t/U expansion for the Hubbard model

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We describe a unitary transformation which eliminates terms coupling states with differing numbers of doubly occupied sites from the Hamiltonian of the Hubbard model. The S matrix for the transformation, and the transformed Hamiltonian, H', are generated by an iterative procedure which results in an expansion in powers of the hopping integral t divided by the on-site energy U. For a half-filled band and in the space with no doubly occupied sites, H' is equivalent to a spin Hamiltonian. We discuss the implications of our results for H' on theories of high-temperature superconductivity.

The Hubbard model[1,2] is the simplest possible Hamiltonian which captures the essential physics of fermion systems with short-range repulsive interactions. The Hamiltonian of this model is $H=T+V$ where the kinetic part represents hops between neighboring sites,

$$T=-t\sum_{ij\sigma}N_{ij}C_{i\sigma}^{\dagger}C_{j\sigma}\ , \tag{1}$$

and the interaction part gives contributions only from electrons on the same site,

$$V=U\sum_{i}n_{i\uparrow}n_{\downarrow}\ . \tag{2}$$

[In Eq. (1) $N_{ij}=1$ if i and j are labels for neighboring sites and equals zero otherwise.] Despite its apparent simplicity, the properties of the Hubbard model are well understood only for the case of a one-dimensional lattice.[3] The difficulty of the model is generally felt to result from the fact that it does capture the essential elements of the complex behavior of strongly-correlated Fermi systems and interest in the model has increased in recent years. (See, for example, Refs. 4–9.) This has been especially true since the discovery of high-T_c superconductivity in copper-oxide systems[10,11] which are believed to be qualitatively described by the Hubbard model.

Our transformation is based on a separation of the kinetic part of H into terms which increase the number of doubly occupied sites by 1, terms which decrease the number of doubly occupied sites by 1, and terms which leave the number of doubly occupied sites unchanged:

$$T=T_0+T_1+T_{-1}\ , \tag{3a}$$

where

$$T_0=-t\sum_{ij\sigma}N_{ij}(n_{i\bar{\sigma}}C_{i\sigma}^{\dagger}C_{j\sigma}n_{j\bar{\sigma}}+h_{i\bar{\sigma}}C_{i\sigma}^{\dagger}C_{j\sigma}h_{j\bar{\sigma}})\ , \tag{3b}$$

$$T_1=-t\sum_{ij\sigma}N_{ij}n_{i\bar{\sigma}}C_{i\sigma}^{\dagger}C_{j\sigma}h_{j\bar{\sigma}}\ , \tag{3c}$$

$$T_{-1}=-t\sum_{ij\sigma}N_{ij}h_{i\bar{\sigma}}C_{i\sigma}^{\dagger}C_{j\sigma}n_{j\bar{\sigma}}\ . \tag{3d}$$

In Eqs. (3) $\bar{\sigma}$ is up for σ down and down for σ up, $n_{i\sigma}=C_{i\sigma}^{\dagger}C_{i\sigma}$, and $h_{i\sigma}=1-n_{i\sigma}$; the separation is formally achieved by multiplying each term in Eq. (1) on the left by $1=n_{i\bar{\sigma}}+h_{i\bar{\sigma}}$ and on the right by $1=n_{j\bar{\sigma}}+h_{j\bar{\sigma}}$. Note that $T_m^{\dagger}=T_{-m}$ and that

$$[V,T_m]=mUT_m\ . \tag{4}$$

Equation (4) expresses the fact that the interaction energy changes by mU after one of the hops in T_m.

We seek a unitary transformation which eliminates hops between states with differing numbers of doubly occupied sites

$$H'=e^{iS}He^{-iS}=H+\frac{[iS,H]}{1!}+\frac{[iS,[iS,H]]}{2!}+\cdots\ . \tag{5}$$

A recursive scheme for determining a transformation which has this property to any desired order in t/U is described below. The last two terms in the untransformed Hamiltonian,

$$H\equiv H'^{(1)}=V+T_0+T_1+T_{-1}\ , \tag{6}$$

may be eliminated by choosing

$$iS=iS^{(1)}=U^{-1}(T_1-T_{-1})\ . \tag{7}$$

Substituting Eqs. (7) and (6) into Eq. (5) and using Eq. (4) gives

$$\begin{aligned}H'^{(2)}&\equiv e^{iS^{(1)}}He^{iS^{(1)}}\\&=V+T_0+U^{-1}([T_1,T_{-1}]+[T_0,T_{-1}]\\&\qquad+[T_1,T_0])+O(U^{-2})\ .\end{aligned} \tag{8}$$

To proceed further we define

$$T^{(k)}(m_1,m_2,\ldots,m_k)\equiv T^{(k)}[m]=T_{m_1}T_{m_2}\ldots T_{m_k}\ , \tag{9a}$$

and note, using Eq. (4), that

$$[V,T^{(k)}[m]]=U\sum_{i=1}^{k}m_iT^{(k)}[m]\equiv UM^{(k)}[m]T^{(k)}[m]\ . \tag{9b}$$

$H'^{(k)}$ will contain terms of order t^kU^{1-k} which couple states with differing numbers of doubly occupied sites, i.e., with $M^{(k)}[m]\neq 0$ and which can be expressed in the form

$$H'^{[k]}=U^{1-k}\sum_{\{m\}}C^{(k)}[m]T^{(k)}[m]\ . \tag{10}$$

It follows from Eq. (9b) that

$$H'^{(k+1)}\equiv e^{iS^{(k)}}He^{-iS^{(k)}} \tag{11}$$

will contain $M[m]\neq 0$ terms only at order $t^{k+1}U^{-k}$, if we generalize Eq. (7) by choosing

$$iS^{[k]}=iS^{(k)}-iS^{(k-1)}$$
$$=U^{-k}\sum_{\{m\}\ni M[m]\neq 0}\frac{C^{(k)}[m]T^{(k)}[m]}{M^{(k)}[m]}\ . \tag{12}$$

Equation (12) generates an expansion for S in powers of (t/U) which when truncated at order (k) leaves H' free of $M[m]\neq 0$ terms up to order k. For example,

$$iS^{[2]}=U^{-2}([T_1,T_0]+[T_{-1},T_0]) \tag{13}$$

yields

$$H'^{(3)}=V+T_0+U^{-1}[T_1,T_{-1}]+U^{-2}\{T^{(3)}(1,0,-1)+T^{(3)}(-1,0,1)-[T^{(3)}(0,1,-1)+T^{(3)}(1,-1,0)$$
$$+T^{(3)}(-1,1,0)+T^{(3)}(0,-1,1)]/2\}+\cdots\ , \tag{14}$$

where we have dropped the $M[m]\neq 0$ at third order which will be eliminated from H' by $S^{[3]}$.

The expressions for H' and S' rapidly become lengthy as the order increases[12] but simplify in the most physically relevant situations. In particular, when t/U is small enough for the present expansion to be convergent, we may expect that the ground state and its low-lying excitations lie, after the unitary transformation, entirely within the subspace with the minimum number of doubly occupied sites. For any state in this subspace, $|\Psi\rangle_L$, and any filling of the Hubbard band

$$T_{-1}|\Psi\rangle_L\equiv 0\ , \tag{15}$$

Eq. (15) simply expresses the fact that the interaction energy cannot be lowered below its minimum value and may be demonstrated explicitly. Equation (15) may be generalized to higher orders:

$$T^{(k)}[m]\,|\Psi\rangle_L\equiv 0\ , \tag{16a}$$

if

$$M_n^{(k)}[m]\equiv\sum_{i=n}^{k}m_i<0 \tag{16b}$$

for any value of n. Equations (16) can be used to eliminate many terms from the expansion for H' so that, in the minimum $\langle V\rangle$ subspace,[12]

$$H_L'^{(4)}=V+T_0-U^{-1}T^{(2)}(-1,1)+U^{-2}\{T^{(3)}(-1,0,1)-[T^{(3)}(-1,1,0)+T^{(3)}(0,-1,1)]/2\}$$
$$+U^{-3}\{T^{(4)}(-1,0,-1,0)+T^{(4)}(-1,1,-1,1)+T^{(4)}(0,-1,0,1)-T^{(4)}(-1,0,0,1)$$
$$-[T^{(4)}(-1,1,0,0)+T^{(4)}(0,0,1,1)+T^{(4)}(-1,-1,1,1)]/2\}+O(U^{-5})\ . \tag{17}$$

Further simplification occurs when the Hubbard band is half filled. In this case the minimum $\langle V\rangle$ subspace has one electron at each site and no hops are possible without increasing the number of doubly occupied sites, i.e., $T_0|\Psi_L\rangle\equiv 0$ and, for higher-order terms,

$$T^{[k]}[m]\,|\Psi_L\rangle\equiv O \text{ if } M_n^{(k)}[m]<0 \text{ or } M_{n+1}^{(k)}[m]=0 \text{ and } m_n\neq 1\ .$$

At half filling these considerations lead to[12]

$$H_{HL}'^{(5)}=-U^{-1}T^{(2)}(-1,1)+U^{-2}T^{(3)}(-1,0,1)+U^{3}[T^{4}(-1,1,-1,1,)+T^{(4)}(-1,0,0,1)-\tfrac{1}{2}T^{(4)}(-1,-1,1,1)]$$
$$+U^{-4}[-\tfrac{3}{2}T^{(5)}(-1,0,1,-1,1)-\tfrac{3}{2}T^{(5)}(-1,1,-1,0,1)+T^{(5)}(-1,0,0,0,1)+\tfrac{1}{2}T^{(5)}(-1,-1,1,0,1)$$
$$+\tfrac{1}{2}T^{(5)}(-1,0,-1,1,1)+\tfrac{1}{4}T^{(5)}(-1,-1,0,1,1)]+\cdots\ . \tag{18}$$

For a half-filled band there is a one-to-one correspondence between states in the $\langle V\rangle=0$ subspace of the Hubbard model and states in the Hilbert space of spin $-\frac{1}{2}$ objects located on each lattice site

$$|n_{1\uparrow},n_{1\downarrow},n_{2\uparrow}n_{2\downarrow},\ldots,n_{N\uparrow},n_{N\downarrow}\rangle$$
$$\rightarrow|\sigma_1\rangle^{(1)}|\sigma_2\rangle^{(2)}\ldots|\sigma_N\rangle^{(N)}\ , \tag{19}$$

where $\sigma_i=|\uparrow\rangle$ for $n_{i\uparrow}=1$ and $\sigma_i=|\downarrow\rangle$ for $n_{i\downarrow}$. (Recall that $n_{i\uparrow}+n_{i\downarrow}=1$.) Similarly, there is a spin Hamiltonian acting in the spin space which corresponds to H'_{NL} acting in the occupation number subspace. The spin Hamiltonian may be expressed as

$$H_S^{(k)}=\frac{1}{2^N}\sum_{m_1,\ldots,m_N=0}^{3}\prod_{l=1}^{N}\sigma_{m_l}^{(l)}T_r(\sigma_{m_1}^{(1)}\ldots\sigma_{m_N}^{(N)}H_{NL}'^{(k)})\ , \tag{20}$$

where σ_0, σ_1, σ_2, and σ_3 are the four Pauli spin matrices. For example,

$$H_{HL}'^{(2)}=\frac{-t^2}{U}\sum_{\substack{i_1,j_1\\ i_2,j_2}}N_{i_2,j_2}N_{i_1,j_1}(h_{i_2\bar{\sigma}_2}C_{i_2\sigma_2}^{\dagger}C_{j_2\sigma_2}n_{j_2\bar{\sigma}_2})$$
$$\times(n_{i_1\bar{\sigma}_1}C_{i_1\sigma_1}^{\dagger}C_{j_1\sigma_1}h_{j_1\bar{\sigma}_1})\ . \tag{21}$$

When the right factor in parentheses operates on a state in

the $\langle V\rangle=0$ subspace it produces zero if sites i_1 and j_1 had the same spin occupied and otherwise gives a state with site i_1 doubly occupied and site j_1 empty and all other sites singly occupied. The left factor in parentheses gives zero unless it operates on a state where site j_2 is doubly occupied and site i_2 is empty so that we can set $j_2=i_1$ and $i_2=J_1$. It follows that, using spin notation and noting that $N_{i,j}^2=N_{i,j}$,

$$H_{HL}^{\prime(2)}=\frac{-t^2}{U}\sum_{i,j}N_{i,j}(|\uparrow\rangle^{(i)}|\downarrow\rangle^{(j)}+|\downarrow\rangle^{(i)}|\uparrow\rangle^{(j)}) \times({}^{(i)}\langle\uparrow|\,{}^{(j)}\langle\downarrow|\,{}^{(i)}+\langle\downarrow|\,{}^{(j)}\langle\uparrow|)\ , \tag{22}$$

which can be rewritten using Eq. (2) as

$$H_2^{\prime(2)}=\frac{-t^2}{2U}\sum_{i,j}N_{i,j}(1-\boldsymbol{\sigma}^{(i)}\cdot\boldsymbol{\sigma}^{(j)})\ . \tag{23}$$

This is the familiar result in the large U limit, that the half-filled-band Hubbard model is equivalent to the Heisenberg model. We have carried out this procedure for translating $H_{HL}^{\prime}$ into a spin Hamiltonian to higher order. (The task becomes quite laborious in high order and we use a computer program to do the bookkeeping.) We find that[13]

$$H_s^{\prime}=\frac{-t^2U^{-1}}{2}{\sum_{1,2}}'N_{1,2}(1-\boldsymbol{\sigma}^{(1)}\cdot\boldsymbol{\sigma}^{(2)})+t^4U^{-3}\Big[2{\sum_{12}}'N_{1,2}(1-\boldsymbol{\sigma}^{(1)}\cdot\boldsymbol{\sigma}^{(2)})+\tfrac{1}{2}{\sum_{1,2,3}}'N_{12}N_{13}(\boldsymbol{\sigma}^{(2)}\cdot\boldsymbol{\sigma}^{(3)}-1)$$
$$+\tfrac{1}{8}{\sum_{1,2,3,4}}'N_{12}N_{23}N_{34}N_{41}[1-\boldsymbol{\sigma}^{(1)}\cdot\boldsymbol{\sigma}^{(2)}-\boldsymbol{\sigma}^{(1)}\cdot\boldsymbol{\sigma}^{(3)}-\boldsymbol{\sigma}^{(4)}\cdot\boldsymbol{\sigma}^{(4)}-\boldsymbol{\sigma}^{(2)}\boldsymbol{\sigma}^{(3)}-\boldsymbol{\sigma}^{(2)}\cdot\boldsymbol{\sigma}^{(4)}-\boldsymbol{\sigma}^{(3)}\cdot\boldsymbol{\sigma}^{(4)}]$$
$$+5[(\boldsymbol{\sigma}^{(1)}\cdot\boldsymbol{\sigma}^{(2)})(\boldsymbol{\sigma}^{(3)}\cdot\boldsymbol{\sigma}^{(4)})+(\boldsymbol{\sigma}^{(1)}\cdot\boldsymbol{\sigma}^{(4)})(\boldsymbol{\sigma}^{(2)}\cdot\boldsymbol{\sigma}^{(3)})-(\boldsymbol{\sigma}^{(1)}\cdot\boldsymbol{\sigma}^{(3)})(\boldsymbol{\sigma}^{(2)}\cdot\boldsymbol{\sigma}^{(4)})]\Big]+O(t^6U^{-5})\ . \tag{24}$$

The primes on the sums indicate that they run over sets of distinct site labels. We emphasize that terms proportional to odd powers of t in Eq. (24) [which is equivalent to Eq. (18)] vanish identically. This fact reflects the invariance of the Hubbard Hamiltonian spectrum at half filling under $t\rightarrow -t$ which may be established by making a particle-hole transformation. Note that $H_s^{\prime}$ involves sums only over sets of sites connected by near-neighbor links, that it is explicitly invariant under rotations in spin-space, and that it annihilates a ferromagnetic (all spins parallel) state. This last property follows simply from the Pauli exclusion principle.

We emphasize that Eq. (24) is valid for any lattice in any number of dimensions. Both Eq. (17) and its spin version at half filling have been derived previously[6,14,15] for terms up to order t^2/U. These leading-order terms are the basis upon which much of the theory for high-temperature superconductivity is based.[16-19] The essential elements of the resonating valence bond (RVB) theory, developed by Anderson and co-workers[16,20-22] and by others[17,23] are the natural favoring of nearest-neighbor singlet pairing of the spins which gives $\langle\boldsymbol{\sigma}^{(1)}\cdot\boldsymbol{\sigma}^{(2)}\rangle=-3$ and the separation of spin and charge degrees of freedom, which is intimately connected to the t/U expansion. We define a valence-bond state as one in which the spin on each site (i) forms a spin singlet with one of its neighbors on site j $(|\uparrow\rangle^{(i)}|\downarrow\rangle^{(j)}-|\downarrow\rangle^{(i)}|\uparrow\rangle^{(j)})/\sqrt{2})$. For such a state, $\langle\boldsymbol{\sigma}^{(i)}\cdot\boldsymbol{\sigma}^{(j)}\rangle=-3$ if sites i and j are connected by a "spin bond" and is zero otherwise. The RVB state, proposed as the underlying cause of high-T_c superconductivity, is a linear combination of all possible valence-bond states. We are interested here in how the higher-order terms in Eq. (24) might affect the RVB state for the case relevant to high-T_c superconductivity, that of a two-dimensional square lattice. The classical ground state in this case is the Néel state, illustrated schematically in Fig. 1(a). Including for now only the t^2/U term the expectation value of $H_s^{\prime}$ in the corresponding quantum state is

$$\langle H_s^{\prime}\rangle_N=-4t^2/U\ , \tag{25}$$

which may be compared with the expectation value for any valence-bond (VB) state

$$\langle H_s^{\prime}\rangle_{\rm VB}=-7t^2/2U\ , \tag{26}$$

and with the ground-state energy,

$$\langle H_s^{\prime}\rangle_0\simeq -4\cdot 8t^2/U\ , \tag{27}$$

estimated from numerical calculations[24,25] for the Heisenberg model. The huge degeneracy of valence-bond states [several valence bond states are illustrated schematically in Figs. 1(b)-1(d)] allows fluctuations in the RVB state which will lower its energy below $-7t^2/U$. Existing numerical evidence suggests that the ground state is closer to

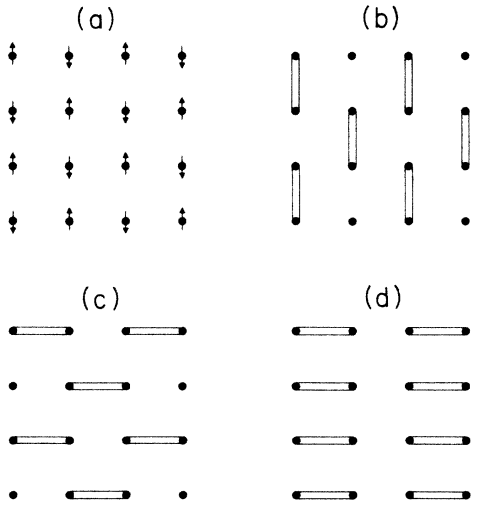

FIG. 1. Schematic illustration of some states of a spin-$\frac{1}{2}$ system on a square lattice. (a) Ising state with antiferromagnetic order. (b)-(d) Three different valence-bond states. Note that states (b) and (d) have no elementary plaquettes with more than one bond on the perimeter.

a Néel state and, unlike the RVB state, has a nonzero staggered moment. (However, the evidence is not yet conclusive.[26]) This expectation has been a principal source of reservations about the RVB theory for high-T_c superconductivity. When the t^4/U^3 terms are included

$$\langle H_s' \rangle_N = -4t^2/U + 24t^4/U^3 + \cdots . \quad (25')$$

More significantly, the degeneracy among valence-bond states is lifted! The largest effect comes from the last of the terms in large parentheses in Eq. (24), which gives a large positive contribution to the energy whenever two bonds exist along the perimeter of an elementary plaquette of the square lattice. Arrangements of the valence bonds which entirely avoid having two bonds on the perimeter of an elementary plaquette, are illustrated schematically in Figs. 1(b) and 1(c). These states are the lowest energy VB states when t^4/U^3 terms are included, and for them we find that for the valence-band lattice states

$$\langle H_s' \rangle_{\mathrm{VBL}} = -7t^2/2U + 12t^4/U^3 + \cdots . \quad (26')$$

These VB states have lower energy than the Ising state for $t/U > 1\sqrt{24} \simeq 0.2$. For comparison, $\langle H' \rangle_s$ for the valence-bond lattice depicted in Fig. 1(d) is $-7t^2/U + 69t^4/2U^3$. For the high-T_c superconductors t/U is now known precisely but it is generally believed that $10^{-2} \lesssim (t/U)^2 \lesssim 10^{-1}$. The higher-order terms discussed above certainly play a role in favoring valence-bond states over Néel states. Moreover, by breaking the degeneracy among valence-bond states they can have a profound effect both on the nature of the RVB state and on the nature of its low-lying excitations.

Note added in proof. After this work was completed, we learned that some of our results for the half-filled case have been obtained previously. See Ref. 27 and work quoted therein.

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