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Mobile holes in a two-dimensional Heisenberg antiferromagnet

Toshihiro Itoh, Masao Arai, and Takeo Fujiwara
Department of Applied Physics, University of Tokyo, Bunkyo-ku, Tokyo 113, Japan
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The t-t'-t''-J model is investigated by a rigorous diagonalization in a two-dimensional square lattice as large as $\sqrt{20}\times\sqrt{20}$, which has no additional degeneracy. The ground state of one hole in the t-J model is at a momentum $\mathbf{k}$ near $(\pm\pi/2, \pm\pi/2)$ with a total spin $S=\frac{1}{2}$ and that of two holes is at $\mathbf{k}=(0,0)$ with $S=0$. The hole pairing and nonclustering may be preferable for the ground state of the t-t'-t''-J model in the region of $t'>0$ and $t''\lesssim 0$.

The recent discovery of high-T_c superconductivity in cuprate oxide compounds has stimulated a wide interest in the motion of holes in two-dimensional Heisenberg antiferromagnets. It seems to be a common understanding that one of the simple starting models for high-T_c superconductivity would be a two-band system (Cu $3d_{x^2-y^2}$ and O $p_{x/y}$ or $p\sigma$) of strongly correlated fermions on a two-dimensional plane, what is called the d-p model.[1] The doped holes occupy oxygen $p\sigma$ orbitals on the CuO_2 plane and the Cu^{2+} is stable in a hole-doped system. The local spin ($S=\frac{1}{2}$) on a copper site might form a local singlet state with hole spins doped on surrounding oxygen sites.[2] This local singlet state behaves just as one composite particle. Therefore, a mobile hole of a local singlet in the d-p model may be projected on a model where a hole moves around in an antiferromagnetic spin system in a two-dimensional square lattice. The oxygen sites without holes play a simple role of superexchange path for local-spin pairs. From this viewpoint, holes can transfer not only to the nearest-neighbor sites but to several farther neighbor sites. Finally, we would arrive at the t-t'-t''-J model in a two-dimensional square lattice;

$$H=\Big[-t\sum_{\langle i,j\rangle_1}\tilde{c}^\dagger_{i\sigma}\tilde{c}_{j\sigma}-t'\sum_{\langle i,j\rangle_2}\tilde{c}^\dagger_{i\sigma}\tilde{c}_{j\sigma}-t''\sum_{\langle i,j\rangle_3}\tilde{c}^\dagger_{i\sigma}\tilde{c}_{j\sigma}+\text{H.c}\Big]+J\sum_{\langle i,j\rangle_1}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_in_j)\,, \tag{1}$$

where $\tilde{c}^\dagger_{i\sigma}=c^\dagger_{i\sigma}(1-n_{j-\sigma})$ is a creation operator of electrons in a Hilbert space subtracting double occupancy and $\mathbf{S}_i=\frac{1}{2}\sum_{ss'}c^\dagger_{is}\sigma_{ss'}c_{is'}$ is a local-spin operator. The transfer integrals t, t', and t'' are for the first (a distance of $R=1$ in units of the lattice constant), second ($R=\sqrt{2}$), and third ($R=2$) nearest neighbors, respectively, and $J(>0)$ is an exchange integral for the nearest-neighbor local-spin pairs in a two-dimensional square lattice. Figure 1 shows a cluster of $\sqrt{20}\times\sqrt{20}$ sites used in this paper and the neighbor pairs for the transfer integrals t, t', and t''. We will use units of energy $t=1$.

The ground state of a Heisenberg antiferromagnetic

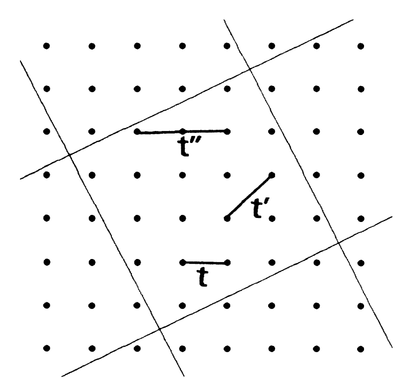

FIG. 1. $\sqrt{20}\times\sqrt{20}$ cluster in a two-dimensional square lattice and the transfer integrals t, t', and t''.

spin system on a square lattice without a hole was studied by several authors and is commonly believed to be an antiferromagnetic ordered state with rather well-defined sublattice magnetization.[3] Once a single hole is introduced in a $J/t\to 0$ limit, the ground state is known exactly and is ferromagnetic (Nagaoka ferromagnetism).[4] For a finite value of J, the t-J model ($t'=t''=0$) with doped holes has been studied by various methods, e.g., the many-body tight-binding method[5,6] and the spin-wave theory.[7,8] The bandwidth of the t-J model is of order of J (Refs. 5–7) and the effects of t' and t'' are not negligible, though the values of t' and t'' may be small in comparison with that of t.

It was also studied by an exact diagonalization of small systems with a periodic boundary condition.[9–15] Conclusion of numerical investigations is rather controversial at the present stage, because the ground state degenerates in $L=\sqrt{10}\times\sqrt{10}$ and 4×4 due to an additional symmetry caused by the finiteness of the system size and a periodic boundary condition. Hasegawa and Poilblanc[13] and Elser, Huse, Shraiman, and Siggia[14] reported the properties of the ground state of one hole in $L=\sqrt{18}\times\sqrt{18}$ sites. However, Hasegawa and Poilblanc[13] used a system of $L=4\times4$ for two holes and suffered from the size restriction. Bonča and Prelovšek[12] treated the t-t'-t''-J model with $t'=t''$ in $L=4\times4$. Riera[15] treated the t-t'-J-J' model starting from the Hubbard model on a square lattice of $L=4\times4$ with a constraint between transfer and exchange integrals as $J=4t^2/U$ and $J'=4t'^2/U$. Hole clustering is expected in a large J limit. The t term destroys

TABLE I. The energy of the lowest state of one hole E_1 and the two-hole binding energy $E_{B,2}$ for the t-J model as a function of J and $\mathbf{k}$ ($L=\sqrt{20}\times\sqrt{20}$ and $t=1$).

$\mathbf{k}$	$J=0.0$	0.25	0.5	0.75	1.0	1.5	2.0
(0,0)	−3.8039	−7.6226	−12.2429	−17.1591	−22.3251	−32.9321	−43.6323
$(\frac{1}{5}\pi,\frac{3}{5}\pi)$	−3.8961	−7.9716	−12.9906	−18.1084	−23.2823	−33.7329	−44.2702
$(\frac{2}{5}\pi,\frac{1}{5}\pi)$	−3.8552	−7.8693	−12.8403	−17.9522	−23.1364	−33.6199	−44.1902
$(\frac{3}{5}\pi,\frac{4}{5}\pi)$	−3.9495	−7.7721	−12.6318	−17.6834	−22.8240	−33.2460	−43.7747
$(\frac{4}{5}\pi,\frac{2}{5}\pi)$	−3.9104	−7.9101	−12.8952	−17.9913	−23.1486	−33.5736	−44.0922
$(\pi,0)$	−3.8731	−7.8997	−12.9047	−18.0038	−23.1609	−33.5882	−44.1135
(π,π)	−4.0000	−7.6460	−12.2169	−16.9748	−22.0339	−32.3338	−42.6984
$E_{B,2}$	1.1296	−0.2420	−0.4798	−0.6817	−0.8717	−1.2360	−1.5890

the Néel order. Emery, Kivelson, and Lin[16] suggested that the t term introduces the frustration and causes the phase separation with the hole-rich ferromagnetism in the $J/t\to 0$ limit of the t-J model. The t' and t'' terms are not contradiction to the Néel order and may stabilize the system against the phase separation.

We report here the ground-state properties for one and two holes of the model Hamiltonian (1) with a periodic boundary condition; they are the t-J model in $L=\sqrt{20}\times\sqrt{20}$ and the t-t'-t''-J model in $L=\sqrt{18}\times\sqrt{18}$. The key quantities are a two-hole binding energy $E_{B,2}=(E_2-E_0)-2(E_1-E_0)$ and a four-hole binding energy $E_{B,4}=(E_4-E_0)-2(E_2-E_0)$. The region $E_{B,2}<0$ would correspond to hole pairing and the region $E_{B,4}<0$ to hole clustering.

For a rigorous diagonalization, we used the Lanczos (for an eigenenergy) and the conjugate gradient (for an eigenfunction) methods.[17] The original Lanczos method is often more efficient than the modified Lanczos method.[18] Our experience tells that, for the t-J model, convergence of the modified Lanczos method is rather poor and not efficient enough. In the present investigation, we classify eigenstates by the total momentum $\mathbf{k}$ and the value of the z component of the total spin (S_z). The resulting eigenfunctions are generally complex quantities and a matrix to be diagonalized is Hermitian but not real symmetric. A direct application of the conjugate gradient method requires a matrix to be real symmetric. However, an eigenvalue problem of an $n\times n$ Hermite matrix $H=A+iB$ is equivalent to that of a $2n\times 2n$ real symmetric matrix

$$H'=\begin{pmatrix} A & -B \\ B & A \end{pmatrix},$$

where A and B are $n\times n$ real symmetric and antisymmetric matrices, respectively, and the conjugate gradient method can work with a doubled size of matrices. The number of states of two holes of $S_z=0$ in $L=\sqrt{20}\times\sqrt{20}$ is 9 237 800, which can be reduced into several blocks of equal size, 461 890 states, by the momentum classification. The system size $L=\sqrt{18}\times\sqrt{18}$ is the smallest one that does not have any additional accidental degeneracy. The system size $L=\sqrt{20}\times\sqrt{20}$ may not be large enough, but is in itself important. This size allows a momentum $\mathbf{k}=(\pi,0)$ and we can see whether these states on a pseudo-Fermi surface ($k_x\pm k_y=\pm\pi$) could be the ground state. Our results of $L=\sqrt{10}\times\sqrt{10}$, 4×4, and $\sqrt{18}\times\sqrt{18}$ all coincide with those already published[9–14] and we will not repeat them except in a case where it is essentially important or new.

One hole in t-J model. The ground state turns out to be the Nagaoka ferromagnetism ($S=S_{max}$) when J/t is less than $(J/t)_1\simeq 0.1$ ($L=\sqrt{10}\times\sqrt{10}$), 0.075 ($L=4\times 4$), 0.05–0.1 ($L=\sqrt{18}\times\sqrt{18}$), 0–0.05 ($L=\sqrt{20}\times\sqrt{20}$). As shown by Hasegawa and Poilblanc,[13] the ground state in $L=\sqrt{18}\times\sqrt{18}$ is at $\mathbf{k}=(\pi/3,\pi/3)$ in $(J/t)_2\simeq 0.2>J/t>(J/t)_1$ and $\mathbf{k}=(\frac{2}{3}\pi,0)$ in $J/t>(J/t)_2$. Then they suggested that the ground state in the t-J model would have a crossover from $\mathbf{k}=(\pi/2,\pi/2)$ to $(\pi,0)$ at $J/t\simeq 0.2$ with increasing J/t. However, the present calculation shows clearly that this situation is specific to $L=\sqrt{10}\times\sqrt{10}$ and $\sqrt{18}\times\sqrt{18}$ and the ground state in $L=\sqrt{20}\times\sqrt{20}$ is at $\mathbf{k}=(\pi/5,\frac{3}{5}\pi)$, irrespective of $J/t[>(J/t)_1]$. The important point is that, in this system size, possible momentums are $\mathbf{k}=(0,0)$, $(\pi/5,\frac{3}{5}\pi)$, $(\frac{2}{5}\pi,\pi/5)$, $(\frac{3}{5}\pi,\frac{4}{5}\pi)$, $(\frac{4}{5}\pi,\frac{2}{5}\pi)$, $(\pi,0)$, and (π,π) and, among them, the ground state is at the second but not the sixth. Therefore, we expect that the true ground state might be at a $\mathbf{k}$ point near $(\pi/2,\pi/2)$ inside the pseudo-Fermi surface. The energy of the lowest state for each $\mathbf{k}$ in $L=\sqrt{20}\times\sqrt{20}$ is summarized in Table I as a function of J/t. We assume a simple

TABLE II. The parameter a_0–a_3 for one-hole lowest-state energy $E(\mathbf{k})$ of the t-J model ($L=\sqrt{18}\times\sqrt{18}$, $\sqrt{20}\times\sqrt{20}$, and $t=1$).

L	J	a_0	a_1	a_2	a_3
18	0.25	−7.294	−0.006	0.148	0.033
18	0.5	−11.622	−0.026	0.349	0.090
18	1.0	−20.667	−0.097	0.496	0.164
18	1.5	−29.935	−0.168	0.478	0.169
18	2.0	−39.305	−0.242	0.473	0.178
20	0.25	−7.859	−0.008	0.142	0.044
20	0.5	−12.786	−0.030	0.344	0.108
20	1.0	−23.786	−0.091	0.489	0.171
20	1.5	−33.456	−0.154	0.475	0.173
20	2.0	−43.993	−0.220	0.468	0.178

TABLE III. A momentum **k** of the one-hole ground state (top) and $E_{B,2}$ (bottom) for the t-t'-t''-J model ($L=\sqrt{18}\times\sqrt{18}$, $J=0.5$, and $t=1$).

t''	$t'=-0.6$	-0.4	-0.2	0.0	0.2	0.4	0.6
-0.6	(π,π)	(π,π)	(π,π)	(π,π)	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$
	0.6099	0.5847	0.5271	0.0733	−0.1068	−0.6139	−0.6698
-0.4	(π,π)	(π,π)	(π,π)	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$
	0.5691	0.5116	0.3852	−0.3872	−0.5476	−0.6265	−0.6640
-0.2	(π,π)	(π,π)	(π,π)	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$
	0.4613	0.3254	−0.2413	−0.4813	−0.5860	−0.6399	−0.6671
0.0	(π,π)	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$
	0.1552	0.0823	−0.0580	−0.5359	−0.6115	−0.6551	−0.6788
0.2	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$	$(\frac{2}{3}\pi,0)$
	0.0993	0.1327	0.1642	−0.1381	−0.6189	−0.6689	−0.6978
0.4	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\frac{2}{3}\pi,0)$
	0.1841	0.2290	0.2587	0.2077	−0.1714	−0.6700	−0.7188
0.6	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\pi/3,\pi/3)$	$(\frac{2}{3}\pi,0)$
	0.2921	0.3217	0.3340	0.3151	0.2186	−0.2120	−0.7263

form of the lowest-state energy as a function of **k** in

$$E(\mathbf{k})=\alpha_0+\alpha_1[\cos(k_x)+\cos(k_y)]+\alpha_2\cos(k_x)\cos(k_y)+\alpha_3[\cos(2k_x)+\cos(2k_y)]\,. \quad (2)$$

The values of these parameters α_0–α_3 depend on J and are summarized in Table II for $L=\sqrt{18}\times\sqrt{18}$ and $\sqrt{20}\times\sqrt{20}$. The values of these parameters are quite similar in these two system sizes. The value of α_1 is very small in a region of $J/t\simeq 0.25-1.0$. These values of α_0–α_3 suggest that the ground state is at **k** near $(\pi/2,\pi/2)$ inside the pseudo-Fermi surface in a width range of J/t. The nonvanishing α_1 indicates that a quantum fluctuation of spins is still important for a hole motion in a large J/t limit. Trugman,[5] Maekawa, Inoue, and Tohyama,[6] and Elser, Huse, Shraiman, and Siggia[14] also suggested the ground-state momentum to be at $\mathbf{k}=(\pi/2,\pi/2)$.

Two holes in t-J model. The ground state of two holes, in $L=\sqrt{10}\times\sqrt{10}$, is degenerated at $\mathbf{k}=(0,0)$ and $(\frac{2}{5}\pi,\frac{4}{5}\pi)$ and, in $L=4\times4$, at $\mathbf{k}=(0,0)$ and $(\pi,0)$. We first observed here that the ground state of two holes in $L=\sqrt{18}\times\sqrt{18}$ and $\sqrt{20}\times\sqrt{20}$ is nondegenerate at $\mathbf{k}=(0,0)$ and is a spin singlet (the total spin $S=0$). This observation is not affected by a value of J/t. Therefore, Nagaoka's theorem[4] is not applicable in this case and phase separation with the hole-rich ferromagnetism may not be expected. The two-hole binding energy $E_{B,2}$ is summarized in Table I as a function of J/t, which is proportional to a value of J when J is relatively large. The hole density-density correlation function shows, as in smaller systems, that the nearest-neighbor correlation increases with increasing J and those of farther neighbors decrease.[19] This observation can be explained by an argument that two holes favorably form a nearest-neighbor pair so that a loss of exchange bonds can be reduced to seven rather than eight for distant two holes. The absolute values of spin-spin correlation functions increase with increasing J for several near-neighbor sites.[19]

t-t'-t''-J model. We investigated effects of t' and t'' carefully in the t-t'-t''-J model of $L=\sqrt{18}\times\sqrt{18}$ in the case of $J=0.5$.

The ground state of one hole is $S=\frac{1}{2}$ and its momentum is listed in Table III. There are three possible cases of the ground-state momentum. It shifts to $(\frac{2}{3}\pi,0)$ with positive increasing t', to $(\pi/3,\pi/3)$ with increasing t'' and to (π,π) with negative but increasing absolute values of t' and t''. We expect the same form as Eq. (2) of the lowest-state energy $E(\mathbf{k})$ and that t' and t'' modulate coefficients α_2 and α_3, respectively. Therefore, the ground state would shift to $\mathbf{k}=(\pi,0)$ with increasing t' and to $\mathbf{k}=(\pi/2,\pi/2)$ with increasing t''.

The ground state of two holes is $S=0$ and at $\mathbf{k}=(0,0)$ in a very wide range of t' and t'', especially when the two-hole binding energy E_{B2} is negative. The ground state is not at $\mathbf{k}=(0,0)$ in a region of ($t''=0.4$, $0\geq t'\geq -0.2$) and ($t''=0.6, 0.2\geq t'$), and states with several momentums **k** give nearly the same lowest-state energies. The values of $E_{B,2}$ are also summarized in Table III. The

TABLE IV. $E_{B,4}$ for the t-t'-t''-J model ($L=\sqrt{18}\times\sqrt{18}$, $J=0.5$, and $t=1$).

t''	$t'=-0.4$	-0.2	0.0	0.2	0.4
-0.4	2.5879	0.8053	1.0671	1.8940	3.0693
-0.2	1.8223	0.6117	0.6777	1.3732	2.4273
0.0	0.2981	0.2064	0.1251	0.5810	1.4409
0.2	−0.0768	−0.0717	−0.1058	−0.1540	0.0651
0.4	−0.2400	−0.1831	−0.1858	−0.2148	−0.2641

change of the momentum of the one-hole ground state causes the steep change of $E_{B,2}$. The hole pairing is most unfavorable in the region where the one-hole ground state is at $\mathbf{k}=(\pi,\pi)$. A positive t' gives a negative two-hole binding energy and is preferable for hole pairing. This result is not inconsistent to the recent work by Yoshioka.[20]

The values $E_{B,4}$ were calculated in $L=4\times4$ because of consuming computational time, though this system size may be too small to study the t-t'-t''-J model. The values of $E_{B,4}$ for $J=0.5$ are all summarized in Table IV. The region $t''\lesssim0$ is preferable for nonclustering ($E_{B,4}>0$). This tendency was seen also in the case of $J=1$.[19]

The desirable region for hole pairing and nonclustering, which may be a necessary condition for superconductivity, is in $t'>0$ and $t''\lesssim0$.

In conclusion, we showed that the ground state of one hole in the t-J model has a total spin $S=\frac{1}{2}$ and is nondegenerate at $\mathbf{k}$ near $(\pi/2,\pi/2)$. The ground state of two holes in the t-J model has been first shown to be nondegenerate $S=0$ at $\mathbf{k}=(0,0)$ and phase separation with the hole-rich ferromagnetism may not be expected. The hole pairing and nonclustering would be preferable for the ground state of the t-t'-t''-J model in the region of $t'>0$ and $t''\lesssim0$.

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