Universal spin response in copper oxide materials

Shiping Feng

*Department of Physics, Beijing Normal University, Beijing 100875, China**
and National Laboratory of Superconductivity, Academia Sinica, Beijing 100080, China

Zhongbing Huang

Department of Physics, Beijing Normal University, Beijing 100875, China
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The spin response in the copper oxide materials at finite temperatures in the underdoped and optimal doped regimes is studied within the framework of the fermion-spin theory. The integrated dynamical spin structure factor is almost temperature independent, the integrated susceptibility shows the particularly universal behavior as $I(\omega,T) \propto \arctan[a_1\omega/T + a_3(\omega/T)^3]$, and the spin-lattice relaxation time is weakly temperature dependent, which are consistent with experiments and numerical simulations. [S0163-1829(98)02017-7]

After ten years of intense experimental and theoretical studies of the copper oxide superconductors, there is now a consensus that these materials should be described as strongly correlated electron systems,[1] since all of the copper oxide materials have in common the existence of a perovskite parent compound which is insulating and has the antiferromagnetic long-range-order (AFLRO), and changing the carrier concentration by ionic substitution or increase of the oxygen content turns these compounds into correlated metals leaving short-range antiferromagnetic correlations still intact.[1,2] The short-range antiferromagnetic correlations results in several peculiar physical properties of the copper oxide materials: they are responsible for the NMR and nuclear quadrupole resonance (NQR), and especially for the temperature dependence of the spin-lattice relaxation rate.[1,3] A series of the neutron-scattering measurements[4–6] on the copper oxide materials $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{6+x}$ show that there is an anomalous temperature T dependence of the spin fluctuations near the antiferromagnetic zone center in the underdoped and optimal doped regimes, and the low-frequency dynamical susceptibility in the optimal doped regime follows a surprisingly simple scaling function as $\chi''(\omega) \propto \arctan(\omega/T)$. The NMR and NQR spin-lattice relaxation time T_1 is weakly T dependent. These unusual magnetic properties of the copper oxide materials suggest that the normal state cannot be described by the conventional Fermi-liquid theory.

As emphasized by many researchers,[7] the essential physics of the copper oxide materials is contained in the doped antiferromagnet, which may be effectively described by the two-dimensional (2D) t-J model acting on the space with no doubly occupied sites. The t-J model is reduced as the Heisenberg model in the undoped case. In spite of its simple form the t-J model proved to be very difficult to analyze, analytically as well as numerically, because of the electron single occupancy on-site local constraint. The local nature of the constraint is of prime importance, and its violation may lead to some unphysical results.[8] Recently a fermion-spin theory based on the charge-spin separation is proposed[9,10] to incorporate this constraint, where the electron on-site local constraint for single occupancy is satisfied even in the mean-field approximation (MFA). The magnetic in the undoped parent compounds is now quite well understood:[1] here, the system of interacting localized Cu^{2+} spins is well described by the 2D Heisenberg model, and then it is clearly of great interest to investigate in detail the crossover from the rather conventional local moment system at zero doping to the electronic state that forms the basis for the high-temperature superconductivity. Therefore in this paper, we only study the spin dynamics of the copper oxide materials within the fermion-spin theory in the underdoped and optimal doped regimes. According to the fermion-spin formulism,[9,10] the electron operators can be decomposed as $C_{i\uparrow} = h_i^\dagger S_i^-$ and $C_{i\downarrow} = h_i^\dagger S_i^+$, with the spinless fermion operator h_i keeps track of the charge (holon), while the pseudospin operator S_i keeps track of the spin (spinon). Within the fermion-spin theory, it has been shown[11] that AFLRO vanishes around doping $\delta = 5\%$ for the reasonable value of the parameter $t/J = 5$. The mean-field theory in the underdoped and optimal doped regimes without AFLRO has been developed,[10] where the mean-field order parameters are defined as $\chi = \langle S_i^+ S_{i+\eta}^- \rangle = \langle S_i^- S_{i+\eta}^+ \rangle$, $\chi_z = \langle S_i^z S_{i+\eta}^z \rangle$, $C = (1/Z^2)\Sigma_{\eta,\eta'}\langle S_{i+\eta}^+ S_{i+\eta'}^- \rangle$, $C_z = (1/Z^2)\Sigma_{\eta,\eta'}\langle S_{i+\eta}^z S_{i+\eta'}^z \rangle$, and $\phi = \langle h_i^\dagger h_{i+\eta} \rangle$ with $\hat{\eta} = \pm\hat{x}, \pm\hat{y}$, and Z is the number of nearest neighbor sites. In this case, the low-energy behavior can be described[10] by the effective Hamiltonian $H = H_t + H_J$ with

$$H_t = -t\sum_{i\eta} h_i h_{i+\eta}^\dagger (S_i^+ S_{i+\eta}^- + S_i^- S_{i+\eta}^+) + \text{H.c.} + \mu\sum_i h_i^\dagger h_i,$$

$$\text{(1a)}$$

$$H_J = J_{\text{eff}}\sum_{i\eta} [\tfrac{1}{2}(S_i^+ S_{i+\eta}^- + S_i^- S_{i+\eta}^+) + S_i^z S_{i+\eta}^z], \quad \text{(1b)}$$

where $J_{\text{eff}} = J[(1-\delta)^2 - \phi^2]$, and μ is the chemical potential which enforce $\langle h_i^\dagger h_i \rangle = \delta$.

In the framework of the charge-spin separation, the basic low-energy excitations are holons and spinons. The charge dynamics can be discussed based on the Ioffe-Larkin combination rule,[12] however, since the spin fluctuations couple

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only to spinons, and therefore no composition law is required in discussing the spin dynamics,[12] but the strongly correlation between holons and spinons still is considered through the holon's order parameters ϕ entering in the spinon propagator, which means that the spinon moves in the background of holons, and the cloud of distorted holon background is to follow spinons, therefore the dressing of the spinon by holon excitations is the key ingredient in the explanation of the spin dynamics. According to Ioffe-Larkin combination rule,[12] we[13] have discussed the optical conductivity, Drude weight, and resistivity of the copper oxide materials in the underdoped and optimal doped regimes by considering fluctuations around the mean-field solution, where the dominant dynamical effect is due to the strongly spinon-holon interaction in Hamiltonian (1). We believe that this strongly spinon-holon interaction also will dominate the spin dynamics within the same regimes. The mean-field spinon Green's functions $D^{(0)}(k,\omega)$ and $D_z^{(0)}(k,\omega)$ and mean-field holon Green's function $g^{(0)}(k,\omega)$ have been given in Ref. 10. In this paper, we limit the holon part to the first-order (mean-field level) since some physical properties can be well described at this level,[10] and spin fluctuations couple only to
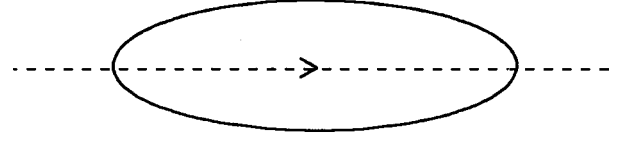

FIG. 1. The spinon's second-order self-energy diagram. The solid and dashed lines correspond to the holon and spinon propagators, respectively.

spinons as mentioned above. However, the second-order correction for the spinon is necessary for the discussion of the spin dynamics. The second-order spinon self-energy diagram from the holon pair bubble is shown in Fig. 1. Since the spinon operators obey the Pauli algebra, we map the spinon operator into the spinless-fermion representation in terms of the 2D Jordan-Wigner transformation[14] for the formal many particle perturbation expansion. After then the spinon Green's function in the spinon self-energy diagram shown in Fig. 1 is replaced by the mean-field spin Green's function $D^{(0)}(k,\omega)$. In this case, we obtain the second-order spinon self-energy as

$$\Sigma_s^{(2)}(k,\omega) = -(Zt)^2 \frac{1}{N^2}\sum_{pp'} (\gamma_{k-p}+\gamma_{p'+p+k})^2 B_{k+p'}\left(\frac{n_F(\xi_{p+p'})[1-n_F(\xi_p)]+[1+n_B(\omega_{k+p'})][n_F(\xi_p)-n_F(\xi_{p+p'})]}{\omega+\xi_{p+p'}-\xi_p+\omega_{k+p'}+i0^+} \right.$$
$$\left. - \frac{n_F(\xi_{p+p'})[1-n_F(\xi_p)]-n_B(\omega_{k+p'})[n_F(\xi_p)-n_F(\xi_{p+p'})]}{\omega+\xi_{p+p'}-\xi_p-\omega_{k+p'}+i0^+} \right), \tag{2}$$

where $\gamma_k=(1/Z)\sum_\eta e^{ik\cdot\hat\eta}$, $\epsilon=1+2t\phi/J_{\rm eff}$, $B_k=ZJ_{\rm eff}[(2\epsilon\chi_z+\chi)\gamma_k-(\epsilon\chi+2\chi_z)]/\omega_k$, $n_F(\xi_k)$ and $n_B(\omega_k)$ are the Fermi and Bose distribution functions, respectively, the mean-field holon excitation spectrum $\xi_k=2Z\chi t\gamma_k+\mu$, and the mean-field spinon excitation spectrum ω_k is given in Ref. 10. Then the full spinon Green's function is obtained as $D^{-1}(k,\omega)=D^{(0)-1}(k,\omega)-\Sigma_s^{(2)}(k,\omega)$. Since the local constraint of the t-J model has been treated exactly in the previous mean-field theory,[10] and it is naturally satisfied in the above perturbation expansion based on this mean-field theory.

We are now ready to discuss the spin dynamics. The dynamical spin response, as manifested by the dynamical spin structure factor $S(k,\omega)$ and the susceptibility $\chi(k,\omega)$, are given as $S(k,\omega)=Re\int_0^\infty dt e^{i\omega t}\langle S_k^+(t)S_k^-(0)\rangle=2ImD(k,\omega)/(1-e^{-\beta\omega})$ and $\chi''(k,\omega)=(1-e^{-\beta\omega})S(k,\omega)=2ImD(k,\omega)$. The properties of $S(k,\omega)$ and $\chi''(k,\omega)$ in different k directions have been discussed,[15] and the results showed that there is the anomalous temperature T dependence of the spin fluctuations near the antiferromagnetic point $Q=(\pi,\pi)$. In this paper we are interested in the universal behavior of the integrated dynamical response. The integrated dynamical spin structure factor and integrated susceptibility are expressed as

$$\bar S(\omega)=S_L(\omega)+S_L(-\omega)=(1+e^{-\beta\omega})S_L(\omega),$$

$$S_L(\omega)=\frac{1}{N}\sum_k S(k,\omega), \tag{3}$$

and

$$I(\omega,T)=\frac{1}{N}\sum_k \chi_s''(k,\omega), \tag{4}$$

respectively. We have performed a numerical calculation for the integrated spin structure factor (3) and integrated susceptibility (4). The result of the integrated spin structure factor for the parameter $t/J=2.5$ with the temperature $T=0.3J$ (solid line), $T=0.4J$ (dashed line), and $T=0.5J$ (dotted line) at the doping (a) $\delta=0.08$, and (b) $\delta=0.15$ is plotted in Fig. 2. From Fig. 2, it is shown that the integrated spin structure factor is almost temperature independent and the shape appears to be particularly universal in the underdoped and optimal doped regimes. $\bar S(\omega)$ is decreased with increasing energies for $\omega<0.5t$, and almost constant for $\omega\geq0.5t$, which is consistent with the experiments[16] and numerical simulations.[17] In correspondence with the integrated spin structure factor, the result of integrated susceptibility at the doping $\delta=0.15$ for the parameter $t/J=2.5$ with the temperature $T=0.2J$ (solid line), $T=0.3J$ (dashed line), and $T=0.4$
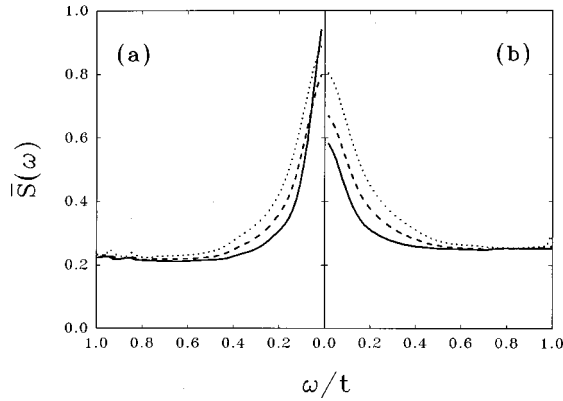
FIG. 2. The integrated dynamical spin structure factor at the doping (a) $\delta = 0.08$ and (b) $\delta = 0.15$ for $t/J = 2.5$ with the temperature $T = 0.3J$ (solid line), $T = 0.4J$ (dashed line), and $T = 0.5J$ (dotted line).

(dotted line) is plotted in Fig. 3. For comparison, the function $b_1 \arctan[a_1 \omega/T + a_3(\omega/T)^3]$ with $b_1 = 0.23$, $a_1 = 2.0$, and $a_3 = 1.4$ is also plotted in Fig. 3 (dot-dashed line). Our results show that the integrated susceptibility is almost constant above $\omega/T > 1$ and then begin to decrease with decreasing ω/T for $\omega/T < 1$. It is quite remarkable that our theoretical results of the integrated susceptibility are scaled approximately as $I(\omega,T) \propto \arctan[a_1 \omega/T + a_3(\omega/T)^3]$, which is in very good agreement with the experiments.[16]

The temperature dependence of the susceptibility converges to a universal function of ω/T is very significant because of its relation to other normal state properties, such as the temperature dependences of the spin-lattice relaxation time. The NQR spin-lattice relaxation time T_1 is expressed as

$$\frac{1}{T_1} = \frac{2 K_B T}{g^2 \mu_B^2 \hbar} \lim_{\omega \to 0} \frac{1}{N} \sum_k F_\alpha^2(k) \frac{\chi''(k,\omega)}{\omega}, \qquad (5)$$

where g is the g factor, μ_0 is the Bohr magneton, and the form factors $F_\alpha(k) = (F_\perp(k), F_\parallel(k))$, with $F_\perp(k)$ and $F_\parallel(k)$
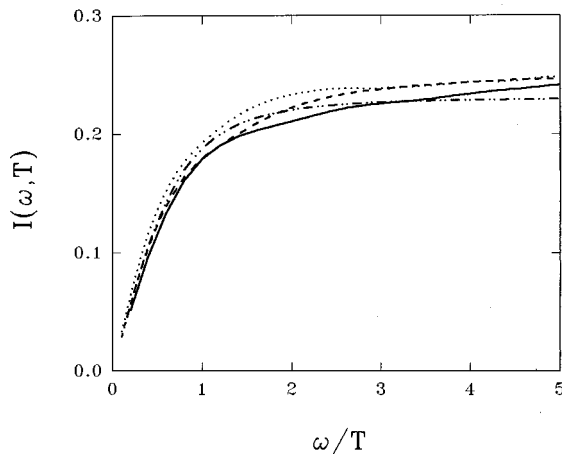

FIG. 3. The integrated susceptibility at the doping $\delta = 0.15$ for $t/J = 2.5$ with the temperature $T = 0.2J$ (solid line), $T = 0.3J$ (dashed line), and $T = 0.4J$ (dotted line). The dot-dashed line is the function $b_1 \arctan[a_1 \omega/T + a_3(\omega/T)^3]$ with $b_1 = 0.23$, $a_1 = 2.0$, and $a_3 = 1.4$.
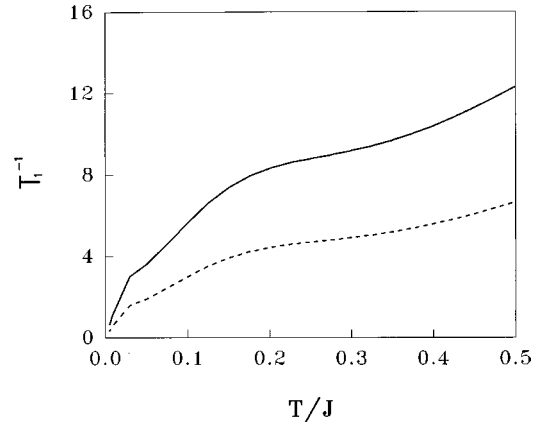

FIG. 4. The spin-lattice relaxation time at the doping $\delta = 0.15$ with $t/J = 2.5$ for the field applied parallel to C axis (solid line) and perpendicular to C axis (dashed line).

are for the field applied parallel and perpendicular to the C axis, respectively. The form factors have dimension of energy, and magnitude determined by atomic physics, and k dependence determined by geometry. For the comparison with experiments, the form factors $F_\perp(k)$ and $F_\parallel(k)$ are chosen as proposed in Ref. 18. The spin-lattice relaxation time T_1 in Eq. (5) has been evaluated numerically and the results for $t/J = 2.5$ with the doping $\delta = 0.15$ for the field applied parallel to C axis (solid line) and perpendicular to C axis (dashed line) are plotted in Fig. 4, where we have chosen units $\hbar = K_B = 1$. From Fig. 4, it is shown that T_1 is very weakly dependent on T in the optimal doped regime. Some experiments[5] show that $1/T_1$ approaches nearly the temperature independent at high temperature for $La_{2-x}Sr_x CuO_4$, and the weakly temperature dependent for $YBa_2Cu_3O_7$, in the optimal doped regime. Although the simplest t-J model cannot be regarded as the complete model for the quantitative comparison with the copper oxide materials, but our results are in qualitative agreement with these remarkable experiments.[5]

In the fermion-spin theory, the charge and spin degrees of freedom of the physical electron are separated as the holon and spinon, respectively. Although both holons and spinons contributed to the charge and spin dynamics, but it has been shown that the scattering of holons dominates the charge dynamics,[13] while the present results shows that scattering of spinons dominates the spin dynamics. The spin dynamics probe local magnetic fluctuations and are a very detailed and stringent test of microscopic theories. Our theoretical results within the fermion-spin formulism leads to the behaviors similar to that seen in the experiments and numerical simulations. To our present understanding, the main reasons why the present theory is successful in studying the normal-state property of the strongly correlated copper oxide materials are that (1) the electron single occupancy on-site local constraint is exactly satisfied during the above analytic calculation. Since the anomalous normal-state property of the copper oxide materials are caused by the strong electron correlation in these systems,[1-3] and can be effectively described by the t-J model,[7] but the strong electron correlation in the t-J model manifests itself by the electron single occupancy on-site local constraint, which means that the electron Hilbert space is

severely restricted due to the strong electron repulsion interaction. This is why the crucial requirement is to treat this constraint exactly during the analytic discussions. (2) Since the local constraint is satisfied even in the MFA within fermion-spin theory, the extra gauge degree of freedom occurring in the slave-particle approach does not appear here,[9,10] then spinons and holons within the fermion-spin theory are by themselves gauge invariant, they are real and can be interpreted as physical excitations. In this case, there are two relaxation times for spinons and holons, respectively, the spinon relaxation time is responsible to the spin dynamics, while holon relaxation time is responsible to the charge dynamics. This important issue to the copper oxide materials within the charge-spin separation has been emphasized by Laughlin.[19]

In summary, we have studied the spin dynamics of the copper oxide materials in the underdoped and optimal doped regimes within the framework of the fermion-spin theory.

Our results show that the strongly correlated renormalization effects for the spinon due to the strongly spinon-holon interaction are very important for the spin dynamics. The integrated dynamical spin structure factor, integrated susceptibility, and spin-lattice relaxation time are discussed, and the results are qualitative consistent with the experiments and numerical simulations.

*Mailing address.

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