Role of next-nearest-neighbor hopping in the t-t'-J model

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A next-nearest-neighbor hopping t' in the t-t'-J model has a different sign between the hole- and electron-doped systems of high-T_c cuprates: $t' < 0$ for the hole-doped system and $t' > 0$ for the electron-doped system. We show that the sign is responsible for the remarkable difference of antiferromagnetic (AF) phases between the two systems. To reveal this and clarify the role of t', we examine magnetic excitations of the t-t'-J model by employing exact diagonalization techniques for 4×4 and $\sqrt{18}\times\sqrt{18}$ lattices. In the low-doping region (two-hole case of the $\sqrt{18}\times\sqrt{18}$ lattice), AF spin correlations are stabilized for the case of $t' > 0$, i.e., electron-doping case, but not for the case of $t' < 0$. In the high-doping region (four-hole case of the 4×4 lattice and more) magnetic excitations are mainly controlled by the geometry of the Fermi surface of the noninteracting system.

One of the remarkable differences between hole- and electron-doped systems of high-T_c materials is the behavior of their antiferromagnetic (AF) phases;[1] in a typical hole-doped system, $La_{2-x}Sr_xCuO_4$, the AF long-range order disappears with an extremely small amount of x but in $Nd_{2-x}Ce_xCuO_4$, which is an electron-doped system, it continues up to $x = 0.15$. A microscopic origin of the stabilization of the AF phase in $Nd_{2-x}Ce_xCuO_4$ has been discussed[2,3] by assuming extraneous oxygens, which probably sit on empty apical sites. In this communication, however, we propose an inherent mechanism in the CuO_2 plane, which stabilizes the AF correlations in the electron-doped system and distinguishes between hole and electron dopings. It is a next-nearest-neighbor hopping t'. To reveal this feature and clarify the role of t', we study the dynamical spin structure factor $S(\mathbf{Q},\omega)$ of the so-called t-t'-J model by using exact-diagonalization techniques for 4×4 and $\sqrt{18}\times\sqrt{18}$ lattices.

The importance of t' has been emphasized by Lee[4] based on an idea that at low doping the t' term causes a different physics as compared with that of the original t-J model, since a hole can propagate on the same sublattice without disturbing spins. Recently the t' term has again been introduced into model Hamiltonians of cuprates to reproduce the observed Fermi surfaces (FS's).[5–7] These two important effects of t', however, have not been investigated on an equal footing for the t-t'-J model. Moreover, there is no study in which sign difference of t' between the hole- and electron-doped systems (which will be shown later) are correctly taken into account. By investigating the effects of t' on magnetic excitations, we show below that in the low-doping region the AF correlations are stabilized in the electron-doped system, and in the high-doping region, the magnetic excitations are mainly controlled by the geometry of the FS.

One of the simplest models to describe the CuO_2 plane is considered to be the t-J model defined as

$$H = -t\sum_{\langle i,j\rangle_1\sigma}(\tilde{c}^\dagger_{i\sigma}\tilde{c}_{j\sigma}+\text{H.c.}) + J\sum_{\langle i,j\rangle_1}\mathbf{S}_i\cdot\mathbf{S}_j, \quad (1)$$

where $\tilde{c}_{i\sigma} = c_{i\sigma}(1-n_{i-\sigma})$, $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$, $c_{i\sigma}$ is the annihilation operator of an electron with spin σ at site i, $\mathbf{S}_i$ is the spin operator, and the summation $\langle i,j\rangle_1$ runs over nearest-neighbor (NN) pairs. The electron in this model corresponds to a d^9 state in the real CuO_2 plane and a hole created by doping is supposed to be a $d^9\underline{L}$ state (Zhang-Rice local singlet state) for hole-doped system and a d^{10} state for electron-doped system. ($\underline{L}$ denotes a ligand hole.) Thus, the hopping term in Eq. (1) stands for an exchange process of the d^9 and $d^9\underline{L}$ (or d^{10}) states. Due to the large hopping integral between NN oxygen sites in the CuO_2 plane, we should also include the exchange process between next-nearest-neighbor (NNN) sites in the t-J model (1). The term is expressed as

$$H' = -t'\sum_{\langle i,j\rangle_2\sigma}(\tilde{c}^\dagger_{i\sigma}\tilde{c}_{j\sigma}+\text{H.c.}), \quad (2)$$

where the summation $\langle i,j\rangle_2$ runs over NNN pairs. A resultant model, $H + H'$, is called the t-t'-J model.

Realistic parameter values for the model have been evaluated by using Cu_2O_7 and Cu_2O_8 clusters for t and t', respectively.[8,9] Let us briefly review how to estimate t and t'. In the hole-doped case of the Cu_2O_7 cluster, the ground state is represented well by the bonding state of special configurations in which the d^9 state is on one CuO_4 unit and the $d^9\underline{L}$ state is on the other unit. As the corresponding antibonding state appears in the first-excited state, the half of the energy difference between the ground and first-excited states corresponds to an en-

ergy required to exchange the d^9 and $d^9\underline{L}$ states, i.e., $-t$. As the bonding state is lower in energy than the antibonding state, the sign of t for the hole-doped system becomes positive. Similar procedures have determined the values of t and t' for both the hole- and electron-doped systems, and interestingly it has been found that the signs of t and t' are different between the two systems: $t > 0$ and $t' < 0$ for the hole-doped system, and $t < 0$ and $t' > 0$ for the electron-doped system.[8,9] The obtained sign difference originates from the fact that the $d^9\underline{L}$ state has a positive charge, while the d^{10} has a negative one as compared with the d^9 state. The ratio of $|t'/t|$ has lain in the region of 0.2–0.4. We note here that the geometry of the FS of noninteracting system with the evaluated values of t and t' is consistent with that obtained by angle-resolved photoemission (ARPES) measurements and band-structure calculations. The FS's for $t'/t = -0.4$ are shown in Fig. 1. In the hole-doped case, the $(0,0)$ point (Γ point) has minimum energy and the (π,π) point (M point) has maximum one because of $t > 0$ and $t' < 0$. The FS thus shrinks around the Γ point with doping. The FS shapes near half filling are analogous to the ARPES results for the hole-doped systems.[10,11] On the other hand, in the electron-doped case ($t < 0$ and $t' > 0$), the energy minimum and maximum are at the M and Γ points, respectively. Since the d^{10} state carrying an electron is considered to be a hole in the t-t'-J model as stated above, the FS shrinks around the M point with doping, which is also consistent with recent ARPES measurements for $Nd_{2-x}Ce_xCuO_4$.[12] These consistencies of the FS shapes with experiments are expected to persist even when strong correlation is introduced into the system because the exact diagonalization calculation of the one-particle excitation spectra of the t-J model[13] has shown the existence of the FS analogous to that of the noninteracting system.

The dynamical spin structure factor $S(\mathbf{Q},\omega)$ is given by ($\hbar = 1$)

$$S(\mathbf{Q},\omega) = \sum_n \left|\langle n|\, S^z_{\mathbf{Q}}\, |0\rangle\right|^2 \delta\left(\omega - E_n + E_0\right), \qquad (3)$$

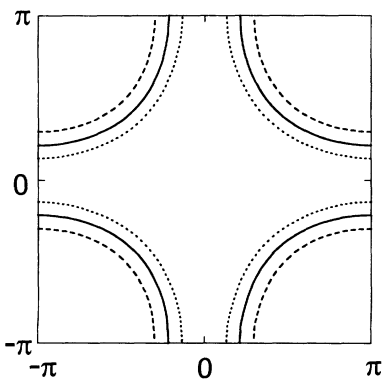

FIG. 1. Fermi surfaces of the noninteracting system for $t' = -0.4t$. The solid curves denote the Fermi surface at half filling. The dotted and dashed curves denote the Fermi surface for $t = 1$ (hole-doping) and -1 (electron-doping), respectively, at doping concentration 0.2.

with $S^z_{\mathbf{Q}} = N^{-1/2}\sum_i e^{i\mathbf{Q}\cdot\mathbf{R}_i} S^z_i$, where N is the number of the lattice sites, $\mathbf{R}_i$ is the position vector at site i, and S^z_i is the z component of the spin operator. $|n\rangle$ is the nth eigenvector with eigenvalue E_n, and $|0\rangle$ denotes the ground state. Usual Lanczos-type algorithm is applied for calculation of $S(\mathbf{Q},\omega)$.

In the present study, we take $J/|t| = 0.4$ and $|t'/t| \leq 0.4$ as realistic values, and we choose $|t| = 1$ as our unit of energy. In order to avoid the confusion of the signs of t and t', we use only the sign of t' hereafter; a negative sign of t' implies hole doping and $t = 1$, while a positive one implies electron doping and $t = -1$. Indeed, the sign of t is less important because the change of sign of t makes no difference for the following results.[14]

We first examine the t' dependence of $S(\mathbf{Q},\omega)$ for a $\sqrt{18}\times\sqrt{18}$ lattice with two holes. In the parameter region of $-0.23 \leq t' \leq 0.4$, the ground state has total spin $S = 0$ and momentum $\mathbf{k} = (0,0)$.[15] Since spin correlation function $S(\mathbf{Q})$ shows a maximum at AF wave vector $\mathbf{Q} = (\pi,\pi)$, we show calculated spectral weights for $\mathbf{Q} = (\pi,\pi)$ in Fig. 2, where the results for $t' = -0.2$, 0, and $t' = 0.4$ are seen. We find that the intensity of the peaks increases with the increase of the value of t'. The increase of the intensity indicates the enhancement of the AF spin correlation. In order to clarify the enhancement, we show spin excitation energy at various $\mathbf{Q}$'s in Fig. 3, which is defined as the energy difference between the ground state and the first excited state for which the transition probability in Eq. (3) is nonzero. It is found that, with the increase of t', the spin excitation energies increase except the energy for $\mathbf{Q} = (\pi,\pi)$. At $t' = 0.4$, the maximum excitation energy is nearly identical to that of the half-filled case where the corresponding value is 1.03 for $\mathbf{Q} = (2\pi/3, 0)$. These behaviors also imply the enhancement of the AF correlation. At $-0.4 \leq t' < -0.23$, the ground states have $S = 1$, i.e., ferromagnetic state. As we are interested in the $S = 0$ ground state, we do not discuss the magnetic excitations in this parameter region.

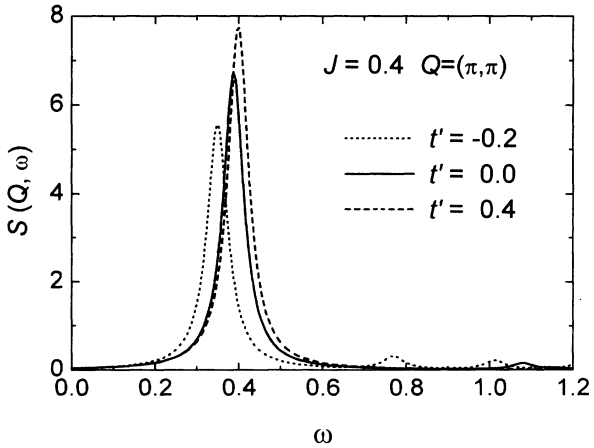

FIG. 2. $S(\mathbf{Q},\omega)$ as a function of ω for a $\sqrt{18}\times\sqrt{18}$ lattice with two holes at $J = 0.4$ and $|t| = 1$. The solid, dotted, and dashed lines denote the case of $(t,t') = (1,0)$, $(1,-0.2)$, and $(-1,0.4)$, respectively. The δ function is broadened by using a small shift, 0.03, from the real axis.

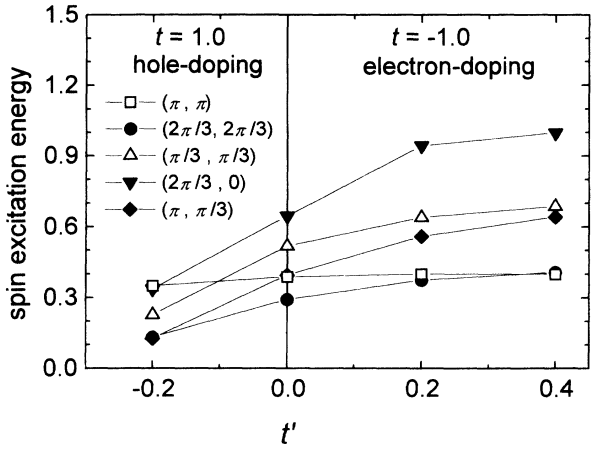

FIG. 3. Spin excitation energy as a function of t' for a $\sqrt{18} \times \sqrt{18}$ lattice with two holes at different wave vectors. $J = 0.4$; $t = 1$ for the negative value of t' (hole-doping) and $t = -1$ for the positive one (electron-doping). The definition of the excitation energy is given in the text.

The fact that the magnetic excitation for $\mathbf{Q} = (\pi, \pi)$ becomes stronger with increasing t' can be interpreted as a result of the stabilization of AF configurations in which NN spins are arranged in antiparallel (Néel-like) and two holes sit on NN sites, since the configurations are expected to show spin-wave excitation similar to that of the half-filled case. The stabilization of these configurations is simply understood through the following considerations: by applying translational and rotational operations to the configurations, we can construct a new basis, which is a linear combination of them. The diagonal matrix element of the Hamiltonian with respect to the new state contains t' because the t' term can move an electron without disturbing the Néel-like spin arrangement. For a subspace with momentum $\mathbf{k} = (0, 0)$ and irreducible representation B_{1g}, to which the ground state belongs, the diagonal element has a term $-t'$. When the sign of t' is positive (electron doping), the configurations mentioned above eventually become stable and has a larger weight in the ground state.[16] Indeed, as a result of the stabilization of the configurations, the hole-hole correlation between NN sites increases by 42% for $t' = 0.4$ as compared with the $t' = 0$ case.[17] Therefore, we conclude that at $t' > 0$ the AF configurations become stable and thus the AF spin correlations are enhanced. In other words, the AF correlations are stabilized by motion of electrons caused by positive t'. The motion does not affect the Néel-like spin arrengement and lowers the total energy of the system.

The difference of magnetic excitation between the hole- and electron-doped systems becomes clear now. In the electron-doped system, i.e., in the region of $t' > 0$, the AF correlations can be stabilized, while the hole-doped system does not show the tendency. This difference is qualitatively consistent with the experimental result[1] mentioned before. The consistency indicates that the sign of t' is an important factor to stabilize the AF state and the difference of the phase diagram is inherent in the CuO_2 plane. $Nd_{2-x}Ce_xCuO_4$ in the AF phase also shows insulating behavior.[18] In contrast with the experiment, our model becomes metallic by the introduction of carriers. In order to explain the insulating behavior simultaneously, some additional effects that lead to the localization of carriers may be needed in our model, such as impurity effect.

Recently, Psaltakis and Papanicolaou[19] have studied the t-t'-J model within a $1/N$ expansion and have detected a stable AF phase near half filling in the $T = 0$ phase diagram. We point out here that the parameter values of t' used in their paper correspond to those for the electron-doped system, although they have not commented on the type of carriers. We can also confirm that no stable AF phase exists in the case of inverse sign of t' by using their equation for classical energy.[19] The existence of the AF phase, thus, seems to support our result that AF correlations are enhanced for the electron-doped system.

To investigate magnetic excitations in high-doping region, we next examine $S(\mathbf{Q}, \omega)$ for a 4×4 lattice with 4, 6, and 8 holes (doping concentration $\delta = 0.25$, 0.375, and 0.5, respectively). In this doping region, spin correlation strongly depends on the value of t'. For example, at $\delta = 0.25$, $S(\mathbf{Q})$ shows a maximum at $\mathbf{Q} = (\pi/2, \pi/2)$ for $t' = -0.4$ and at $\mathbf{Q} = (\pi, \pi)$ for $t' = 0$.[20] This imlpies that at $\delta = 0.25$ the $\mathbf{Q} = (\pi, \pi)$ excitation is no longer a characteristic excitation in the t-t'-J model in contrast with the previous low-doping case (two hole case of the $\sqrt{18} \times \sqrt{18}$ lattice). In Fig. 4, we show the δ dependences of the spin excitation energies for several $\mathbf{Q}$'s, where the results for $t' = -0.4$ and 0 are presented.[21] The wave vector of the lowest-energy state depends on δ and t'. The distribution of other excited states also differs between the cases of $t' = -0.4$ and 0: in the former the excited states are distributed within $0.6t$ in energy; on the other hand, in the latter the highest-energy state is located at $2.1t$ for $\delta = 0.5$. These dependences of the spin exci-

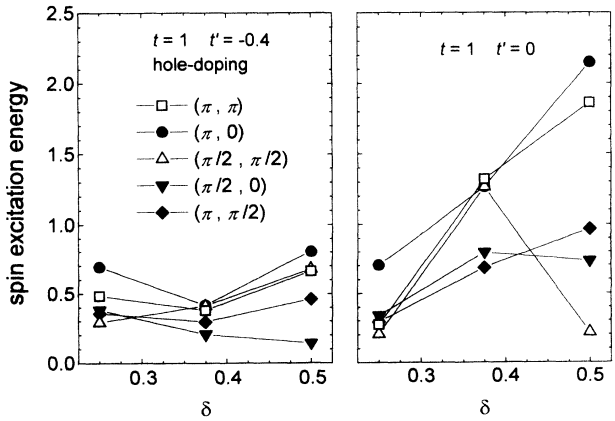

FIG. 4. Spin excitation energy as a function of doping ($0.25 \leq \delta \leq 0.5$) for $J = 0.4$ at different wave vectors. A 4×4 lattice is employed. The left panel is for $t' = -0.4$ (hole-doping), and the right panel is for $t' = 0$. The data for $t' = 0$ are taken from Ref. 22.

tation energies on both δ and t' may be interpreted as a result of the change of the FS shapes. As an example, let us consider spin excitation for $\mathbf{Q} = (\pi, \pi)$ in the noninteracting system. For the case of $t' = 0$ where FS at half filling has well-known square shape that exhibits complete nesting with wave vector (π, π), the spin excitation has an energy gap at $\delta > 0$ because the (π, π) vector cannot connect two points on the FS. The magnitude of the gap increases with increasing δ. On the other hand, for the case of $t' = -0.4$ (see Fig. 1) no gap is expected for the $\mathbf{Q} = (\pi, \pi)$ excitation up to $\delta = 0.42$. Similar behaviors are seen in the result of the t-t'-J model in Fig. 4: the excitation energy for $\mathbf{Q} = (\pi, \pi)$ increases rapidly for $t' = 0$ but shows small change for $t' = -0.4$. For other $\mathbf{Q}$ vectors, we can also qualitatively explain the doping dependences of their excitation energies by taking into account the FS shapes of the noninteracting system. Therefore, it is considered that the FS shapes play an important role on the spin excitation of the t-t'-J model in the high doping region. Of course, the 4×4 lattice used here is too small to discuss spin excitation at thermodynamic limit. Thus, our argument presented should be confirmed quantitatively by using larger lattices.

In summary, we have examined the dynamical spin structure factors of the t-t'-J model by using the exact diagonalization method for 4×4 and $\sqrt{18} \times \sqrt{18}$ lattices, and have shown that the sign differences of t and t', especially t', between hole- and electron-doped systems are of importance to understand the difference of antiferromagnetic states near half filling; the model with positive t', which corresponds to the electron-doped system, reveals the stabilization of antiferomagnetic correlation, which is consistent with experiment. In the high-doping region, we have found that the spin excitations are characterized by the geometry of the FS of the noninteracting system. We conclude that the t' term should be included in the t-J model in order to explain the difference of the magnetic and electronic properties between the hole- and electron-doped systems.

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[14]Note that, since the change of sign of t in Eq. (1) is equivalent to the shift of phase of its hopping term by (π, π), eigenstates for the case of $t = 1$ coincide with those for the case of $t = -1$ by shifting their momentum by (π, π). Thus, we can obtain same results between the cases of, for example, $t > 0$, $t' < 0$ and $t < 0$, $t' < 0$ by taking into account the difference of the momentum.

[15]The ground state for a 4×4 lattice with two holes has $S = 0$ in all parameter region, but in the region of $-0.4 \leq t' < 0$ the ground state belongs to $\mathbf{k} = (\pi, 0)$ and $(0, \pi)$ subspaces, but not $(0, 0)$.

[16]This argument is related to that of the stabilization of the Nagaoka's ferromagnetic state in the case of the negative t'. See E. Gagliano, A. Bacci, and E. Dagotto, Phys. Rev. B **42,** 6222 (1990).

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[20]In the case of four holes, the momentum of the ground state is $(0, 0)$ for $-0.4 \leq t' \leq 0$, but $(\pi, 0)$ [or $(0, \pi)$] for $0 < t' \leq 0.4$. We thus discuss magnetic excitations only for the former region to avoid the difference of the momentum of the ground state.

[21]The ground state for all the cases presented here belongs to the momentum $\mathbf{k} = (0, 0)$ space.

[22]E. Dagotto *et al.*, Phys. Rev. B **45,** 10 741 (1992).