Influence of the additional second-neighbor hopping on the spin response in the t-J model

Xianglin Ke and Feng Yuan
Department of Physics, Beijing Normal University, Beijing 100875, China

Shiping Feng
Department of Physics, Beijing Normal University, Beijing 100875, China
and Institute of Theoretical Physics, Academia Sinica, Beijing 100080, China

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The influence of the additional second-neighbor hopping t' on the spin response of the t-J model in the underdoped and optimally doped regimes is studied within the fermion-spin theory. Although the additional second-neighbor hopping t' is systematically accompanied by the reduction of the dynamical spin structure factor and susceptibility, the qualitative behavior of the dynamical spin structure factor and susceptibility of the t-t'-J model is the same as in the case of t-J model. The integrated dynamical spin structure factor spectrum is almost t' independent, and the integrated dynamical spin susceptibility still shows the particularly universal behavior as $I(\omega,T)\propto\arctan[a_1\omega/T+a_3(\omega/T)^3]$.

Following the initial discovery of the antiferromagnetic (AF) spin fluctuation in copper oxide materials,[1] extensive experimental and theoretical studies have been carried out in order to clarify the relationship between the AF spin fluctuation and superconductivity.[2–4] The single common feature of copper oxide materials is the two-dimensional (2D) CuO_2 plane,[2,5] and it seems evident that the exotic behaviors are dominated by this plane. It has been shown from the experiments that the anomalous magnetic properties in copper oxide materials mainly depend on the extent of dopings, and the regimes have been classified into the undoped, the underdoped, the optimally doped, and the overdoped, respectively.[2–4] The undoped copper oxide materials are insulating systems[2] and well understood in terms of the 2D antiferromagnet with an AF long-range order (AFLRO).[3,4] This AFLRO is reduced dramatically with dopings[6,7] and vanishes around the doping $\delta=5\%$. But a series of inelastic neutron scattering measurements shows that the AF short-range spin fluctuation in copper oxide materials persists in the underdoped and optimally doped regimes.[8–10] It is widely believed that the same correlations that lead to the insulating AF state at small doping also lead to the superconductivity in the underdoped and optimally doped regimes.[4,5] Since the copper oxide superconductors are doped Mott insulators, many authors[11,12] have suggested that the essential physics of these materials can be effectively described by the 2D t-J model acting on space with no doubly occupied sites, where t is the nearest-neighbor hopping matrix element and J is the nearest-neighbor magnetic exchange interaction. This model has been used to study the spin dynamics of copper oxide materials in the underdoped and optimally doped regimes, and the results obtained[4,13–15] from the analytical methods and numerical simulations are in qualitative agreement with the experiments.[8–10]

However, the recent angle-resolved photoemission spectroscopy measurements[16] on copper oxide materials show that although the highest-energy filled electron band is well described by the t-J model in the direction between the (0,0) point and the (π,π) point in momentum space, but both the experimental data near $(\pi,0)$ point and overall dispersion may be properly accounted by generalizing the t-J model to include the second- and third-nearest neighbors hopping terms t' and t''. These photoemission results also show that the electron bandwidth is reduced from the several eV expected from the band theory to of order J, which indicates that the coupling of the electron to the AF background plays an essential role in the electronic structure.[16] On the other hand, the short-range AF spin correlation in the underdoped and optimally doped regimes is responsible for the nuclear magnetic resonance (NMR), nuclear quadrupole resonance (NQR), and especially for the temperature dependence of the spin-lattice relaxation rate.[3] It is believed that both experiments from the angle-resolved photoemission spectroscopy and neutron scattering measurements produce interesting data that introduce important constraints on the microscopic models and theories. In this case, a natural question is what is the effect of these additional hoppings on the spin dynamics of the t-J model. In this paper, we study this issue within t-t'-J model. Our results show that although the additional second-neighbor hopping t' is systematically accompanied by the reduction of the dynamical spin structure factor and susceptibility in the underdoped and optimally doped regimes, the qualitative behavior of the dynamical spin structure factor and susceptibility is the same as in the case of the t-J model.[13–15] The integrated dynamical spin structure factor of the t-t'-J model is almost t' independent, and the integrated dynamical spin susceptibility still shows the particularly universal behavior as $I(\omega,T)\propto\arctan[a_1\omega/T+a_3(\omega/T)^3]$.

We start from the 2D t-t'-J model which can be written as

$$H=-t\sum_{i\hat{\eta}\sigma}C^{\dagger}_{i\sigma}C_{i+\hat{\eta}\sigma}+t'\sum_{i\hat{\tau}\sigma}C^{\dagger}_{i\sigma}C_{i+\hat{\tau}\sigma}+\mu\sum_{i\sigma}C^{\dagger}_{i\sigma}C_{i\sigma}+J\sum_{i\hat{\eta}}\mathbf{S}_i\cdot\mathbf{S}_{i+\hat{\eta}},\tag{1}$$

where $\hat{\eta}=\pm\hat{x},\pm\hat{y}$, $\hat{\tau}=\pm\hat{x}\pm\hat{y}$, $C^{\dagger}_{i\sigma}$ ($C_{i\sigma}$) are the electron creation (annihilation) operators, $\mathbf{S}_i=C^{\dagger}_i\sigma C_i/2$ are spin op-

erators with $\sigma=(\sigma_x,\sigma_y,\sigma_z)$ as the Pauli matrices, and μ is the chemical potential. The t-t'-J model (1) is supplemented by the on-site local constraint $\Sigma_\sigma C^\dagger_{i\sigma}C_{i\sigma}\leqslant 1$; i.e., there are no doubly occupied sites. The t-J model was originally introduced[11] as an effective Hamiltonian of the large-U Hubbard model, where the on-site Coulomb repulsion U is very large as compared with the electron hopping energy t, which leads to electrons becoming strongly correlated to avoid double occupancy. Furthermore, many authors[12,17] derived the t-J model or t-t'-J model from a multiband large-U Hubbard model described with the 2D CuO_2 plane. Therefore the strong electron correlation in the t-J or t-t'-J model manifests itself by the electron single-occupancy on-site local constraint. This on-site local constraint can be treated exactly in analytical calculations within the fermion-spin theory,[18] $C_{i\uparrow}=h^\dagger_i S^-_i$ and $C_{i\downarrow}=h^\dagger_i S^+_i$, where the spinless fermion operator h_i keeps track of the charge (holon), while the pseudospin operator S_i keeps track of the spin (spinon); then the fermion-spin theory naturally incorporates the physics of the charge-spin separation. In the fermion-spin representation, the t-t'-J model can be expressed[18] as

$$H=t\sum_{i\hat{\eta}} h^\dagger_{i+\hat{\eta}}h_i(S^+_i S^-_{i+\hat{\eta}}+S^-_i S^+_{i+\hat{\eta}}) - t'\sum_{i\hat{\tau}} h^\dagger_{i+\hat{\tau}}h_i(S^+_i S^-_{i+\hat{\tau}}+S^-_i S^+_{i+\hat{\tau}}) + \mu\sum_i h^\dagger_i h_i + J_{eff}\sum_{i\hat{\eta}}(\mathbf{S}_i\cdot\mathbf{S}_{i+\hat{\eta}}), \tag{2}$$

where $J_{eff}=J[(1-\delta)^2-\phi_1^2]$, the holon particle-hole order parameter $\phi_1=\langle h^\dagger_i h_{i+\hat{\eta}}\rangle$, and S^+_i and S^-_i are the pseudospin raising and lowering operators, respectively. As a consequence, the kinetic part in the t-t'-J model has been expressed as the holon-spinon interactions in the fermion-spin representation, which dominates the physics in the underdoped and optimally doped regimes as in the case of the t-J model.[14]

Within the framework of the charge-spin separation, it has been shown[19] that the charge dynamics can be discussed based on the combination rule from spinons and holons, but no composition law is required for discussing the spin dynamics, since the spin fluctuation couples only to spinons, but the strong correlation between holons and spinons is considered through the holon's order parameters entering in the spinon propagator. In this case, the spin dynamics of the t-J model in the underdoped and optimally doped regimes has been discussed[14] within the fermion-spin theory by considering spinon fluctuations around the mean-field solution, where the spinon part is treated by the loop expansion to second order. Following their discussions,[14] we can obtain the dynamical spin structure factor and susceptibility in the present t-t'-J model as

$$S(k,\omega)=\mathrm{Re}\int_0^\infty dt e^{i\omega(t-t')}D(k,t-t') = 2[1+n_B(\omega)]\,\mathrm{Im}\,D(k,\omega), \tag{3a}$$

$$\chi''(k,\omega)=(1-e^{-\beta\omega})S(k,\omega)=2\,\mathrm{Im}\,D(k,\omega), \tag{3b}$$

respectively, where the full spinon Green's function $D^{-1}(k,\omega)=D^{(0)-1}(k,\omega)-\Sigma^{(2)}_s(k,\omega)$, with the mean-field spinon Green's function $D^{(0)-1}(k,\omega)=(\omega^2-\omega_k^2)/B_k$, and the second-order spinon self-energy from the holon pair bubble,

$$\Sigma^{(2)}_s(k,\omega)=\left(\frac{Z}{N}\right)^2\sum_{pp'}\gamma^2_{12}(k,p,p')\frac{B_{k+p}}{2\omega_{k+p}} \times\left(\frac{F_1(k,p,p')}{\omega+\xi_{p+p'}-\xi_{p'}-\omega_{k+p}} - \frac{F_2(k,p,p')}{\omega+\xi_{k+p'}-\xi_{p'}+\omega_{k+p}}\right), \tag{4}$$

where $\gamma_{12}(k,p,p')=t(\gamma_{k+p+p'}+\gamma_{k-p})-t'(\gamma'_{k+p+p'}+\gamma'_{k-p})$, $\gamma_{\mathbf{k}}=(1/Z)\Sigma_{\hat{\eta}}e^{i\mathbf{k}\cdot\hat{\eta}}$, $\gamma'_{\mathbf{k}}=(1/Z)\Sigma_{\hat{\tau}}e^{i\mathbf{k}\cdot\hat{\tau}}$, Z is the number of nearest-neighbor or second-nearest-neighbor sites, $B_k=\Delta_1[2\chi^z_1(\epsilon\gamma_k-1)+\chi_1(\gamma_k-\epsilon)]-\Delta_2(2\chi^z_2\gamma'_k-\chi_2)$, $\Delta_1=2ZJ_{eff}$, $\Delta_2=4Z\phi_2 t'$, $\epsilon=1+2t\phi_1/J_{eff}$, $F_1(k,p,p')=n_F(\xi_{p+p'})[1-n_F(\xi_{p'})]+[1+n_B(\omega_{k+p})][n_F(\xi_{p'})-n_F(\xi_{p+p'})]$, $F_2(k,p,p')=n_F(\xi_{p+p'})[1-n_F(\xi_p)]-n_B(\omega_{k+p})[n_F(\xi_{p'})-n_F(\xi_{p+p'})]$, $n_F(\xi_k)$ and $n_B(\omega_k)$ are the fermion and boson distribution functions, respectively, the mean-field holon spectrum $\xi_k=2Zt\chi_1\gamma_k-2Zt'\chi_2\gamma'_k-\mu$, and the mean-field spinon spectrum

$$\begin{aligned}\omega_k^2=&\Delta_1^2\left(\left[\alpha C^z_1+\frac{1}{4Z}(1-\alpha)-\alpha\epsilon\chi^z_1\gamma_k-\frac{1}{2Z}\alpha\epsilon\chi_1\right]\right.\\ &\left.\times(1-\epsilon\gamma_k)+\frac{1}{2}\epsilon\left[\alpha C_1+\frac{1}{2Z}(1-\alpha)-\alpha\chi_1\gamma_k-\frac{1}{2}\alpha\chi^z_1\right]\right.\\ &\left.\times(\epsilon-\gamma_k)\right)+\Delta_2^2\left(\left[\alpha\chi^z_2\gamma'_k-\frac{3}{2Z}\alpha\chi_2\right]\gamma'_k\right.\\ &\left.+\frac{1}{2}\left[\alpha C_2+\frac{1}{2Z}(1-\alpha)-\frac{1}{2}\alpha\chi^z_2\right]\right)\\ &+\Delta_1\Delta_2\left(\alpha\chi^z_1\gamma'_k(1-\epsilon\gamma_k)+\frac{\alpha}{2}(\chi_1\gamma'_k-C_3)(\epsilon-\gamma_k)\right.\\ &\left.+\alpha\gamma'_k(C^z_3-\epsilon\chi^z_2\gamma_k)-\frac{1}{2}\alpha\epsilon(C_3-\chi_2\gamma_k)\right),\end{aligned} \tag{5}$$

with the spinon correlation functions $\chi_1=\langle S^+_i S^-_{i+\hat{\eta}}\rangle$, $\chi_2=\langle S^+_i S^-_{i+\hat{\tau}}\rangle$, $\chi^z_1=\langle S^z_i S^z_{i+\hat{\eta}}\rangle$, $\chi^z_2=\langle S^z_i S^z_{i+\hat{\tau}}\rangle$, $C_1=(1/Z)\Sigma_{\hat{\eta}'}\langle S^+_{i+\hat{\eta}}S^-_{i+\hat{\eta}'}\rangle$, $C^z_1=(1/Z)\Sigma_{\hat{\eta}'}\langle S^z_{i+\hat{\eta}}S^z_{i+\hat{\eta}'}\rangle$, $C_2=(1/Z)\Sigma_{\hat{\tau}'}\langle S^+_{i+\hat{\tau}}S^-_{i+\hat{\tau}'}\rangle$, $C_3=(1/Z)\Sigma_{\hat{\tau}}\langle S^+_{i+\hat{\eta}}S^-_{i+\hat{\tau}}\rangle$, $C^z_3=(1/Z)\Sigma_{\hat{\tau}}\langle S^z_{i+\hat{\eta}}S^z_{i+\hat{\tau}}\rangle$, and the holon particle-hole order parameter $\phi_2=\langle h^\dagger_i h_{i+\hat{\tau}}\rangle$. In order not to violate the sum rule of the correlation function $\langle S^+_i S^-_i\rangle=1/2$ in the case without AFLRO, the important decoupling parameter α has been introduced in the mean-field calculation, which can be regarded as the vertex correction.[20]

For small dopings, the spin fluctuation scattering remains commensurate at the AF wave vector $Q=(\pi,\pi)$ position.[2,3] With increasing dopings, there is a commensurate-incommensurate transition in the spin fluctuation geometry, and the incommensurate scattering in the underdoped and optimally doped regimes corresponds to four 2D rods at (π

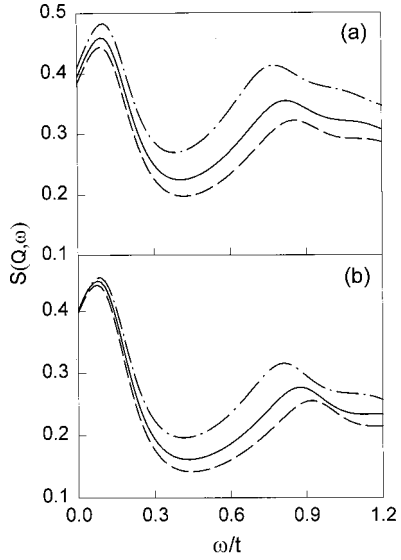

FIG. 1. The dynamical structure factor $S(Q,\omega)$ at the doping (a) $\delta=0.06$ and (b) $\delta=0.12$ with the temperature $T=0.2J$ for the parameters $t/J=2.5$, $t'/J=0.3$ (solid line), and $t'/J=0.5$ (dashed line). The dash-dotted line is the corresponding result of the t-J model.

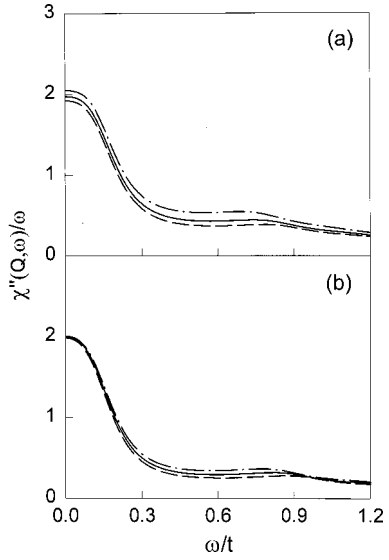

FIG. 2. The dynamical susceptibility $\chi''(Q,\omega)$ at the doping (a) $\delta=0.06$ and (b) $\delta=0.12$ with the temperature $T=0.2J$ for the parameters $t/J=2.5$, $t'/J=0.3$ (solid line), and $t'/J=0.5$ (dashed line). The dash-dotted line is the corresponding result of the t-J model.

$\pm 2\pi\delta$d$,\pi)$ and $(\pi,\pi\pm 2\pi\delta_d)$ with δ_d is the deviation of the peak position from the AF wave vector Q position.[2,3] This incommensurate scattering is the main new feature that appears into the superconducting phase of copper oxide materials.[2] In this paper, we are interested in the influence of the additional second-neighbor hopping on the spin dynamics of the t-J model. To make the discussion simpler, we only study the spin response of the t-t'-J model near the AF wave vector Q. We have performed a numerical calculation for the dynamical spin structure factor $S(Q,\omega)$ and dynamical spin susceptibility $\chi''(Q,\omega)$ of the t-t'-J model, and the results of the $S(Q,\omega)$ and $\chi''(Q,\omega)$ spectra at the doping (a) $\delta=0.06$ and (b) $\delta=0.12$ with the temperature $T=0.2J$ for the parameters $t/J=2.5$, $t'/J=0.3$ (solid line), and $t'/J=0.5$ (dashed line) are plotted in Fig. 1 and Fig. 2, respectively. For comparison, the corresponding results[14] of the t-J model (dash-dotted line) are also shown in Fig. 1 and Fig. 2, respectively. From Fig. 1 and Fig. 2, we find that although the additional second-neighbor hopping t' is systematically accompanied by a clear reduction of the dynamical spin structure factor and susceptibility in the underdoped and optimally doped regimes, the qualitative behavior of the dynamical spin structure factor and susceptibility in the t-t'-J model is the same as in the case of the t-J model.[14] The spin structure factor spectrum is separated into low- and high-frequency parts, respectively, but the high-frequency part is suppressed in the susceptibility; then the low-frequency peak dominates the dynamical spin susceptibility, the neutron scattering, and NMR processes, which is consistent with the experiments.[2,8,9]

One of the most important features of the spin dynamics in copper oxide materials is the universal behavior of the integrated dynamical spin response.[2,10] This universal behavior is very significant because of its relation to many other normal-state properties of copper oxide materials. The integrated dynamical spin response is manifested by the integrated dynamical spin structure factor and integrated dynamical spin susceptibility, and can be expressed as

$$\begin{aligned}\overline{S}(\omega)&=S_L(\omega)+S_L(-\omega)\\&=(1+e^{-\beta\omega})S_L(\omega)\\&=(1+e^{-\beta\omega})\frac{1}{N}\sum_k S(k,\omega),\end{aligned}\tag{6a}$$

$$I(\omega,T)=\frac{1}{N}\sum_k \chi''(k,\omega),\tag{6b}$$

respectively. The numerical results of the integrated dynamical spin structure factor $\overline{S}(\omega)$ at the doping (a) $\delta=0.06$ and (b) $\delta=0.12$ with the temperature $T=0.2J$ for the parameters $t/J=2.5$, $t'/J=0.3$ (solid line), and $t'/J=0.5$ (dashed line) are shown in Fig. 3. The dash-dotted line is the corresponding result[14] of the t-J model. These results indicate that the integrated spin structure factor of the t-t'-J model is almost t' independent in the underdoped and optimally doped regimes. Moreover, $\overline{S}(\omega)$ is decreased with increasing energies for $\omega<0.5t$ and constant for $\omega>0.5t$. In correspondence with the integrated dynamical spin structure factor, the numerical results of the integrated dynamical spin susceptibility at the doping $\delta=0.12$ with the temperature $T=0.2J$ for the parameters $t/J=2.5$, $t'/J=0.3$ (solid line), and $t'/J=0.5$ (dashed line) are shown in Fig. 4. The dash-dotted line is the corresponding result[14] of the t-J model. Our results show that the integrated susceptibility increases with increasing ω/T for $\omega/T<1$, and then is almost constant for $\omega/T>1$. Although the value of the integrated dynamical spin susceptibility of the t-t'-J model is weakly t' dependent, the shape still is particularly universal, and can be scaled approximately as $I(\omega,T)=b_1\arctan[a_1\omega/T+a_3(\omega/T)^3]$ as in the case of the t-J model.[14] These results are in very good agreement with the experiments.[10]

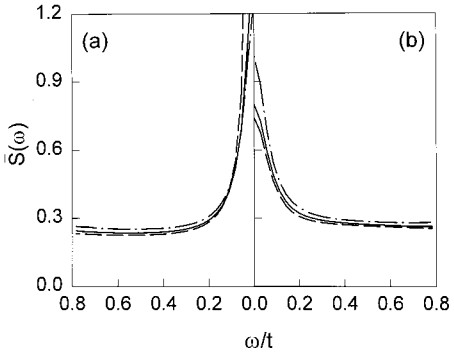

FIG. 3. The integrated dynamical structure factor $\bar{S}(\omega)$ at the doping (a) $\delta=0.06$ and (b) $\delta=0.12$ with the temperature $T=0.2J$ for the parameters $t/J=2.5$, $t'/J=0.3$ (solid line), and $t'/J=0.5$ (dashed line). The dash-dotted line is the corresponding result of the t-J model.

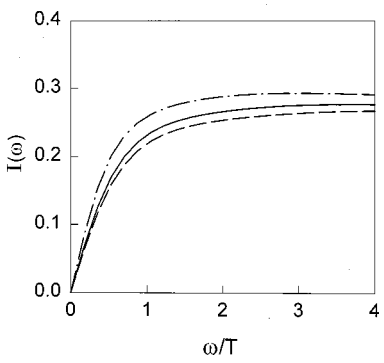

FIG. 4. The integrate dynamical susceptibility $I(\omega)$ at the doping $\delta=0.12$ with the temperature $T=0.2J$ for the parameters $t/J=2.5$, $t'/J=0.3$ (solid line), and $t'/J=0.5$ (dashed line). The dash-dotted line is the corresponding result of the t-J model.

The t-J model is characterized by a competition between the kinetic energy (t) and magnetic energy (J). The magnetic energy J favors the magnetic order for spins, while the kinetic energy t favors delocalization of holes and tends to destroy the magnetic order. Only in this sense is the additional second-neighbor hopping t' in the t-J model equivalent to an increase in the kinetic energy, and its influence on the spin dynamics of the t-J model may be similar to the effect of dopings. On the other hand, the scattering of spinons dominates the spin dynamics, and the qualitative behavior of the spin dynamics in the t-J model is not changed dramatically with dopings in the underdoped and optimally doped regimes.[14] These are why at least for small values of t' the qualitative behavior of the spin dynamics in the t-t'-J model is the same as these obtained from the t-J model. Since the scattering of holons dominates the charge dynamics,[21] and some qualitative physical properties of the charge dynamics are changed dramatically with dopings in the t-J model,[21] then it is possible that the additional second neighbor hopping t' may affect the qualitative behavior of the charge dynamics of the t-J model.

In summary, we have discussed the influence of the additional second-neighbor hopping t' on the spin response in the t-J model in the underdoped and optimally doped regimes within the fermion-spin theory. Our results show that although the additional second-neighbor hopping t' is systematically accompanied by the reduction of the dynamical spin structure factor and susceptibility, the qualitative behavior of the dynamical spin structure factor and susceptibility of the t-t'-J model is the same as in the case of t-J model. The integrated spin structure factor spectrum is almost t' independent, and the integrated dynamical spin susceptibility still shows the particularly universal behavior as $I(\omega,T)\propto\arctan[a_1\omega/T+a_3(\omega/T)^3]$.

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