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* In Kazan State University the Electron Paramagnetic Resonance (EPR) was discovered by Zavoisky E.K. in 1944.

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 $^{63}(1/T_1)$ data in right up to optimally doped $La_{2-x}Sr_xCuO_4$.

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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 ω/T scaling for the averaged over the Brillouin zone the imaginary part of the dynamic spin susceptibility, $\chi''(\omega,T)=\int\chi''(\mathbf{q},\omega,T)\mathrm{d}^2\mathbf{q}\approx\chi''(\omega,T\to 0)f(\omega/T)$, 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:

$$H_{t-J}=\sum_{i,j,\sigma}t_{ij}X_i^{\sigma 0}X_j^{0\sigma}+J\sum_{i>j}(\mathbf{S}_i\mathbf{S}_j-\frac{1}{4}n_in_j),\qquad (1)$$

written in terms of the Hubbard operators $X_i^{\sigma 0}$ that create an electron with spin σ at site i and $\mathbf{S}_i$ 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:

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

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

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

$$\chi(\mathbf{k}) = \frac{4\,|\,c_1\,|}{Jg_-(g_+ + \gamma_\mathbf{k})}, \tag{3}$$

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 $c_1 = (1/4)\sum_\rho \left\langle S_i^z S_{i+\rho}^z \right\rangle$, the index ρ runs over NN, and $\gamma_\mathbf{k} = (1/2)(\cos k_x + \cos k_y)$. The parameter g_+ is related to AF correlation length ξ via the expression $\xi = 1/(2\sqrt{g_+ - 1}) \approx (J\sqrt{g\_}/k_B T)\exp(2\pi\rho_S / k_B T)$, where ρ_S is spin stiffness. The values of the parameters of the theory [9]: c_1, $g\_$, and ρ_S are given in Table **1**.

Table 1. *The calculated in the $T\to 0$ limit antiferromagnetic spin-spin correlation function between the nearest neighbours c_1, the parameter $g\_$, and the spin stiffness constant ρ_S.*

Doping	c_1	$g\_$	$2\pi\rho_S / J$	ξ_0
δ=0	-0.1152	4.1448	0.38	–
δ=0.04	-0.1055	3.913	0.3	$1/(2\delta)$
δ=0.15	-0.0617	2.947	0.13	$1/\delta$

The relaxation shape function is given by [11]

$$F(\mathbf{k},\omega) = \frac{\tau_\mathbf{k}\Delta_{1\mathbf{k}}^2\Delta_{2\mathbf{k}}^2/\pi}{[\omega\tau_\mathbf{k}(\omega^2 - \Delta_{1\mathbf{k}}^2 - \Delta_{2\mathbf{k}}^2)]^2 + (\omega^2 - \Delta_{1\mathbf{k}}^2)^2}, \tag{4}$$

where $\tau_\mathbf{k} = \sqrt{2/(\pi\Delta_{2\mathbf{k}}^2)}$, and $\Delta_{1\mathbf{k}}^2$ and $\Delta_{2\mathbf{k}}^2$ are related to the frequency moments

$$\left\langle \omega_\mathbf{k}^n \right\rangle = \int_{-\infty}^{\infty} \omega^n F(\mathbf{k},\omega) d\omega, \tag{5}$$

as $\Delta_{1\mathbf{k}}^2 = \left\langle \omega_\mathbf{k}^2 \right\rangle$, $\Delta_{2\mathbf{k}}^2 = (\left\langle \omega_\mathbf{k}^4 \right\rangle / \left\langle \omega_\mathbf{k}^2 \right\rangle) - \left\langle \omega_\mathbf{k}^2 \right\rangle$, the expression for the second moment is given by

$$\left\langle \omega_\mathbf{k}^2 \right\rangle = i\left\langle [\dot{S}_\mathbf{k}^z, S_{-\mathbf{k}}^z] \right\rangle / \chi_\mathbf{k} = -\left(8Jc_1 - 4t_{eff}T_1\right)\left(1-\gamma_\mathbf{k}\right)/\chi_\mathbf{k}, \tag{6}$$

where $T_1 = p\sum_\mathbf{k} \gamma_\mathbf{k} f_\mathbf{k}^h$, $p = (1+\delta)/2$, and $f_k^h = [\exp(-E_\mathbf{k} + \mu)/k_B T + 1]^{-1}$ is the Fermi function of holes, where the number of *extra* holes, δ, due to doping, per one plane Cu^{2+}, can be identified with the Sr content x in $La_{2-x}Sr_xCuO_4$. The excitation spectrum of holes is given by, $E_\mathbf{k} = 4t_{eff}\gamma_\mathbf{k}$, 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 $t_{eff} = \delta J/0.2$, in order to match the insulator-metal transition. The chemical potential μ is related to δ by $\delta = p\sum_\mathbf{k} f_\mathbf{k}^h$. Note that $F(\mathbf{k},\omega)$ is real, even in both $\mathbf{k}$ and ω, and normalized to unity $\int_{-\infty}^{\infty} d\omega F(\mathbf{k},\omega) = 1$. The detailed expression for $\left\langle \omega_\mathbf{k}^4 \right\rangle$ is given in [5].

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

$$\chi_L(\mathbf{k},\omega) = \frac{\chi_\mathbf{k}\omega\Gamma_\mathbf{k}}{[\omega - \omega_\mathbf{k}^{sw}]^2 + \Gamma_\mathbf{k}^2} + \frac{\chi_\mathbf{k}\omega\Gamma_\mathbf{k}}{[\omega + \omega_\mathbf{k}^{sw}]^2 + \Gamma_\mathbf{k}^2}, \tag{7}$$

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

$$\omega_\mathbf{k}^{sw} = 2\int_0^{\infty} \omega F(\mathbf{k},\omega) d\omega, \tag{8}$$

where the integration over ω in Eq. (8) has been performed analytically and exactly [7].

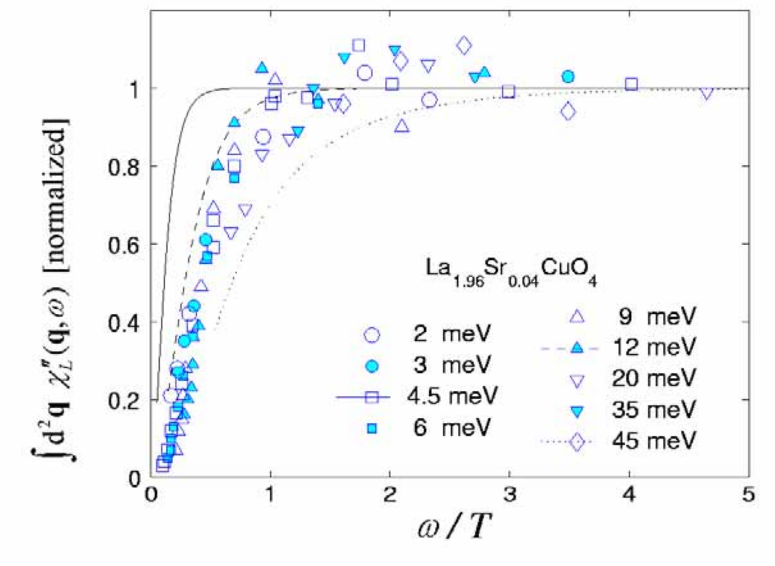

Figure 1. The averaged over the Brillouin zone the imaginary part of dynamic spin susceptibility $\chi''_L(\omega) = \int \chi''_L(\mathbf{q},\omega)\mathrm{d}^2\mathbf{q}$ *versus* ω/T. Symbols: NS data for $La_{1.96}Sr_{0.04}CuO_4$ at various ω values from Ref. [13], the lines show the calculated $\chi''_L(\omega)$.

The damping of paramagnon-like excitations $\Gamma_\mathbf{k}$ is given by $\Gamma_\mathbf{k} = \sqrt{\langle\omega_\mathbf{k}^2\rangle - (\omega_\mathbf{k}^{sw})^2}$.

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

$$^{63}(1/T_1) = \frac{2k_BT}{\omega_0}\sum_{|\mathbf{k}|>1/\xi_{eff}} {}^{63}F(\mathbf{k})^2\chi_L(\mathbf{k},\omega_0)\,, \qquad (9)$$

where $\omega_0 = 2\pi\times 34$ MHz ($\ll T, J$) is the measuring NQR frequency. The hyperfine formfactor for plane ^{63}Cu sites is given by, $^{63}F(\mathbf{k})^2 = (A_{ab} + 4\gamma_\mathbf{k}B)^2$, where $A_{ab} = 1.7\cdot10^{-7}$ eV and $B = (1+4\delta)\cdot 3.8\cdot10^{-7}$ eV are the Cu on-site and transferred hyperfine couplings, respectively [12]. The *effective* correlation length ξ_{eff} is given by, $\xi_{eff}^{-1} = \xi_0^{-1} + \xi^{-1}$ [5,13]. Thus from now on we replace ξ by ξ_{eff} and ξ_0 values are presented in the Table **1**.

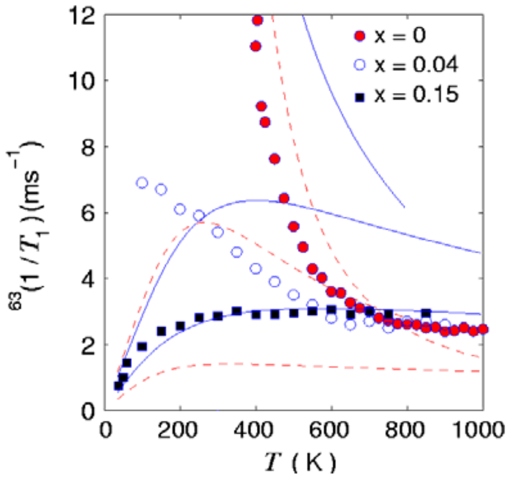

Figure 2. Temperature and doping dependence of the plane copper nuclear spin-lattice relaxation rate $^{63}(1/T_1) = 2W$. Experimental data for $La_{2-x}Sr_xCuO_4$ from Ref. [4]. Solid lines show the results of the calculations with Lorentzian form of the susceptibility and taking into account the damping of the paramagnon-like excitations using Eq. (7). The dashed lines show the results of the calculations without damping of the paramagnon-like excitations, after Refs. [5,6], i.e., using Eq. (11).

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

$$^{63}(1/T_1)_{Diff} = \frac{^{63}F(0)^2 k_BT\chi(\mathbf{k}=0)}{\pi\hbar D}\Lambda\,, \qquad (10)$$

where $\Lambda = [1/(4\pi)]\ln[1 + D^2/(\omega_0^2\xi_{eff}^4)]$ and $D = \lim_{q\to0}[\pi q^2 F(\mathbf{q},0)]^{-1}$ is the spin diffusion constant.

3. Results

Figure 1 shows the averaged over the Brillouin zone and normalized imaginary part of dynamic spin susceptibility $\chi''(\omega,T)$ *versus* ω/T. It suggests ω/T scaling for underdoped high-T_c layered cuprates with a deviations at small ω 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 $F(\mathbf{k},\omega)$ is related to the imaginary part of the dynamic spin susceptibility $\chi''(\mathbf{k},\omega)$ as [5,11],

$$\chi''(\mathbf{k},\omega) = \omega\chi_{\mathbf{k}}F(\mathbf{k},\omega) \quad . \tag{11}$$

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_BT in agreement with [12]. At low T, where $\xi_{eff} \approx const$, 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_2CuO_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 ω/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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