Ground state of $U=\infty$ Hubbard model. Exact solution for two holes

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A many-electron singlet state is constructed and the exact solution of the two-hole Schrödinger equation with the $U=\infty$ Hubbard Hamiltonian is found. It is shown that the singlet-state energy is lower than the energy of the saturated ferromagnetic state.

Nagaoka[1] studied the limiting case of infinite Coulomb repulsion in the Hubbard model[2] and formulated the following proposition which has now been raised to the rank of a theorem: In alternate (A) lattices in the presence of a single hole the ground state is a saturated ferromagnet (F). It is argued in a number of papers[3–7] that the F state is the ground state for a macroscopic number of holes, i.e., for electron densities $n>n_c$ (the critical density n_c depends on the type of lattice). Anderson *et al.*[8] showed by a variational method that in this range of electron densities the F state is stable with respect to the flipping of a single spin.

It follows from Refs. 9 and 10 that for two holes the F state is not the ground state. In this letter we show that the singlet-state is the most likely candidate for the ground state of an electronic system described by Hubbard's model with $U=\infty$.

The Hubbard Hamiltonian, defined on an ideal d-dimensional lattice of N sites, with coordination number z and periodic boundary conditions, in the case of infinite Coulomb repulsion ($U=\infty$) has the form

$$H_\infty=\sum_{\mathbf{fm}\sigma} t(\mathbf{f}-\mathbf{m})X_{\mathbf{f}}^{\sigma 0}X_{\mathbf{m}}^{0\sigma},\quad t(0)=0,\quad t(\delta)=t(-\delta). \tag{1}$$

This Hamiltonian describes a collection of $N_e\leqslant N$ electrons which tunnel to the empty lattice sites. Every site is either empty (0) or is occupied by an electron with spin projection σ. The algebra of Hubbard's X operators is well known.[2]

The problem of the ground state consists of constructing the N_e electron wave functions $|\psi_S\rangle$, which are classified according to the magnitude of the total spin S of the system (because H_∞ commutes with all components of the operator S), and finding the lowest eigenvalue, $E=E(S)$, of the Schrödinger equation:

$$H_\infty|\psi_S\rangle=E(S)|\psi_S\rangle. \tag{2}$$

We note that for any spin configuration the energy of a fully occupied lattice ($N_e=N$) is zero and 2^N-fold degenerate.

The exact solution of Eq. (2) is known—it is the saturated F state with $S=S_{\max}=N_e/2$ (ideal gas of spinless fermions). In particular, the minimum energy of the system with two holes ($N_e=N-2$) is

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$$E_{\min}(S_{\max}) = -[\epsilon(Q) + \epsilon(Q-\Delta k)], \tag{3}$$

where

$$\epsilon(k) = \sum_{\vec{\delta}} t(\vec{\delta}) \exp(ik\vec{\delta}) \tag{4}$$

is the single-electron spectrum, $\epsilon(Q) = \epsilon_{\max}$, $\epsilon(Q-\Delta k)$ is the energy level closest to $\epsilon_{\max}$, and $\Delta k_i = 2\pi/N^{1/d}$.

As an alternative to the F state we consider the *singlet state* ($S=0$, N_e is an even number). The many-electron singlet functions with the common number

$$L_0 = (N_e)! \Big/ \left(\frac{N_e}{2}+1\right)! \left(\frac{N_e}{2}\right)!$$

can be constructed by the method of Rumer diagrams.[11] The following points are important for further discussion.

First, this method can be extended to operators by introducing the creation operators for singlet pairs:

$$B^+_{\mathbf{lm}} = \frac{1}{\sqrt{2}} (X^{\uparrow 0}_{\mathbf{l}} X^{\downarrow 0}_{\mathbf{m}} - X^{\downarrow 0}_{\mathbf{l}} X^{\uparrow 0}_{\mathbf{m}}) = B^+_{\mathbf{ml}}, \tag{5}$$

where **l** and **m** are lattice sites (positions in the indexing circle). For a fixed configuration of N_0 holes the jth Rumer state (Rumer diagram with no intersections) on the remaining collection of an even number of sites can then be written as a product of the jth type

$$|\theta^{(j)}_{\mu}\rangle = B^+_{ab} B^+_{cd} \ldots B^+_{fn} |0\rangle \tag{6}$$

of $(N-N_0)/2$ creation operators which operate on the vacuum $|0\rangle$, where μ is a hole configuration (enumeration of the positions occupied by holes). The number of Rumer diagrams, i.e., products of the type (6), is equal to L_0. The general singlet function for the μth hole configuration is a linear combination of Rumer states:

$$|\theta_{\mu}\rangle = \sum_{j=1}^{L_0} c_j |\theta^{(j)}_{\mu}\rangle. \tag{7}$$

Second, we introduce the concept of evolutionary states which arise as a result of the action of an elementary tunneling operator on the Rumer states $|\theta^{(j)}_{\mu}\rangle$. We consider the case in which the electrons (holes) tunnel to the nearest neighbor (n.n.) sites. The requirement that the tunneling (to n.n.) must be equivalent in all directions imposes rigorous constraints on the choice of coefficients in Eq. (7) and on the following states:

for a single hole in a lattice consisting of an odd number of sites

$$H_{\infty} |\theta_{\mathbf{f}}\rangle = \sum_{\vec{\Delta}} t(\vec{\Delta}) |\theta_{\mathbf{f}+\vec{\Delta}}\rangle, \tag{8}$$

where $\vec{\Delta}$ are vectors directed from the site $\mathbf{f}$ to its z and n.n.;

for two holes in a lattice consisting of an even number of sites

$$H_\infty |\theta_{\mathbf{fm}}\rangle = \sum_{\vec{\Delta}} t(\vec{\Delta}) [|\theta_{\substack{\mathbf{f}+\vec{\Delta},\mathbf{m} \\ \mathbf{f}+\vec{\Delta}\neq\mathbf{m}}}\rangle + |\theta_{\substack{\mathbf{f},\mathbf{m}+\vec{\Delta} \\ \mathbf{f}\neq\mathbf{m}+\vec{\Delta}}}\rangle], \tag{9}$$

where the restrictions on the summation reflect the effect of the "excluded volume." Here $|\theta_{\mathbf{f}}\rangle$ and $|\theta_{\mathbf{fm}}\rangle$ are the functions (7) for one and two holes, respectively, and are invariant under the symmetry operations for the given lattice. The extension of Eq. (9) to a large number of holes is obvious.

Fourier transform (8) immediately yields the eigenvalue of the Schrödinger equation $E_1(\mathbf{k})=\epsilon(\mathbf{k})$ and $[E_1(\mathbf{k})]_{\min}=\epsilon(0)$, where the index 1 denotes the energy of a system with a single hole. For A-lattices we have $\epsilon(0)=-W$, which corresponds to the energy of the F state with a single hole; i.e.,

$$E_1(S=0)=E_1(S=S_{\max}). \tag{10}$$

Nagaoka's theorem disregards this point.

We represent the singlet wave function of a system with two holes in the form

$$|\psi_0\rangle = \sum_{\mathbf{fm}} C_{\mathbf{fm}} |\theta_{\mathbf{fm}}\rangle, \tag{11}$$

where $|\theta_{\mathbf{fm}}\rangle = |\theta_{\mathbf{mf}}\rangle$ is the normalized singlet vacuum for two holes which occupy the sites $\mathbf{f}$ and $\mathbf{m}$, and $\langle\theta_{\mathbf{f'm'}}|\theta_{\mathbf{fm}}\rangle = \delta_{\mathbf{f'f}}\delta_{\mathbf{m'm}}$. The holes occupy different sites, but the restrictions $\mathbf{f}\neq\mathbf{m}$ can be omitted by requiring that $|\theta_{\mathbf{ff}}\rangle=0$. Then, once again, the wave function $|\psi_0\rangle$ does not contain diagonal terms, but formally it contains the so-called nonphysical amplitudes $C_{\mathbf{ff}}$; clearly, $C_{\mathbf{fm}}=C_{\mathbf{mf}}$.

The Schrödinger equation (2) with the function (11) leads, on the basis of Eq. (9), to the following equations for the amplitudes:

$$EC_{\mathbf{f},\mathbf{f}+\mathbf{r}} = \sum_{\substack{\vec{\Delta} \\ (\vec{\Delta}\neq\mathbf{r})}} t(\vec{\Delta}) [C_{\mathbf{f}+\vec{\Delta},\mathbf{f}+\mathbf{r}} + C_{\mathbf{f},\mathbf{f}+\mathbf{r}-\vec{\Delta}}], \tag{12}$$

where $E=E_2(0)$, $\mathbf{m}=\mathbf{f}+\mathbf{r}$, $t(\vec{\Delta})=t(-\vec{\Delta})=-|t|$. The "exceptional volume" effect, when $\mathbf{r}$ coincides with one of the vectors $\vec{\Delta}$, is important in Eq. (12). The amplitudes are sought in the form

$$C_{\mathbf{f},\mathbf{f}+\mathbf{r}} = N^{-2} \sum_{\mathbf{Pk}} \exp[i(\mathbf{PR}+\mathbf{kr})] C_{\mathbf{P}}(\mathbf{k},E), \tag{13}$$

where $\mathbf{R}=(\mathbf{m}+\mathbf{f})/2=\mathbf{f}+\mathbf{r}/2$, $\mathbf{P}=\mathbf{k}_1+\mathbf{k}_2$ is the total momentum of the holes, and $\mathbf{k}=(\mathbf{k}_1-\mathbf{k}_2)/2$ is their relative momentum (all momenta assume N values in the first Brillouin zone). The functions (13) with the Fourier amplitudes

$$C_{\mathbf{P}}(\mathbf{k},E) = \frac{\Omega_{\mathbf{P}}(\mathbf{k})}{E-\Omega_{\mathbf{P}}(\mathbf{k})}, \quad \Omega_{\mathbf{P}}(\mathbf{k}) = \epsilon\left(\frac{\mathbf{P}}{2}+\mathbf{k}\right) + \epsilon\left(\frac{\mathbf{P}}{2}-\mathbf{k}\right), \tag{14}$$

TABLE I.

d	N	$e(0)$	$e(S_{\max})$
1	8	-1,848	-1,707
2	4 × 4	-1,892	-1,500
3	4 × 4 × 4	-1,970	-1,666

where $\epsilon(\mathbf{k})$ is the single-electron spectrum (4) in the n.n. approximation, are the solutions of Eq. (12). Substituting (13) and (14) in (12), we obtain the dispersion relation

$$N^{-1}\sum_{\mathbf{k}}[E-\Omega_{\mathbf{P}}(\mathbf{k})]^{-1}=0, \quad E=E(0), \tag{15}$$

which is the *exact solution* of the problem of finding the spectrum for two holes against the background of a singlet state in the Hubbard model with $U=\infty$. The most interesting solution of the dispersion equation (15) is $E_{\min}(0)$—the lower limit of the spectrum. It is obvious that this is one of the states for which $\mathbf{P}=0$ and $\Omega_0(\mathbf{k})=2\epsilon(\mathbf{k})$ [the center-of-mass momentum $\mathbf{P}$ is a parameter in Eq. (15)]. This solution must be compared with Eq. (3).

For A lattices we have $|\epsilon_{\min}|=\epsilon_{\max}=W=z|t|$, $\epsilon(\mathbf{k})=W\omega_{\mathbf{k}}$, $\omega_0=-1$, $\omega_{\mathbf{Q}}=1$, the spectrum exhibits the properties $\omega_{\mathbf{k}+\mathbf{Q}}=-\omega_{\mathbf{k}}$, $\sum_{\mathbf{k}}\omega_{\mathbf{k}}=0$ (dimensionless momenta are used), and it is easy to prove that the dispersion relation can be represented as follows:

$$N^{-1}\sum_{\mathbf{k}}[e^2-4\omega_{\mathbf{k}}^2]^{-1}=0, \tag{16}$$

where (here and below) the energy of the system $e=E(0)/W$ is put in dimensionless form by dividing by the half-width of the band.

In the one-dimensional case (closed chain) the maximum root of Eq. (16) can be found explicitly. The minimum energies of the singlet ($S=0$) and F states ($S=S_{\max}$) for two holes can be represented in the form

$$e(0)=-2\sqrt{\lambda(N)}, \quad e(S_{\max})=-2\lambda(N), \quad \lambda(N)=\frac{1}{2}\left(1+\cos\frac{2\pi}{N}\right). \tag{17}$$

It follows from Eq. (17) that for arbitrarily large but finite values of N we have $e(S_{\max})-e(0)\approx(2\pi/N)^2/4>0$.

In Table I the minimum energy of the singlet state $e(0)$, found from Eq. (16), for A lattices with $z=2d$ is compared with the minimum energy $e(S_{\max})$ of the F state, calculated in units of W using Eq. (3); the cases with a small number of sites are typical.

These numerical examples and analysis of the solutions (16) for large N enable us to draw the following conclusion: For an electronic system described by the Hubbard

Hamiltonian with $U=\infty$ with tunneling to nearest neighbors, in lattices with an even number of sites and two holes the energy of the singlet state is lower than the energy of the saturated ferromagnetic state:

$$E_2(0) < E_2(S_{\max}). \tag{18}$$

In conclusion, we wish to point out the important fact that there exists an electron–hole symmetry of the following type. Analysis of the two-electron singlet state on an empty lattice, $B^+_{\mathbf{fm}}|0\rangle \equiv |\theta^{el}_{\mathbf{fm}}\rangle$, gives rise to Eqs. (9). Thus the hole states $|\theta_{\mathbf{fm}}\rangle$ against the background of the "singlet vacuum" are equivalent to two-electron singlet states $|\theta^{el}_{\mathbf{fm}}\rangle$ and the spectrum of the singlet pair is described by the same dispersion relation (15). As usual, $e(0) < e(S=1)$, i.e., the energy of the singlet pair is lower than the energy of the triplet pair. In addition, in lattices with an even number of sites the N_e-electron singlet state is energetically equivalent to the state with $(N - N_e)$ holes against the background of the "singlet vacuum" (they are described by equations having the same structure).

The "singlet vacuum" and the "ferromagnetic vacuum", against the background of which the holes move, are spatially uniform and there are probably no other states which could play the role of the ground state in this model. On the basis of inequality (18) which we derived above, the singlet state is the ground state. Since in the gaseous limit $(n=N_e/N \ll 1)$ the ground state obviously does not exhibit long-range magnetic order, due to the indicated type of electron–hole symmetry long-range magnetic order also does not exist in the gaseous limit in the hole concentration. We can thus predict that the singlet state with any even number of electrons is the ground state of the Hubbard model with $U=\infty$.

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