Exact ground state of the Hubbard model on a double-layer square lattice

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A group of analytical wave functions is confirmed to be the ground state of a Hubbard model on a double-layer square lattice in the case of half-filling and in the case with one or two doped holes for a range of parameters. The method is based on the variational principle, and no approximations are applied. In the case of half-filling, the ground state is a product of local pairs. In the case of one or two holes, the doped holes are freely moving in the above background. In both cases there exists a long-range order of the evenness and oddness with respect to the layer parity.

I. INTRODUCTION

Recently, great theoretical effort has been undertaken in the study of two-dimensional (2D) strongly correlated fermion models, which have been suggested as the basis in the description of the properties of CuO_2 layers in high-T_c copper-oxide superconductors. Although the mechanism of superconductivity in these materials remains the main issue, increasing research has been devoted to the understanding of the normal-state properties, especially the transition from the insulating antiferromagnets to the metallic phases by the process of doping of the carriers. The simplest (but still very complex) problem is the behavior of a single doped hole in a background formed by the fermions at half-filling. It is believed that the solution of this problem may give useful information on the general properties of the doped carriers.

Despite the strongest interest, there still exist significant difficulties in this study. In general, the Hamiltonian of a two-dimensional model cannot be exactly diagonalized. At this stage, it seems useful to construct special analytical wave functions which can be rigorously verified to be the eigenstates, or even more, to be the ground states of some models in more than one dimension. These rigorous results can provide reliable information on the general features of strongly correlated systems, and can serve as benchmarks for approximate theories. In recent years some progress has been made in this line. Lieb has proved several theorems on the eigenstates of the Hubbard model.[1] From the analysis of SO(4) symmetry of the Hubbard model in d dimensions, Yang and Zhang have specified a group of eigenstates which are of the η-pairing type and have off-diagonal long-range order.[2,3] Essler, Korepin, and Schoutens have constructed an extended model in d dimensions, and obtained its exact eigenstates also by using the η-pairing theory.[4] From an operator identity, Brandt and Giesekus have obtained the exact ground-state energy for the Hubbard and periodic Anderson model on a peculiar d-dimensional perovskitelike lattice at the limit of infinite interaction strength ($U\rightarrow\infty$).[5] By use of the same method, Strack has found the exact ground-state energy of the periodic Anderson model in $d=1$ and the extended Emery model in $d=1,2$ at the limit of $U\rightarrow\infty$ for special parameter values.[6] At the same time, several analytical wave functions have been specified as the exact ground states for frustrated Heisenberg models or the extended multiband Hubbard model on special lattices in $d=2$ or 3.[7–10] In these works the eigenstates are constructed from a sophisticated selection of the lattice structure and the values of parameters, and then some of them are proved to be the ground state by matching their energies to a lower bound of the ground-state energy, which is usually determined by the variational principle.[11–13] The method of finding a lower bound of ground-state energy has been further developed in recent years.[14]

The theory of η-pairing symmetry of the Hubbard model[2–4] provides a systematic method of finding a special group of eigenstates for finite U. Unfortunately, in the repulsive case ($U>0$) these states are not the ground state.[2] On the other hand, a set of analytical wave functions have been specified as the exact ground states for an extended Hubbard model on a double-layer CuO_2 lattice with two orbits per Cu site in both the insulating case and the case with a few itinerant carriers.[10] The inclusion of two planes and two orbits per Cu site in this model produces a U(2)×U(2) symmetry, in addition to the SO(4) symmetry with respect to the spins and the η pairs. Perhaps it is this additional symmetry that creates the possibility of finding the exact ground states in the case of finite repulsion. It is interesting to notice that the ground state of a few carriers doped to the insulating background is extended, retaining the state of the background almost unchanged, but their momenta are restricted in two directions.[10] The situation is just like two independent Luttinger liquids, overlapped together, with one-dimensional momenta in two cross directions.

In the present paper, I will present a set of analytical wave functions as the exact ground states in a range of parameter values for a single-band Hubbard model on a double-layer square lattice. The spin-$\frac{1}{2}$ fermions fill the lattice, one orbital per site. The interlayer and intralayer nearest-neighbor (NN) hoppings, the on-site repulsion, and the interlayer NN repulsion are taken into account. This model can be viewed as a double-layer version of the

primary Hubbard model.[15] Such a double-layer lattice can be used to mimic the structure of two nearest CuO_2 planes in the Y-Ba-Cu-O or Bi-Sr-Ca-Cu-O high-T_c materials. This structure has a U(2) symmetry with respect to the layer index, instead of the U(2)×U(2) symmetry of the model described in Ref. 10. At the same time, a chemical potential is introduced to specify the filling status. The ground states are given for the case at half-filling and for the case with one or two doped holes. In a range of parameter values, the ground state at half-filling is a product of local pairs. If a few holes are doped, they are mixed with this background and can move freely on the plane with renormalized mass. Unlike the case in Ref. 10, here the momentum direction is no longer restricted, but their parity, defined here as the evenness or oddness, in the layers coincides with the parity of the local pairs in the background. The parity of the local pairs has long-range order, but there is no antiferromagnetic structure. This is because of the special structure and the conditions under which the ground state is found.

This paper is organized as follows: In Sec. II, we describe the Hamiltonian and present a set of analytical eigenstates for a range of parameter values as candidates of the ground state. In Sec. III, the ground state at half-filling is specified by the variational principle. In Sec. IV, the ground state in the case with one or two holes is specified. In Sec. V, the properties of the system are discussed from the obtained results. The conclusions are summarized in Sec. VI.

II. THE HAMILTONIAN AND THE EXACT EIGENSTATES

The Hamiltonian of the model can be written as

$$H=-\sum_{\substack{\mu,\sigma\\ \langle i,j\rangle}} t_1(a^\dagger_{i\mu\sigma}a_{j\mu\sigma}+\text{H.c.})-\sum_{i,\sigma} t_2(a^\dagger_{i1\sigma}a_{i2\sigma}+\text{H.c.}) + \sum_{\substack{i\\ (\mu\sigma)\neq(\mu'\sigma')}} U n_{i\mu\sigma}n_{i\mu'\sigma'}-\mu_c\sum_{i\mu\sigma} n_{i\mu\sigma} , \tag{1}$$

where $a^\dagger_{i\mu\sigma}$ is the creation operator for the spin-$\frac{1}{2}$ fermion at the ith site of the μth plane ($\mu=1,2$) with spin σ ($\sigma=\uparrow,\downarrow$), t_1 and t_2 are the intralayer and interlayer NN hopping strengths, respectively (the site in a plane is numbered so that the two interlayer NN sites have the same index), U is the Coulomb repulsion of two fermions at one site or on two interlayer NN sites, $n_{i\mu\sigma}=a^\dagger_{i\mu\sigma}a_{i\mu\sigma}$ is the number operator, and μ_c is the chemical potential. The sum for $\mu\sigma$ and $\mu'\sigma'$ in the third term is taken over all the pairs of different combinations ($\mu\sigma$) and ($\mu'\sigma'$). In this model the on-site and interlayer NN repulsion strengths are the same, the other repulsion terms are omitted. This optional choice is applied to guarantee the solubility of the model. The model becomes the primary 2D Hubbard model when the number of planes is reduced to one. For such a double-layer structure, there is a U(2) symmetry with respect to the layer index, in addition to the SO(4) symmetry for the spins and the η pairs.[2,3]

The Hamiltonian can be sorted out into two parts:

$$H=H^{(1)}+H^{(2)} , \tag{2}$$

where $H^{(1)}$ is the first sum on the right-hand side of Eq. (1), and $H^{(2)}$ includes the rest terms. For the system with only $H^{(2)}$, the pairs of the interlayer NN sites are isolated from each other, so one can write the eigenstate of it as

$$\Phi_1=\left(\prod_i \psi^\dagger_{1i}\right)|0\rangle , \tag{3}$$

where $|0\rangle$ denotes the vacuum, and $\psi^\dagger_{1i}$ is a pair-creation operator defined as

$$\psi^\dagger_{1i}=\tfrac{1}{2}\{a^\dagger_{i1\uparrow}a^\dagger_{i1\downarrow}+a^\dagger_{i1\uparrow}a^\dagger_{i2\downarrow}+a^\dagger_{i2\uparrow}a^\dagger_{i2\downarrow}+a^\dagger_{i2\uparrow}a^\dagger_{i1\downarrow}\} . \tag{4}$$

The total number of fermions in state Φ_1 is N, the total number of the sites, corresponding to the case of half-filling, and the eigenenergy is

$$\varepsilon_1=N(U/2-t_2-\mu_c) . \tag{5}$$

At the same time, applying $H^{(1)}$ on state Φ_1 results in zero. This can be verified by the relations of the fermion operators:

$$[a_{i\mu\sigma},\psi^\dagger_{1k}]_-=[a^\dagger_{i\mu\sigma},\psi^\dagger_{1k}]_-=0 \quad \text{for } i\neq k \tag{6}$$

and

$$\sum_{\mu,\sigma}(a^\dagger_{i\mu\sigma}a_{j\mu\sigma}+\text{H.c.})\psi^\dagger_{1i}\psi^\dagger_{1j}|0\rangle=0 \quad \text{for } i\neq j . \tag{7}$$

From these relations, one has

$$H^{(1)}\Phi_1=0 . \tag{8}$$

This means that Φ_1 is also an exact eigenstate of Hamiltonian H with energy ε_1.

More generally, it can be verified that the states

$$\Phi_l=\left(\prod_i \psi^\dagger_{li}\right)|0\rangle \quad (l=1,2,3,4) \tag{9}$$

with

$$\psi^\dagger_{li}=\tfrac{1}{2}\sum_{\mu,\mu'} \nu_{\mu\uparrow}(l)\nu_{\mu'\downarrow}(l)a^\dagger_{i\mu\uparrow}a^\dagger_{i\mu\downarrow} ,$$

and

$$\nu_{\mu\sigma}(l)=\begin{cases} 1 & \text{for } \mu=1 \text{ or } l=1 \text{ or } l=3 \text{ and } \sigma=\uparrow \\ & \text{or } l=4 \text{ and } \sigma=\downarrow \\ -1 & \text{otherwise} , \end{cases}$$

are eigenstates of H at half-filling with energies

$$\varepsilon_l=N\{U/2-\mu_c-[\nu_{2\uparrow}(l)+\nu_{2\downarrow}(l)]t_2/2\} . \tag{10}$$

Here the sign functions $\nu_{\mu\sigma}(l)$, $l=1,2,3,4$, reflect the parity (evenness or oddness) at layer μ of the particle. At the same time, $\psi^\dagger_{li}$, $l=1,2,3,4$, can be regarded as the local expressions for symmetry generators, which form the U(2) algebra for the local interlayer pairing.

Now we consider the case with particle number out of the half-filling. Here we only investigate the states of hole doping. The situation of electron doping can be obtained by the particle-hole transformation. When a single

hole with spin $(-\sigma)$ is doped, the following wave function

$$\Phi^{(l)}_{\mathbf{k},\sigma}=\sqrt{1/N}\sum_j \exp(i\mathbf{k}\cdot\mathbf{r}_j)\left[\prod_{i\neq j}\psi^\dagger_{lj}\right]\times[a^\dagger_{j1\sigma}+\nu_{2\sigma}(l)a^\dagger_{j2\sigma}]|0\rangle\ , \tag{11}$$

with arbitrary 2D momentum $\mathbf{k}$, is an exact eigenstate of H with eigenenergy

$$\varepsilon^{(l)}_{\mathbf{k}\sigma}=\left[1-\frac{2}{N}\right]\varepsilon_l-\nu_{2\sigma}(l)t_2-\mu_c+2t_1[\cos(k_x d)+\cos(k_y d)]\ , \tag{12}$$

where $\mathbf{r}_j$ is the 2D coordinate of the jth site, d is the site spacing of the square lattice. This can be verified by applying the two parts of the Hamiltonian $H^{(1)}$ and $H^{(2)}$ on this wave function. As $H^{(2)}$ is the Hamiltonian of independent interlayer pairs, we have

$$H^{(2)}\Phi^{(l)}_{\mathbf{k},\sigma}=\left[\left[1-\frac{2}{N}\right]\varepsilon_l-\nu_{2\sigma}(l)t_2-\mu_c\right]\Phi^{(l)}_{\mathbf{k},\sigma}\ . \tag{13}$$

By the use of the relations in Eqs. (6) and (7), it can be proved that applying those terms in $H^{(1)}$, which do not involve the operators of the jth site, on the jth term in the sum of the right-hand side of Eq. (11), yields zero. At the same time, for the terms in $H^{(1)}$ involving the jth site, we have the relation

$$\left[\sum(a^\dagger_{i\mu\sigma}a_{j\mu\sigma}+\text{H.c.})\right]\psi^\dagger_{li}[a^\dagger_{j1\sigma}+\nu_{2\sigma}(l)a^\dagger_{j2\sigma}]|0\rangle=\psi^\dagger_{lj}[a^\dagger_{i1\sigma}+\nu_{2\sigma}(l)a^\dagger_{i2\sigma}]|0\rangle\quad\text{for } i\neq j\ . \tag{14}$$

Thus, we obtain

$$H^{(1)}\Phi^{(l)}_{\mathbf{k},\sigma}=2t_1[\cos(k_x d)+\cos(k_y d)]\Phi^{(l)}_{k,\sigma}\ . \tag{15}$$

Combining Eqs. (13) and (15), we can prove

$$H\Phi^{(l)}_{\mathbf{k},\sigma}=\varepsilon^{(l)}_{\mathbf{k},\sigma}\Phi^{(l)}_{\mathbf{k},\sigma}\ . \tag{16}$$

$\psi^\dagger_{li}$ is a creation operator for a local interlayer pair. Here the parities of two particles of the pair are described by a single quantum number, l. It can be seen that Φ_l is just a background formed by the local pairs with the same parity number l. The restriction on the parity of individual pair corresponds to the symmetry breaking caused by the correlation effect of the model. It is interesting to notice that a single hole is simply imbedded in this background, and can move freely in the plane with arbitrary 2D momentum, but its parity is also restricted by the parity of the background, as can be seen from the sign factor $\nu_{2\sigma}(l)$ in Eq. (11). This situation is different from that of the multiband double-layer model on a CuO_2 lattice, where the parity of a single carrier is not restricted, but the direction of the momentum is restricted in the principal axes of the oxygen sublattice.[10]

If M holes ($M<N/2$) are doped, the following wave functions are exact eigenstates of the system:

$$\Phi^{(l)}_{\mathcal{K}_M}=N^{-M/2}\sum_{j_1}\sum_{j_2}\cdots\sum_{j_\chi}\cdots\sum_{j_M}\exp\left[\sum_{\chi=1}^{M}i\mathbf{k}_\chi\cdot\mathbf{r}_{j_\chi}\right]\left[\prod_{i\neq j_1,j_2,\ldots,j_\chi,\ldots,j_M}\psi^\dagger_{lj}\right]\prod_{\chi=1}^{M}[a^\dagger_{j_\chi 1\sigma_\chi}+\nu_{2\sigma_\chi}(l)a^\dagger_{j_\chi 2\sigma_\chi}]|0\rangle\ , \tag{17}$$

with eigenenergies

$$\varepsilon^{(l)}_{\mathcal{K}_M}=\left[1-\frac{2M}{N}\right]\varepsilon_l-t_2\sum_{\chi=1}^{M}\nu_{2\sigma_\chi}(l)-M\mu_c+2t_1\sum_{\chi=1}^{M}[\cos(k_{\chi x}d)+\cos(k_{\chi y}d)]\ , \tag{18}$$

where $\mathcal{K}_M$ is an ensemble of M different combined quantum numbers: $(\mathbf{k}_1,\sigma_1),(\mathbf{k}_2,\sigma_2),\ldots,(\mathbf{k}_\chi,\sigma_\chi),\ldots,(\mathbf{k}_M,\sigma_M)$. These eigenstates can also be verified by applying the Hamiltonian to them. In these states the parities of all the doped holes are the same as that of the background. At the same time, the other quantum numbers, $\mathbf{k}$ and σ, are filled by the holes just like a free-fermion system. As the parity is restricted, a pair of sites can only accommodate one hole per spin, and the laminate hopping in this double-layer structure is renormalized to that of a single-layer structure.

III. EXACT GROUND STATE AT HALF-FILLING

In the last section we have presented several analytical eigenstates of the Hamiltonian. These states are far from complete, but they can be used as some candidates in searching the ground state. In order to find out if one of them is the ground state, we should first determine a lower bound of the ground-state energy, and then compare the energies of the candidates with this bound. In doing this we divide the Hamiltonian into N sub-Hamiltonians:

$$H=\sum_{m=1}^{N}H_m\ , \tag{19}$$

where

$$\begin{aligned}H_m=&-\sum_{\mu,\sigma}t_1(a^\dagger_{i\mu\sigma}a_{j\mu\sigma}+\text{H.c.})\\&-\tfrac{1}{4}\sum_{\sigma}t_2(a^\dagger_{i1\sigma}a_{i2\sigma}+a^\dagger_{j1\sigma}a_{j2\sigma}+\text{H.c.})\\&+\tfrac{1}{4}\sum_{(\mu\sigma)\neq(\mu'\sigma')}U(n_{i\mu\sigma}n_{i\mu'\sigma'}+n_{j\mu\sigma}n_{j\mu'\sigma'})\\&-\tfrac{1}{4}\mu_c\sum_{\mu\sigma}(n_{i\mu\sigma}+n_{j\mu\sigma})\ ,\end{aligned} \tag{20}$$

here $i=[(m+1)/2]$, j is such a nearest neighbor of i that $\mathbf{r}_j=\mathbf{r}_i+\hat{\mathbf{x}}d$ if m is odd and $\mathbf{r}_j=\mathbf{r}_i+\hat{\mathbf{y}}d$ if m is even, $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are the unit vectors along the x and y directions, respectively. It can be seen that all the sub-Hamiltonians

are the same, except a dummy index m. So they have the same eigenvalues. If $\varepsilon_{\min}$ is the lowest eigenvalue of H_m for all possible fermion numbers, then $N\varepsilon_{\min}$ is a lower bound of the ground-state energy of H, in accordance with the variational principle.[11–13] $\varepsilon_{\min}$ can be determined by comparing all the eigenvalues of H_m.

If N_m, the fermion number in the subsystem, is zero, the corresponding lowest eigenvalue of H_m is also zero,

$$\varepsilon_m(0)=0 . \tag{21}$$

In the case of $N_m=1$, there are eight eigenstates, and the lowest eigenvalue is

$$\varepsilon_m(1)=-\mu_c/4-|t_1|-|t_2|/4 . \tag{22}$$

After a tedious calculation, the lowest eigenvalues for $N_m=2,3,4$ are

$$\varepsilon_m(2)=-\mu_c/2-|t_2|/2 -(U^2/64+4t_1^2)^{1/2}+U/8 , \tag{23}$$

$$\varepsilon_m(3)=-3\mu_c/4+U/4-|t_2|/4 +\min\{x_1,-|t_1|-|t_2|/2\} , \tag{24}$$

where x_1 is the smallest solution of the equation for x:

$$x^3-(U/2-|t_1|)x^2-(U/2+5|t_1|)|t_1|x +t_1^2U+3|t_1|^3=0 , \tag{25}$$

$$\varepsilon_m(4)=-\mu_c+U/2+\min\{-|t_2|,-|t_2|/2+U/8 -(U^2/64+4t_1^2)^{1/2},x_2\} , \tag{26}$$

where x_2 is the smallest solution of the equation for x:

$$x^3-\frac{5U}{4}x^2+(U^2/4-12t_1^2)x+8t_1^2U=0 . \tag{27}$$

By the use of these results, the lowest eigenvalues in the cases of $N_m=5,6,7,8$ can be obtained from the particle-hole symmetry,

$$\varepsilon_m(5)=-5\mu_c/4+U-|t_2|/4 +\min\{x_1,-|t_1|-|t_2|/2\} , \tag{28}$$

$$\varepsilon_m(6)=-3\mu_c/2+13U/8-|t_2|/2 -(U^2/64+4t_1^2)^{1/2} , \tag{29}$$

$$\varepsilon_m(7)=-7\mu_c/4+9U/4-|t_1|-|t_2|/4 , \tag{30}$$

$$\varepsilon_m(8)=-2\mu_c+3U . \tag{31}$$

So a lower bound of the ground-state energy of H can be determined as

$$\varepsilon_{\text{bound}}=N\min_{0\le N_m\le 8}\{\varepsilon_m(N_m)\} . \tag{32}$$

It depends on the parameters t_1, t_2, U, and μ_c.

In the last section we have found four eigenstates of H in the case of half-filling, Φ_l, $l=1,2,3,4$. If the eigenvalue of one of these candidates saturates the lower bound, it is the true ground state. From this we can obtain that, when

$$|t_2|\ge-\min\{-|t_2|/2+U/8-(U^2/64+4t_1^2)^{1/2},x_2\} \tag{33}$$

and

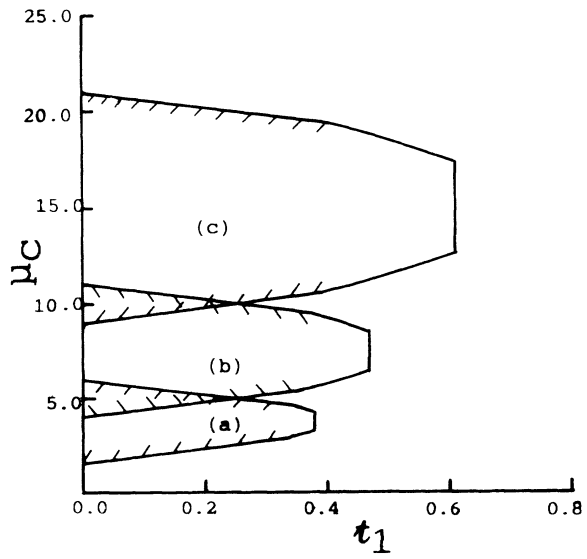

FIG. 1. The regions defined by conditions (33) and (34) are plotted in the μ_c-t_1 plane. $t_2=1$. Region (*a*) is for $U=2.5$, (*b*) is for $U=5.0$, and (*c*) is for $U=10.0$. A portion of the boundaries, which is defined by the equalities of (34) and meets conditions (33) and (38), is marked by shady lines.

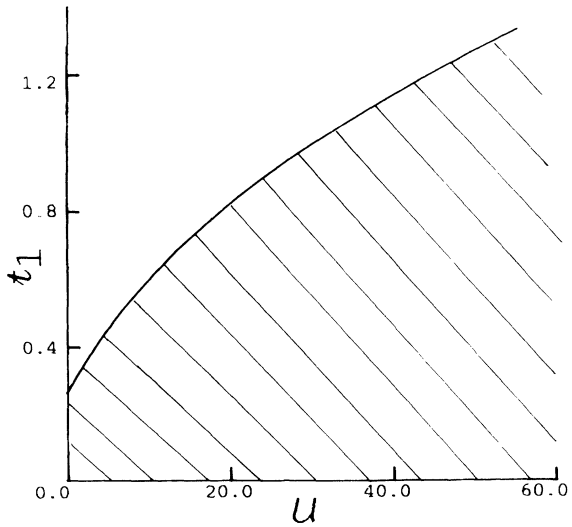

FIG. 2. The region defined by condition (33) is shown by a shady area in the t_1-U plane. $t_2=1$, and μ_c is arbitrary.

$$2U+3|t_2|+4\min\{x_1,-|t_1|-|t_2|/2\}\geq\mu_c\geq U-3|t_2|-4\min\{x_1,-|t_1|-|t_2|/2\}\ , \tag{34}$$

then Φ_1 is the ground state for $t_2\geq 0$ and Φ_2 is the ground state for $t_2\leq 0$, with ground-state energy ε_1 and ε_2, respectively.

For positive t_1, t_2, and U, we illustrate the parameter regions which meet conditions (33) and (34) in Figs. 1 and 2. The regions are plotted on the μ_c-t_1 plane for several choices of U in Fig. 1, and plotted on the t_1-U plane for arbitrary value of μ_c in Fig. 2. The value of t_2 is defined as the energy scale. Only a portion of the boundaries of a region, marked by the shady lines in Fig. 1, is the borders separating the half-filling and the doped areas. These borders will be discussed later. Conditions (33) and (34) are satisfactory for Φ_1 or Φ_2 being the ground state, but may not be necessary. It can be seen that these parameter regions are enlarged if the repulsion strength is increased. At the limit $U\rightarrow\infty$, there is no restriction on the values of t_1 and t_2 for meeting condition (33), and the range of μ_c defined by inequalities (34) also approaches infinity.

IV. THE EXACT GROUND STATE IN THE CASE WITH ONE OR TWO DOPED HOLES

The method mentioned above can be used to determine the ground state not only for the half-filling case, but also for the case with doped carriers. In fact, the lower bound for ground-state energy given by Eq. (32) is valid for any filling status. In this section we consider the case with a few doped holes, which may be of interest in understanding the interplay between the repulsion terms and the itinerant terms in the model.

If a single hole with spin $(-\sigma)$ is doped, from Eqs. (11) and (12), the possible candidate for the ground state is $\Phi^{(l)}_{\mathbf{k},\sigma}$ with

$$l=\begin{cases}1 & \text{for } t_2\geq 0\ ,\\ 2 & \text{for } t_2\leq 0\ ,\end{cases} \tag{35}$$

and

$$\mathbf{k}d=\begin{cases}(0,0) & \text{for } t_1\leq 0\ ,\\ (\pi,\pi) & \text{for } t_1\geq 0\ ,\end{cases} \tag{36}$$

having the eigenenergy

$$\varepsilon_1^{(\text{hole})}=N(U/2-|t_2|-\mu_c)-U+\mu_c+|t_2|-4|t_1|\ . \tag{37}$$

From Eqs. (32) and (37), we can prove that if the conditions

$$-|t_1|-|t_2|/2\leq x_1\ , \tag{38}$$

$$\mu_c=U-|t_2|+4|t_1|\ , \tag{39}$$

and condition (33) are all satisfied, $\varepsilon_1^{(\text{hole})}$ saturates the lower bound of the ground-state energy and the state $\Phi^{(l)}_{\mathbf{k}\sigma}$ with l and $\mathbf{k}$ given by Eqs. (35) and (36) is the exact ground state. The parameter region for these conditions is just a part of the boundaries of the region defined in the last section for the case of half-filling. It is illustrated by the bottom-marked boundary of the region in Fig. 1. Equation (39) specifies the value of chemical potential for one-hole doping status. At the same time, the top-marked boundary in Fig. 1 corresponds to the case with one particle doped.

In a similar way, we can verify that under the same conditions the state $\Phi^{(l)}_{\mathcal{H}_M}$, defined in Eq. (17), with $M=2$ and $\mathcal{H}_2=\{(\uparrow,\mathbf{k}),(\downarrow,\mathbf{k})\}$, and l and $\mathbf{k}$ given by Eqs. (35) and (36), respectively, is the exact ground state with the same energy as $\varepsilon_1^{(\text{hole})}$, and with two holes doped.

In the case with more than two holes doped, we cannot rigorously specify the ground state. Nevertheless, the most possible candidates may be selected from the states described by $\Phi^{(l)}_{\mathcal{H}_M}$. For a given hole number M, the ensemble $\mathcal{H}_M$ with the lowest energy is such that the doped holes occupy the lowest levels defined by the last sum on the right-hand side of Eq. (18) and form a pseudo-Fermi sphere. Meanwhile l is given by Eq. (35). Although the energy of this pseudo-Fermi sphere does not saturate the lower bound of Eq. (32), the per-site energy increment with respect to this bound is only a quantity of the order of M/N:

$$\delta\varepsilon(\mathcal{H}_M)/N\approx\pi|t_1|M/N\ . \tag{40}$$

When a finite number of holes are doped into an infinite lattice, this per-site increment is infinitesimal. This is because the states (17) do not violate the main structure of the background. At the same time, those states which involve a change of the background should cause a finite per-site energy increment. So we can argue that in this situation the pseudo-Fermi sphere is most likely to be the ground state.

V. SOME REMARKS ON THE PROPERTIES OF THE STATES

In this section we qualitatively discuss some properties of the states obtained above. This is far from complete, but may be useful for further investigations.

A. Long-range order

Unlike the single-layer model, the ground state at half-filling Φ_l ($l=1$ or 2) does not exhibit antiferromagnetic order. However, there is another type of long-range order: the order in the interlayer parity l. In the ground state, the parities of all the local pairs are the same. Furthermore, when a hole is doped, it also takes the same parity. For the quantitative description one can define an order parameter as

$$\Delta_l=\left\langle\frac{2}{N}\sum_i\psi^\dagger_{li}\psi_{li}\right\rangle\ ,\quad l=1,2,3,4\ , \tag{41}$$

where $\langle\cdots\rangle$ denotes the statistical average. In the ground state at half-filling, Δ_1 or Δ_2 is 1 and the others are zero. A quantum fluctuation occurs only when holes (or electrons) are doped.

B. Is the system with doped holes a Fermi liquid?

Although the ground states of one and two doped holes are found, the question whether the Fermi-liquid characteristics are resumed in the system with more doped holes is still open. The state of the pseudo-Fermi sphere described in the last section, most likely being the ground state at the limit of $M/N \to 0$, behaves like a Fermi sea containing free holes embedded in a background of local pairs. The only restriction on the holes is their layer parity. Unfortunately, the states described by Eq. (17) represent only a little portion of the degrees of freedom. The other states are still unknown. It can be expected that they should involve some kind of fluctuations of the background. Thus, the energy-momentum relation is not so determinant as that of Eq. (18). As these states may be involved in a large portion of the low-energy excitations, the system is not a standard Fermi liquid, even though the pseudo-Fermi sphere may be a ground state.

VI. SUMMARY

We have defined a Hubbard model on a double-layer square lattice. In this model, the intralayer and interlayer NN hoppings, and the on-site and interlayer NN Coulomb repulsions are included. It represents some main features of the 2D strongly correlated system, but is easy to solve. A set (far from complete) of the exact eigenstates is presented as the candidates of the ground state. By the use of the variational principle, the ground states in the case of half-filling and in the case with one and two doped holes are specified for a certain region of the parameter space. In this procedure no approximation is applied. At half-filling, the ground state is simply a product of local interlayer pairs, having long-range order of the layer parity. If one or two holes are doped, they are simply embedded in this background, and can move in the plane freely, but their layer parity is restricted by the background. In the case with a few (more than two) holes doped, the most possible candidate of the ground state is a pseudo-Fermi sphere with the background unchanged, but the Fermi-liquid characteristics are unlikely to be resumed because of the enormous number of degrees of freedom for the low-energy excitations arising in the background.

A striking difference of these states from those of the single-layer model is the absence of the antiferromagnetic order and the accompanying quantum fluctuations. The structural source of this difference is the additional U(2) symmetry of the layer index. In the parameter regions investigated in this paper, the features governed by this symmetry are dominant over the others. At the same time, the present model also has the SO(4) symmetry of the Hubbard models, with respect to the spins and the η pairs. So it is possible that in the other parameter regions the system may exhibit the same antiferromagnetic order as that of the single-layer model. However, at the strongest correlation limit ($U \to \infty$), the order of the interlayer parity is dominant for any finite values of t_1 and t_2, as has been discussed in Sec. III. It is interesting to investigate the interplay between these different long-range orders in further studies.

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