' which is equivalent to (c) a six-site superblock constituted of two three-site blocks (with parameters t_1,t_2,U).

superscript (n) refers to the renormalized quantities at the nth recursion. However, to renormalize the interblock terms t_1 and t_2 we use the lowest-lying energies of a ''superblock'' containing two such blocks.[10]

At this point we consider the effect of the environment on an isolated block by immersing two such three-site blocks in a single superblock (Fig. 1) of six sites. In the renormalized length-scale these two blocks would look like two ''renormalized'' sites constituting a two-site block. Therefore, the lowest-lying state with one or two particles in the renormalized two-site block now corresponds to that with five or six particles in the six-site superblock with $S_z=1/2$ and 0, respectively. The lowest energies of the two-site block (with renormalized parameters) are

$$e_2^{(1)}=-U'/2-t_1'+2C',$$

$$e_2^{(2)}=(-U'-\sqrt{U'^2+16t_2'^2})/2+2C', \tag{4}$$

where, the subscript and superscript of e correspond to the block size and the particle number (in the renormalized scale), respectively. Primed quantities refer to the renormalized values of the parameters. The lowest-lying states in the six-site superblock are, however,

$$e_6^{(5)}=\tilde{e}_6^{(5)}(t_1,t_2,U)+6C,$$

$$e_6^{(6)}=\tilde{e}_6^{(6)}(t_1,t_2,U)+6C, \tag{5}$$

where $\tilde{e}_6^{(5)}$ and $\tilde{e}_6^{(6)}$ refer to the lowest energies corresponding to $C=0$ in the Hamiltonian (2) in a six-site block for five and six particles, respectively. Now we have

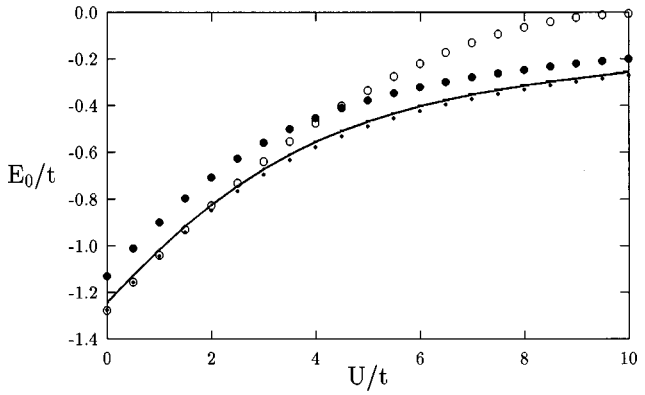

FIG. 2. Plot of E_0/t, the ground-state energy (scaled by the hopping integral) per site, as a function of the coupling constant U/t for the one-dimensional Hubbard chain at half filling. The result from the present calculation is indicated by the solid curve, while the dotted curve shows the exact result. ● shows the result obtained in the existing scheme of the real-space RG (Ref. 1) and ○ shows that obtained from Gutzwiller's approximation.

$$e_2^{(1)}(t_1',t_2',U',C')\simeq\tilde{e}_6^{(5)}(t_1,t_2,U)+6C,$$

$$e_2^{(2)}(t_1',t_2',U',C')\simeq\tilde{e}_6^{(6)}(t_1,t_2,U)+6C. \tag{6}$$

These relations lead to the renormalization of t_1 and t_2 as

$$t_1'=-U'/2+2E_2-\tilde{e}_6^{(5)}(t_1,t_2,U),$$

$$t_2'=\sqrt{-U'^2+(4E_2-U'-2\tilde{e}_6^{(6)})^2}/4, \tag{7}$$

which are to be used together with Eqs. (3). The recursion relations (3) and (7) are used to find the ground-state energy per site for an infinte chain, given by

$$E_0=\lim_{n\to\infty}\frac{C^{(n)}}{3^n}.$$

Instead of a six-site superblock, had we used an infinite superblock the relations (6) would turn out to be exact equalities and consequently we would have obtained the exact ground-state energy.

In Fig. 2 we have plotted the ground-state energy E_0 per site (scaled by the hopping integral t) for the half-filled Hubbard chain as a function of the coupling constant U/t. This agrees reasonably well with the exact solution[11] over the whole range of coupling. It turns out that using the present prescription improves the result by a significant extent compared to that obtained in the existing RG scheme,[1] which is also shown in Fig. 2. At this point it is important to note that although the ground-state energy turns out to be quite satisfactory in this scheme the energy gap is not so well behaved. This scheme fails to reproduce the Mott-Hubbard transition at $U/t=0$ that was present in the existing RG.[1,2] In fact, in the present scheme, a gap, given by $U^{(\infty)}$ (the value of U after infinite iterations), opens up at a finite value of $(U/t)_c \simeq 6.1$. Such a critical $(U/t)_c(\simeq 10.2)$ for a metal-insulator transition in the one-dimensional Hubbard model is obtained in the Gutzwiller approximation (GA) for a variational calculation.[12,13] The present RG approach also constructs it-

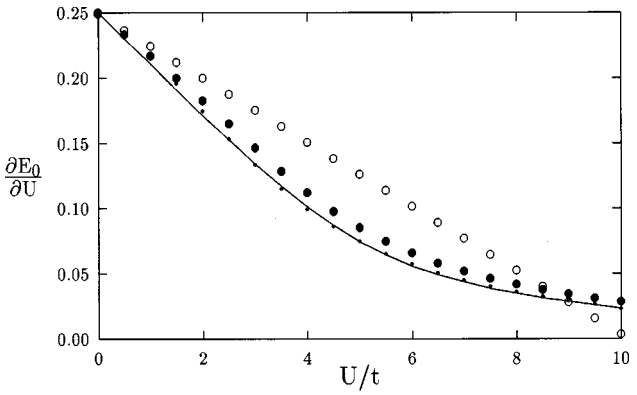

FIG. 3. Plot of $\partial E_0/\partial U$, the derivative of the ground-state energy with respect to the correlation parameter U, as a function of U/t for the one-dimensional Hubbard chain at half filling. This gives the average number of double occupancies $\langle n_{i\uparrow} n_{i\downarrow} \rangle$. The solid curve gives the result from our present calculation and the dotted curve shows the exact result. ● gives the result for the existing real-space RG (Ref. 1), while ○ shows the result from Gutzwiller's approximation.

eratively a variational wave function and thereby yields an upper bound to the ground-state energy.[1] Therefore, a comparison of the present result with that obtained in the GA is interesting at this point. Such a comparison shows (Fig. 2) that the energy is much improved in the present RG scheme compared to the GA especially from the intermediate- to the strong-coupling regime. Therefore, it is clear that although the present scheme generates a fictitious metal-insulator (MI) transition (the so-called Brinkmann-Rice transition[13,14] in a GA), it takes into account the correlation effects neglected in the GA.[13]

It seems that the present scheme yields an upper bound to the exact energy with uniform accuracy over the whole coupling range. To investigate this further we calculate the slope of the energy with respect to U. The plot of $\partial E_0/\partial U \ \ (t=1)$ vs U/t is compared with the exact result[11] in Fig. 3. It turns out to be fairly reliable from the intermediate- to the strong-coupling regime; an improvement over that obtained from the existing scheme is noticeable in this region. The result from the GA is also shown for comparison. $\partial E_0/\partial U$ gives the number of double occupancies ($\langle n_{i\uparrow} n_{i\downarrow} \rangle$) in the system. Therefore, we see that such quantities could be obtained with reasonable accuracy within the present scheme.

Since the gap does not turn out to be reliable in this scheme it is not meaningful to calculate the long-range correlation functions within this scheme. The basic reason for this is that while renormalizing the parameters we have totally neglected the low-lying states of the superblock Hamiltonian in the different subspaces. Only an extension of the present scheme that properly takes into consideration the above fact is expected to correctly yield the gap and the long-range correlation functions. Some more work is required in this direction.

The present scheme, however, seems to be capable of finding out a very good upper bound to the ground-state energy and the derivative of the energy (which gives an expectation value of local operators such as the double occupancy) for interacting fermion models. This could be useful in problems that require a minimization of the energy of a many-fermion system coupled to some other degrees of freedom (e.g., phonons) within a variational approach.[15] Moreover, an estimation of the free energy and its derivatives could be achieved in a finite-temperature version[16] of this scheme and such a genralization would lead to a reliable study of the thermodynamics of the low-dimensional many-fermion models such as the Hubbard model. It is straightforward to generalize the present scheme to the case of the non-half-filled band[17] and to the higher dimension,[1,18] although the latter requires some extensive numerics.

Summarizing, we have worked out a recently proposed modification of the real-space RG scheme for the one-dimensional Hubbard model for a half-filled band. The results seem to be markedly improved for the ground-state energy and its derivative, which gives the average number of double occupancies per site. A comparison with the exact result shows that the energy calculated in the present method gives a very good upper bound over the whole range of the coupling constant. However, this approach generates a fictitious MI transition at a finite U/t as in the GA calculation. It turns out that here the correlation effects are taken into account more satisfactorily compared to the GA. However, it is indicated that the present scheme requires further refinement for the calculation of the energy gap and the long-range correlation functions. A finite-temperature generalization of the present scheme also seems to be of great interest.

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