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Lorentzian form for the imaginary part of the dynamic spin susceptibility: comparison with NQR and Neutron Scattering data in copper oxide superconductors

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We present some new results based on the relaxation function theory for a doped two-dimensional Heisenberg antiferromagnetic system with damping of paramagnon-like excitations. The Lorentzian form for the imaginary part of the dynamic spin susceptibility gives a reasonable agreement with neutron scattering and plane copper nuclear spin-lattice relaxation rate $\chi''(1/T_1)$ data in right up to optimally doped La$_2$-Sr$_x$CuO$_4$.

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Keywords: cuprate superconductors, dynamic spin susceptibility

1. Introduction

Plane copper oxide high-temperature superconductors (high-$T_c$) are the doped $S = 1/2$ two-dimensional Heisenberg antiferromagnetic (2DHAF) systems. In the carrier free regime, the elementary excitations are spin waves [1-3], magnons in the quasiparticle language. Observations by neutron scattering (NS) of the $\omega/\Gamma$ scaling for the averaged over the Brillouin zone the imaginary part of the dynamic spin susceptibility, $\chi''(\omega,T) = \int \chi''(\mathbf{q},\omega,T)d^2\mathbf{q} \approx \chi''(\omega,T \rightarrow 0)/f(\omega/\Gamma)$, in the underdoped high-$T_c$ compounds [2] above $T_c$ is referred to a nearby quantum phase transition [1]. Nuclear Magnetic/Quadrupole Resonance (NMR/NQR) studies [4] revealed the extension of the universal behavior of $\chi''(\omega,T)$ down to the MHz frequency range. In this paper we present some new results based on the relaxation function theory with damping of the paramagnon-like excitations [5-7] in connection with plane copper nuclear spin-lattice relaxation rate as obtained by NQR and imaginary part of the dynamic spin susceptibility $\chi''(\mathbf{k},\omega)$ as obtained by NS experiments.

2. Basic relations

We employ the $t$-$J$ Hamiltonian [8] known as the minimal model for high-$T_c$ cuprates:

$$H_{t,J} = \sum_{i,j,\sigma} t_{ij} X_i^{\sigma 0} X_j^{\sigma 0} + J \sum_{i<j} (S_i S_j - \frac{1}{4} n_i n_j), \quad (1)$$

written in terms of the Hubbard operators $X_i^{\sigma 0}$ that create an electron with spin $\sigma$ at site $i$ and $S_i$ are spin-1/2 operators. Here, the hopping integral $t_{ij} = t$ between the nearest neighbors (NN) describes the motion of electrons causing a change in their spins and $J = 0.12$ eV is the NN AF coupling constant. The spin and density operators are defined as follows:

$$S_i^\sigma = X_i^{\sigma 0}, \quad S_i^z = 0.5 \sum_\sigma \sigma X_i^{\sigma 0}, \quad n_i = \sum_\sigma X_i^{\sigma 0}, \quad (\sigma = -\tilde{\sigma}), \quad (2)$$

with the standard normalization $X_i^{00} + X_i^{++} + X_i^{--} = 1$. 

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The static spin susceptibility as derived within the $t$-$J$ model [9] is given by,

$$
\chi(k) = \frac{4c_1}{Jg_\gamma (g_\gamma + \gamma_k)},
$$

(3)

and has the same structure as in the isotropic spin-wave theory [10] at all doping levels. The NN AF spin-spin correlation function is given by

$$
\chi_{\gamma} = \frac{c_1}{Jg_\gamma (g_\gamma + \gamma_k)}(S_{\gamma}^zS_{\gamma}^z),
$$

(3)

Table 1. The calculated in the $T \rightarrow 0$ limit antiferromagnetic spin-spin correlation function between the nearest neighbours $c_1$, the parameter $g_\gamma$, and the spin stiffness constant $\rho_\gamma$.

<table>
<thead>
<tr>
<th>Doping</th>
<th>$c_1$</th>
<th>$g_\gamma$</th>
<th>$2\pi\rho_\gamma / J$</th>
<th>$\xi_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta=0$</td>
<td>-0.1152</td>
<td>4.1448</td>
<td>0.38</td>
<td>-</td>
</tr>
<tr>
<td>$\delta=0.04$</td>
<td>-0.1055</td>
<td>3.913</td>
<td>0.3</td>
<td>$1/(2\delta)$</td>
</tr>
<tr>
<td>$\delta=0.15$</td>
<td>-0.0617</td>
<td>2.947</td>
<td>0.13</td>
<td>$1/\delta$</td>
</tr>
</tbody>
</table>

The relaxation shape function is given by [11]

$$
F(k,\omega) = \frac{\tau_k\Delta_k^2 / \pi}{[\omega\tau_k(\omega^2 - \Delta_k^2 - \Delta_k^2)] + (\omega^2 - \Delta_k^2)^2},
$$

(4)

where $\tau_k = \sqrt{2/(\pi\Delta_k^2)}$, and $\Delta_k^2$ and $\Delta_k^2$ are related to the frequency moments

$$
\langle \omega_k^2 \rangle = \int_0^\infty \omega' F(k,\omega)d\omega,
$$

(5)

as $\Delta_k^2 = \langle \omega_k^2 \rangle$, $\Delta_k^2 = \langle \omega_k^2 \rangle / \langle \omega_k^2 \rangle - \langle \omega_k^2 \rangle$, the expression for the second moment is given by

$$
\langle \omega_k^2 \rangle = i\left[\langle S_{\alpha}^z \rangle \langle S_{\alpha}^z \rangle \right] / \chi_k = -\left(8JC_1 - 4t_{off} T_i\right)[1-\gamma_k] / \chi_k,
$$

(6)

where $T_i = p\sum_k \gamma_k j_k^2$, $p = (1+\delta)/2$, and $j_k^2 = [\exp(-E_k + \mu) / k_B T + 1]$ is the Fermi function of holes, where the number of extra holes, $\delta$, due to doping, per one plane Cu $^{2+}$, can be identified with the Sr content $x$ in La$_{2-x}$Sr$_x$CuO$_4$. The excitation spectrum of holes is given by, $E_k = 4t_{off} \gamma_k$, where the hoppings, $t$, are affected by electronic and AF spin-spin correlations $c_1$, resulting in effective values [5,8], for which we set $t_{off} = \delta J / 0.2$, in order to match the insulator-metal transition. The chemical potential $\mu$ is related to $\delta$ by $\delta = p\sum_k j_k^2$. Note that $F(k,\omega)$ is real, even in both $k$ and $\omega$, and normalized to unity $\int_0^\infty d\omega F(k,\omega) = 1$. The detailed expression for $\langle \omega_k^2 \rangle$ is given in [5].

We take the Lorentzian form for the imaginary part of the dynamic spin susceptibility,

$$
\chi_L(k,\omega) = \frac{Z_\omega \omega F_k}{[\omega - \omega_k^\omega]^2 + \Gamma_k^2} + \frac{Z_\omega \omega F_k}{[\omega + \omega_k^\omega]^2 + \Gamma_k^2},
$$

(7)

for $k$ around the AF wave vector $(\pi,\pi)$. The spin-wavelike dispersion, renormalized by interactions, is given by the relaxation function [11], given by Eq. (4),

$$
\omega_k^\omega = 2\int_0^\infty \omega F(k,\omega)d\omega,
$$

(8)

where the integration over $\omega$ in Eq. (8) has been performed analytically and exactly [7].
The damping of paramagnon-like excitations $\Gamma_k$ is given by $\Gamma_k = \sqrt{\frac{\omega}{\omega_0}} - \left( \frac{\omega}{\omega_0} \right)^2$.

The plane copper nuclear spin-lattice relaxation rate is given by

$$\frac{^{63}(1/T)}{\omega_0} = \frac{2k_BT}{\omega_0} \sum_{k>\xi_{\text{eff}}}^{\text{Cu}} F(k)^2 \chi_k(k,\omega_0),$$

where $\omega_0 = 2\pi \times 34 \text{ MHz} \ (\ll T_c, J)$ is the measuring NQR frequency. The hyperfine formfactor for plane $^{63}\text{Cu}$ sites is given by, $F(k)^2 = (A_{\text{eff}} + 4\gamma_B k)^2$, where $A_{\text{eff}} = 1.7 \times 10^{-7} \text{ eV}$ and $B = (1 + 4\delta) \times 3.8 \times 10^{-7} \text{ eV}$ are the Cu on-site and transferred hyperfine couplings, respectively [12]. The effective correlation length $\xi_{\text{eff}}$ is given by, $\xi_{\text{eff}} = \xi^{-1} + \xi_{\text{eff}}^{-1} [5,13]$. Thus from now on we replace $\xi$ by $\xi_{\text{eff}}$ and $\xi_0$ values are presented in the Table 1.

The spin diffusive contribution (from small wave vectors $|\mathbf{k}| \ll 1/\xi_{\text{eff}}$) can be calculated from general physical grounds, namely, the linear response theory, hydrodynamics, and fluctuation-dissipation theorem [5-7,11,14],

$$\frac{^{63}(1/T)_d}{\omega_0} = \frac{\pi D}{\omega_0 \xi_{\text{eff}}^2} = \frac{\int q^2 F(q,0) d^2q}{\omega_0 \xi_{\text{eff}}^2},$$

where $\Lambda = \frac{1}{(4\pi)} \ln[1 + D^2 / (\omega_0^2 \xi_{\text{eff}}^2)]$ and $D = \lim_{q \to 0} \pi q^2 F(q,0)$ is the spin diffusion constant.

3. Results

Figure 1 shows the averaged over the Brillouin zone the imaginary part of dynamic spin susceptibility $\chi''(\omega) = \int \chi''(\mathbf{q},\omega) d^2q$ versus $\omega/T$. Symbols: NS data for $\text{La}_{1.96}\text{Sr}_{0.04}\text{CuO}_4$ at various $\omega$ values from Ref. [13], the lines show the calculated $\chi''(\omega)$.

![Figure 1](image1.png)

![Figure 2](image2.png)
Lorentzian form for the imaginary part of the dynamic spin susceptibility: comparison …

susceptibility \( \chi''(\omega, T) \) versus \( \omega / T \). It suggests \( \omega / T \) scaling for underdoped high-\( T_c \) layered cuprates with deviations at small \( \omega \) in qualitative agreement with NS data [1,13].

Figure 2 shows the calculated with Eqs. (7) and (9) plane copper nuclear spin-lattice relaxation rate \( ^{63}(1/T_1) \) (solid lines) without any adjustable parameters. The dashed lines show the calculated \( ^{63}(1/T_1) \) without damping of the paramagnon-like excitations [5], where \( F(k, \omega) \) is related to the imaginary part of the dynamic spin susceptibility \( \chi''(k, \omega) \) as [5,11],

\[
\chi''(k, \omega) = \omega \chi_k F(k, \omega). \tag{11}
\]

It is worth to mention that the temperature dependence of \( ^{63}(1/T_1) \) in both theories is governed by the temperature dependence of the correlation length and by the factor \( k_B T \) in agreement with [12]. At low \( T \), where \( \xi_{\text{eff}} \approx \text{const} \), the plane copper \( ^{63}(1/T_1) \propto T \), as it should. At high \( T \), the correlation length shows weak doping dependence and \( ^{63}(1/T_1) \) of doped samples behaves similarly to that of La\(_2\)CuO\(_4\).

4. Summary

In summary, we developed further a relaxation function theory [5-7] for dynamic spin properties and approved the Lorentzian form for the imaginary part of the dynamic spin susceptibility for layered copper high-\( T_c \) in the normal state. The \( \omega / T \) scaling and spin-lattice relaxation at plane copper sites may be explained within the damped spin-wave-like theory, possessing a reasonable agreement with the observations by means of neutron scattering and magnetic resonance in high-\( T_c \) copper oxides.

Acknowledgments

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References