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Large-U cluster-Hamiltonian expansion of the Hubbard model

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We discuss an expansion of the low-energy effective Hamiltonian of the large-U Hubbard model, in which higher-order terms involve lattice clusters with larger numbers of sites rather than larger powers of the hopping amplitude parameter t. Expressions for each term, valid to all orders in t, can be obtained by exactly diagonalizing the Hubbard model for small clusters. Leading terms in this expansion are derived.

The Hubbard model is a highly simplified and widely studied model for studying strongly correlated fermions on a lattice. The usual and simplest version of the Hubbard Hamiltonian is

$$\mathscr{H} = -t\sum_{ij\sigma} N_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U\sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $N_{ij}=1$ if i,j are nearest-neighbor sites and is zero otherwise. We will refer to N_{ij} below as the link variable. In Eq. (1), $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are the creation and annihilation operators for an electron of spin σ on site i and $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$ is the number operator for spin σ on site i. The one-body term describes hopping of electrons between Wannier orbitals associated with neighboring sites, while the two-body terms describe interactions between two electrons on the same site. One of the virtues of this model Hamiltonian is that it provides a very simple picture of the Mott insulator state in which strong interactions lead to an insulating state where band theory would predict a metallic state. For $t=0$, site representation occupation number states are eigenstates of the Hamiltonian with eigenvalue $E=UN_D$, where $N_D=\Sigma_i n_{i\uparrow}n_{i\downarrow}$ is the number of doubly occupied sites. When the number of electrons per site $n=1$, the ground state has energy $E=0$ and for N sites has degeneracy 2^N. The degeneracy reflects the two possible spin states for the single electron on each site. The ground state is separated from excited states by a Mott-Hubbard gap U. The Mott-Hubbard gap and the associated insulating behavior of the electronic system survive for $t\neq 0$, at least to a finite value of the magnitude of the hopping parameter $|t_c|$. Low-temperature and -energy properties of Hubbard model systems for small t/U depend on the manner in which the ground state degeneracy is lifted for $t\neq 0$.

It is convenient to describe this low-energy portion of the Hubbard model spectrum at large U in terms of an effective Hamiltonian.[1–4] One approach to deriving a systematic expansion of the effective Hamiltonian in powers of t/U, developed previously by one of us,[5,6] is based on an analogy to the Foldy-Wouthuysen[7] transformation derivation of relativistic corrections to the Schrödinger equation. In this approach the number of doubly occupied sites plays a role similar to the number of electron-positron pairs in the Dirac equation. At lowest order the resulting effective Hamiltonian is the so-called "t-J" model which has, despite legitimate concerns[8] about its reliability in the metallic state, been widely used to model the many-body physics of the CuO_2 planes in high-temperature superconductors.[9] In this paper we restrict our attention to the case $n=1$ for which the low-energy Hilbert space evolves for finite t from those states with one electron on each site and no orbital degrees of freedom. As a consequence the effective Hamiltonian can always be expressed as a spin Hamiltonian. It follows from the ap-

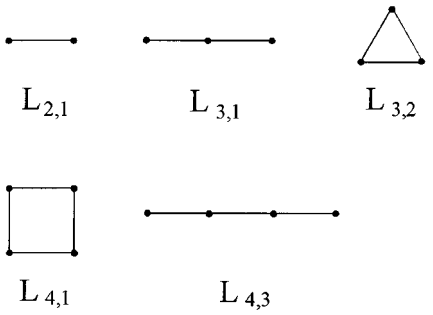

FIG. 1. Schematic illustration of some linkage functions for $N=2$, 3, 4. Sites connected by a solid line have $N_{ij}=1$; otherwise, $N_{ij}=0$.

proach of Refs. 5 and 6 that this Hamiltonian can always be expressed in the form of a sum of coupled cluster Hamiltonians:

$$\mathscr{H}'=\sum_{N,l}\sum_{i_1,\ldots,i_N} L_{N,l}(i_1,\ldots,i_N)\mathscr{H}_{N,l}(\vec{\sigma}_{i_1},\ldots,\vec{\sigma}_{i_N}). \tag{2}$$

Here N is the number of distinct sites in a cluster, $i_1,\ldots,i_N$ range over all lattice sites, $\vec{\sigma}_i=2\vec{s}_i$ is the Pauli spin-matrix operator for site i, l labels the distinct manners in which N sites can be linked by nearest-neighbor hops, and $L_{N,l}(i_1,\ldots,i_N)$ is equal to 1 if the sites are linked in the lth manner and is zero otherwise. $L_{N,l}$ can always be expressed as the product of the $N_{i,j}$ for the various sites in a cluster. The set of possible linkage functions for up to six sites is listed in Ref. 6. Some linkage functions for $N=2,3,4$ are illustrated schematically in Fig. 1. With this form of expansion, the effective Hamiltonian depends on the dimension and type of the lattice only through the link variables. In the t/U expansion of the $n=1$ effective Hamiltonian, terms involving N linked sites appear only at order $2[(N+1)/2]$ or larger. (Here $[x]$ denotes the integer part of x.) In this paper we propose an alternate approach in which the cluster effective Hamiltonians, $\mathscr{H}_{N,l}$, are determined *to all orders in t* iteratively, starting with small N, by exactly diagonalizing the corresponding cluster Hamiltonians. (Spectra for the Hubbard model for some clusters discussed here are illustrated in Fig. 2.) Exact expressions are derived for the leading cluster Hamiltonians.

The starting point for the derivation of the cluster Hamiltonians is the application of Eq. (2) to a system consisting of two linked sites so that $\mathscr{H}'=2\mathscr{H}_{2,1}$. The Hubbard model for the two-site system is readily diagonalized analytically.[10] The low-energy Hilbert space is found by identifying the eigenvalues which approach zero for $t\to 0$. For the two-site Hubbard model there are four such eigenvalues, a triplet with $E=0$ and a singlet with $E=U/2-(4t^2+U^2/4)^{1/2}$. It follows that

$$\mathscr{H}_{2,1}(\vec{\sigma}_1,\vec{\sigma}_2)/U=\frac{1}{16}(1-\sqrt{1+16x})(1-\vec{\sigma}_1\cdot\vec{\sigma}_2)$$

$$\equiv f_2(1-\vec{\sigma}_1\cdot\vec{\sigma}_2), \tag{3}$$

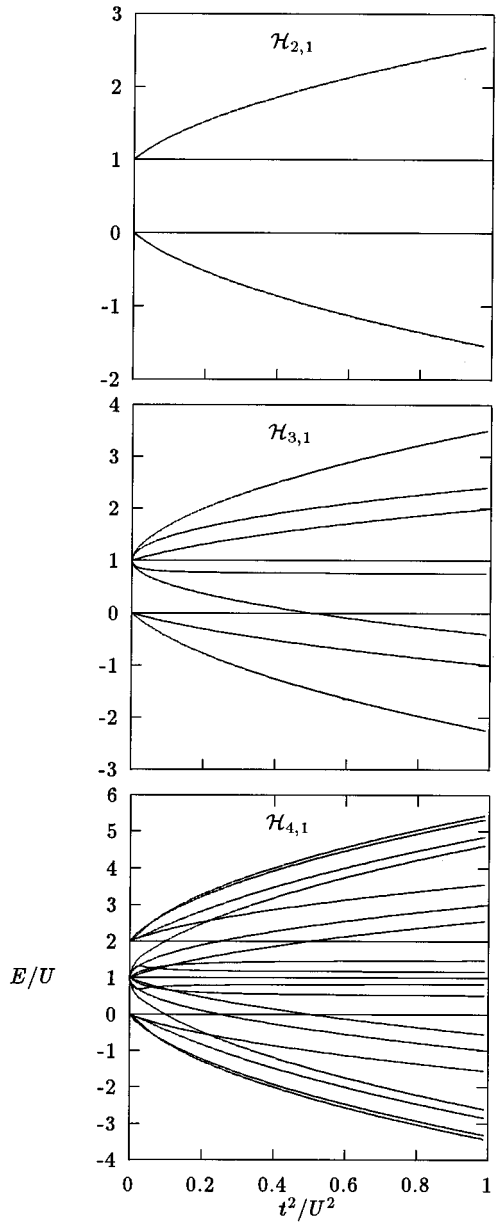

FIG. 2. Plots of the energy eigenvalues of the Hubbard model for clusters of two linked cites, three linearly linked cites, and four cyclically linked cites. The spectra for these clusters may be used to determine cluster effective spin Hamiltonians as described in the text. Note that subspaces associated, in the $t=0$ limit, with different numbers of doubly occupied sites begin to overlap at smaller t/U in larger clusters. As has been shown in Ref. 6 the cluster spin Hamiltonians $\mathscr{H}_{3,1}$ and $\mathscr{H}_{4,1}$ are the only ones that vanish like t^4 in the small t/U limit. $\mathscr{H}_{N,l}$ vanishes at least like t^6 for $N>4$.

where $x=t^2/U^2$. The leading term in the small x expansion of $\mathscr{H}_{2,1}$ is the usual term arising at leading order in the large-U expansion of the Hubbard model; the next two terms are in agreement with the contributions associated with the linkage function $L_{2,1}$ which appear at order t^4 and t^6 in the systematic expansion of Refs. 5 and 6. The higher-order terms represent a subsum to all orders in t of the portion of the perturbation expansion which is associated with the $L_{2,1}$ linkage function.

Next we determine the exact form of the operator $\mathscr{H}_{3,1}$ to all orders in t. This operator is associated with the linkage function $L_{3,1}(1,2,3)=N_{12}N_{13}$. The effective spin Hamiltonian $\mathscr{H}_{3,1}$ must be invariant under spin rotations, in order to respect the spin-rotational symmetry of the underlying Hubbard Hamiltonian. It must also respect the symmetries of the cluster under site interchange operations. In addition the state with all spins parallel must be an eigenstate with eigenvalue zero, since the corresponding state with one electron per site is a zero-energy eigenstate of the Hubbard model. (No hopping is possible if all spins are parallel.) It follows that $\mathscr{H}_{3,1}$ must have the form

$$\mathscr{H}_{3,1}(\vec{\sigma}_1,\vec{\sigma}_2,\vec{\sigma}_3)/U=2f_3^a+f_3^b-f_3^a(\vec{\sigma}_1\cdot\vec{\sigma}_2+\vec{\sigma}_1\cdot\vec{\sigma}_3)-f_3^b(\vec{\sigma}_2\cdot\vec{\sigma}_3), \tag{4}$$

where f_3^a, f_3^b are as yet undetermined functions of x. From Eq. (2) it follows that the low-energy effective spin Hamiltonian for a cluster of three linearly linked sites has the form

$$\mathscr{H}_3'=2.\mathscr{H}_{2,1}(\vec{\sigma}_1,\vec{\sigma}_2)+2.\mathscr{H}_{2,1}(\vec{\sigma}_1,\vec{\sigma}_3)+2.\mathscr{H}_{3,1}(\vec{\sigma}_1,\vec{\sigma}_2,\vec{\sigma}_3). \tag{5}$$

Combining Eq. (3) and Eq. (4) gives

$$\mathscr{H}_3'/U=[4f_2+4f_3^a+2f_3^b]-[2f_2+2f_3^a]\times(\vec{\sigma}_1\cdot\vec{\sigma}_2+\vec{\sigma}_1\cdot\vec{\sigma}_3)-2f_3^b(\vec{\sigma}_2\cdot\vec{\sigma}_3), \tag{6}$$

where f_2 was defined above. This Heisenberg-like Hamiltonian is readily diagonalized. The spectrum consists of three eigenvalues: $E_1'=0$ for a $S=3/2$ multiplet with degeneracy 4, $E_2'=12f_2+12f_3^a$ for a $S=1/2$ doublet, and $E_3'=4f_2+4f_3^a+8f_3^b$ for a $S=1/2$ doublet. To determine f_3^a and f_3^b we must find exact eigenvalues of the Hubbard model for the same cluster, identify the low-energy eigenvalues, and compare with this spectrum.

The diagonalization of the Hubbard cluster Hamiltonian is simplified by the use of group theoretical techniques.[11] The symmetry group of this three-site cluster is C_{2v}. The three-site Hubbard model has Hamiltonian dimension 20: one state each in the sectors with the z component of total spin $S_z=\pm 3/2$ and nine states each in the sectors with $S_z=\pm 1/2$. Each $S=3/2$ multiplet and each $S=1/2$ doublet has one member with $S_z=1/2$. In the $S_z=1/2$ sector, five states belong to the A_1 representation of the C_{2v} group and have eigenvalues

$$E_1=0,\quad E_2=U,$$

$$E_{3,4,5}=U\left[\frac{2}{3}+\frac{2}{3}\sqrt{1+24x}\cos\left(\theta+j\frac{2\pi}{3}\right)\right], \tag{7}$$

where $\theta=\frac{1}{3}\cos^{-1}[-(1+9x)/(1+24x)^{3/2}]$ and $j=0,1,2$. The four additional states correspond to the B_2 representation of the C_{2v} group. The eigenvalues for these states are

$$E_{6,7}=U(1\pm\sqrt{2x}),$$

$$E_{8,9}=U\left(\frac{1}{2}\pm\frac{1}{2}\sqrt{1+8x}\right). \tag{8}$$

We identify the eigenvalues E_1, E_4, and E_9 as belonging to the low-energy sector since they vanish for $x\to 0$.

Comparing the spin-model and Hubbard-model eigenvalues for this cluster and using the expression for f_2 [Eq. (3)] we find

$$f_3^a=-\frac{1}{144}+\frac{1}{16}\sqrt{1+16x}+\frac{1}{18}\sqrt{1+24x}\cos\theta,$$

$$f_3^b=\frac{5}{144}-\frac{1}{16}\sqrt{1+8x}-\frac{1}{36}\sqrt{1+24x}\cos\theta,$$

$$\theta=\frac{2\pi}{3}+\frac{1}{3}\cos^{-1}\left[-\frac{1+9x}{(1+24x)^{3/2}}\right]. \tag{9}$$

For small x we can expand Eq. (9) keeping terms up to order x^3,

$$f_3^a\sim 2x^3,\quad f_3^b\sim-\frac{x^2}{2}+5x^3. \tag{10}$$

The partial results up to this order are in agreement with those obtained in Ref. 6.

Continuing in this way it is possible to uniquely determine all cluster Hamiltonians. For example, the effective Hamiltonian for a three-site Hubbard cluster with cyclic links contains contributions from $\mathscr{H}_{2,1}$, $\mathscr{H}_{3,1}$, and $\mathscr{H}_{3,2}$:

$$\mathscr{H}_3'=2.\mathscr{H}_{2,1}(\vec{\sigma}_1,\vec{\sigma}_2)+2.\mathscr{H}_{2,1}(\vec{\sigma}_1,\vec{\sigma}_3)+2.\mathscr{H}_{2,1}(\vec{\sigma}_2,\vec{\sigma}_3)+2.\mathscr{H}_{3,1}(\vec{\sigma}_1,\vec{\sigma}_2,\vec{\sigma}_3)+2.\mathscr{H}_{3,1}(\vec{\sigma}_2,\vec{\sigma}_3,\vec{\sigma}_1)+2.\mathscr{H}_{3,1}(\vec{\sigma}_3,\vec{\sigma}_1,\vec{\sigma}_2)+6.\mathscr{H}_{3,2}(\vec{\sigma}_1,\vec{\sigma}_2,\vec{\sigma}_3). \tag{11}$$

Symmetry considerations (see Fig. 1) imply that

$$\mathscr{H}_{3,2}/U=f_3^c(3-\vec{\sigma}_1\cdot\vec{\sigma}_2-\vec{\sigma}_1\cdot\vec{\sigma}_3-\vec{\sigma}_2\cdot\vec{\sigma}_3), \tag{12}$$

TABLE I. Analytic all-order expressions for the effective spin Hamiltonians appearing at leading order in the cluster expansion discussed in the text. f_2, f_3^a, f_3^b, and f_3^c are functions of $x\equiv t^2/U^2$ given by Eqs. (3), (9), and (17).

Cluster	Equivalent spin Hamiltonian
Two sites	$f_2(1-\vec{\sigma}_1\cdot\vec{\sigma}_2)$
Three sites linearly linked	$[4f_2+4f_3^a+2f_3^b]-[2f_2+2f_3^a](\vec{\sigma}_1\cdot\vec{\sigma}_2+\vec{\sigma}_1\cdot\vec{\sigma}_3)-2f_3^b(\vec{\sigma}_2\cdot\vec{\sigma}_3)$
Three sites cyclically linked	$[2f_2+4f_3^a+2f_3^b+6f_3^c](3-\vec{\sigma}_1\cdot\vec{\sigma}_2-\vec{\sigma}_1\cdot\vec{\sigma}_3-\vec{\sigma}_2\cdot\vec{\sigma}_3)$

where f_3^c is an as yet unknown function of x. Combining Eq. (11) with Eqs. (3), (4), and (12) we find that

$$\mathscr{H}_3'/U=(2f_2+4f_3^a+2f_3^b+6f_3^c)\times(3-\vec{\sigma}_1\cdot\vec{\sigma}_2-\vec{\sigma}_1\cdot\vec{\sigma}_3-\vec{\sigma}_2\cdot\vec{\sigma}_3). \quad (13)$$

The eigenvalues of this spin Hamiltonian are $\mathscr{E}_1'=0$ and $\mathscr{E}_{2,3}'=6(2f_2+4f_3^a+2f_3^b+6f_3^c)$. Identifying the effective Hamiltonian spectrum with the low-energy portion of the Hubbard-model spectrum for this cluster determines f_3^c uniquely. The symmetry group for this cluster is C_{3v} and there are two states that belong to the A_1 representation with eigenvalues

$$\mathscr{E}_1=0, \quad \mathscr{E}_2=U, \quad (14)$$

one state that belongs to the A_2 representation with eigenvalue

$$\mathscr{E}_3=U, \quad (15)$$

and six states that belong to the E representation with (doubly degenerate) eigenvalues

$$\mathscr{E}_{4,5,6}=U\left[\frac{2}{3}+\frac{2}{3}\sqrt{1+27x}\cos\left(\theta_0'+j\frac{2\pi}{3}\right)\right], \quad (16)$$

where $\theta_0'=(1/3)\cos^{-1}[-1/(1+27x)^{3/2}]$ and $j=0,1,2$. The three eigenvalues that belong to the low-energy cluster are $\mathscr{E}_1$ and $\mathscr{E}_5$ (doubly degenerate). Comparing with the eigenvalues of the spin Hamiltonian Eq. (13) we find

$$f_3^c=-\frac{1}{108}+\frac{1}{48}\sqrt{1+8x}-\frac{1}{48}\sqrt{1+16x}-\frac{1}{36}\sqrt{1+24x}\cos\theta+\frac{1}{54}\sqrt{1+27x}\cos\theta',$$

$$\theta'=\frac{2\pi}{3}+\frac{1}{3}\cos^{-1}\left[-\frac{1}{(1+27x)^{3/2}}\right] \quad (17)$$

[θ was defined in Eq. (9)], which in the small x limit reduces to $f_3^c\sim 5x^3/6$ in agreement with Ref. 6. In Table I we have collected the analytic results for clusters consisting of two and three sites.

To continue to $N=4$, it is important to start with clusters for which only one linkage function is nonzero and add then additional links. For example, the effective Hamiltonian for a linearly linked Hubbard cluster involves only $\mathscr{H}_{2,1}$, $\mathscr{H}_{3,1}$, and $\mathscr{H}_{4,3}$. $\mathscr{H}_{4,3}$ can be determined by comparing with the Hubbard spectrum for this cluster. Once $\mathscr{H}_{4,3}$ is known, $\mathscr{H}_{4,1}$ can be determined from the analytically known[12] spectrum of the cyclically linked $N=4$ Hubbard cluster (see Fig. 1). It should be noted that at small t/U, as shown in Ref. 6, the cluster spin Hamiltonian $\mathscr{H}_{2,1}$ vanishes like t^2, $\mathscr{H}_{3,1}$ and $\mathscr{H}_{4,1}$ vanish like t^4, and all other cluster Hamiltonians vanish at least as fast as t^6. In extending the iterative determination of the cluster effective Hamiltonians, numerical values of the f_N^i functions can be obtained where the necessary cluster Hubbard-model diagonalizations cannot be accomplished analytically.

We note that when the cluster Hamiltonians are analytically continued to complex values of the hopping parameter, singularities occur off the real axis. The two-site cluster Hamiltonian $\mathscr{H}_{2,1}$ has a singularity at $t/U=0.25i$, while $\mathscr{H}_{3,1}$ has a singularity [Eq. (9)] at $t/U=0.20i$ and $\mathscr{H}_{3,2}$ at $t/U=0.19i$ [Eq. (17)]. From the analytically known[12] eigenvalues for the cyclically linked $N=4$ cluster it follows that $H_{4,1}$ has a number of singularities of which the closest to the origin occurs near $t/U=0.14i$. (These singularities have also been discussed in Ref. 13 in connection with a series expansion study of the ground state of the Hubbard.) The presence of these singularities shows that the radius of convergence of the direct Taylor series expansion of the effective Hamiltonians is small, further motivating the cluster resummation discussed here.

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