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Spin dynamics in La_2CuO_4: consistent description by the inclusion of ring exchange

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Abstract

We consider the square lattice Heisenberg antiferromagnet with plaquette ring exchange ($J_\square$) to investigate the spin dynamics in La_2CuO_4. The values for the in-plane exchange parameters, $J = 151.9$ meV and $J_\square = 0.24$ J, are obtained consistently by an accurate fit to the experimentally observed spin-wave dispersion. In a parameter-free calculation for the Raman light scattering intensity we find that the inclusion of ring exchange in the dispersion and the magnon–magnon interaction vertex leads to a 2-magnon peak position in B_{1g} geometry which agrees perfectly with the experimental value.

Understanding the undoped parent compounds of high temperature superconductors is a precondition for the many theories which describe metallic cuprates by doping carriers into a layered antiferromagnet. The conventional starting point for undoped cuprates is the two-dimensional (2D) spin-1/2 Heisenberg model with nearest-neighbor (nn) exchange interaction J. Despite the substantial progress on the theory of the 2D Heisenberg antiferromagnet, some of the experimental facts for La_2CuO_4 have clearly demonstrated that a complete description of the magnetic excitations requires additional physics not contained in the 2D Heisenberg model with J only. Here we show that the inclusion of a sizable ring-exchange coupling $J_\square$ simultaneously allows an accurate description of the spin-wave spectrum and the two-magnon Raman intensity in B_{1g} geometry.

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Specifically we study the spin Hamiltonian

$$H = J\sum_{i,\delta}\mathbf{S}_i\cdot\mathbf{S}_{i+\delta} + J'\sum_{i,\delta'}\mathbf{S}_i\cdot\mathbf{S}_{i+\delta'} + J_\square\sum_{\langle ijkl\rangle}\big[(\mathbf{S}_i\cdot\mathbf{S}_j)(\mathbf{S}_k\cdot\mathbf{S}_l) + (\mathbf{S}_i\cdot\mathbf{S}_l)(\mathbf{S}_k\cdot\mathbf{S}_j) - (\mathbf{S}_i\cdot\mathbf{S}_k)(\mathbf{S}_j\cdot\mathbf{S}_l)\big], \quad (1)$$

where J' is the next-nn exchange coupling. We use the Dyson–Maleev representation for the spin operators and diagonalize the quadratic part of the resulting spin Hamiltonian; the renormalization of the magnon spectrum by quartic terms is consistently accounted for by the inclusion of a set of quantum renormalization factors $\{\gamma\}$, which are determined self-consistently and constitute the corrections to the spectrum to order $1/S$ [2]. The result for the spin-wave spectrum reads

$$E_\mathbf{k} = \sqrt{A_\mathbf{k}^2 - B_\mathbf{k}^2}, \quad B_\mathbf{k} = 4S(J\gamma - J_\square S^2\gamma_\delta^\square)\nu_\mathbf{k}^\delta,$$
$$A_\mathbf{k} = 4S[J\gamma - J'\gamma'(1-\nu_\mathbf{k}^{\delta'}) - J_\square S^2(\gamma_0^\square + \gamma_{\delta'}^\square\nu_\mathbf{k}^{\delta'})], \quad (2)$$

where $v_{\mathbf{k}}^{\delta} = (\cos k_x + \cos k_y)/2$ and $v_{\mathbf{k}}^{\delta'} = \cos k_x \cos k_y$. Eq. (2) is used to fit the experimentally determined magnon spectrum for La_2CuO_4 from Ref. [1] as shown in Fig. 1 and we thereby obtain the following parameter set:

$$J = 151.9 \text{ meV}, \quad J' = 0.025 \text{ J}, \quad J_{\square} = 0.24 \text{ J}. \tag{3}$$

With these parameters we obtain the sublattice magnetization $S_0 = 0.319$ and the spin stiffness $\rho_s = 23.8$ meV which agrees well with previous estimates. Thus, the numbers in (3) provide an accurate, consistent determination of the exchange couplings for La_2CuO_4.

For an independent test of these quantitative results we calculate the Raman response with the fixed coupling constants (3), i.e. without adjustable parameters. We use the effective Loudon–Fleury Hamiltonian in B_{1g} geometry for the coupling of the incoming and outgoing photons to the localized nn spins, which are involved in the two-spin flip Raman process

$$H_R = \Lambda \sum_j \mathbf{S}_j \cdot (\mathbf{S}_{j+\delta_y} - \mathbf{S}_{j+\delta_x}). \tag{4}$$

The Raman light scattering intensity is determined by $I(\omega) = -(1/\pi)\mathrm{Im}\, G(\omega)$ where $G(\omega)$ is the time-ordered response function

$$G(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t e^{\mathrm{i}\omega t} \langle T[H_R(t) H_R(0)] \rangle. \tag{5}$$

$G(\omega)$ is evaluated in the ladder approximation for the magnon–magnon interaction vertex [3]. The effect of the ring exchange is included in the spectrum as well as the renormalized vertex function [4].

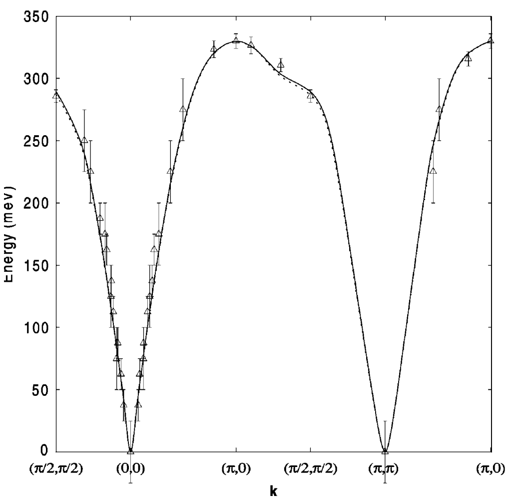

Fig. 1. Spin-wave dispersion along high symmetry directions in the 2D Brillouin zone. The triangles are the experimental results of Ref. [1] for La_2CuO_4 at 10 K. The solid line is the result of a fit to our theoretical result.

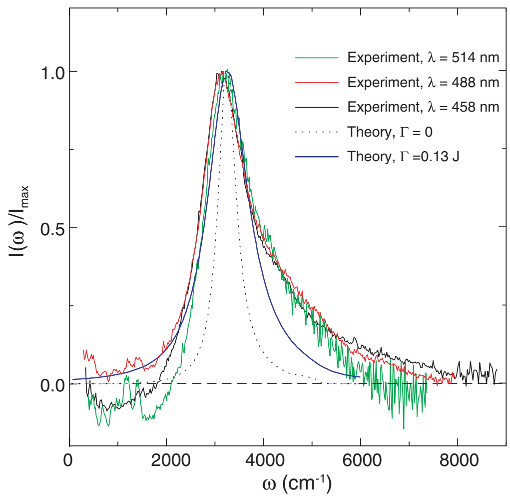

Fig. 2. Comparison of the theoretical result (without and with additional damping $\Gamma = 0.13$ J) to the experimental Raman intensity in La_2CuO_4 in B_{1g} geometry taken from Ref. [5]. The three experimental curves belong to different incoming photon frequencies; the high-energy intensity background was substracted. All data sets were normalized to their corresponding intensity maximum.

In Fig. 2 we compare the theoretical result for the Raman lineshape with the experimental data on La_2CuO_4 from Ref. [5]. Although the peak position depends sensitively on the magnitude of $J_{\square}$ [4], it is in excellent agreement with the data for the parameter set (3). The ring-exchange is also responsible for an asymmetry of the theoretical lineshape, i.e. a foot structure near the upper edge of the spectrum. Its weight, however, is too small to account for the overall linewidth and lineshape. The peak width can only be accounted for, if an additional damping for the magnon lifetime is included. Therefore, other processes must contribute which are not described by the Heisenberg model with ring exchange alone.

The fact the B_{1g} Raman peak position is excellently reproduced confirms the quantitative accuracy of the exchange couplings (3) for La_2CuO_4.

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