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Inelastic neutron scattering peak in Zn substituted $YBa_2Cu_3O_7$

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The effects of nonmagnetic impurities on the $\mathbf{Q} = (\pi, \pi)$ spin-fluctuation spectral weight are studied in the normal state using the framework of the Hubbard model. It is shown that the impurity scattering of the spin fluctuations with momentum transfers near $2\mathbf{k}_F$ could lead to a peak in $\text{Im}\,\chi(\mathbf{Q}, \omega)$ at $\omega = 2|\mu|$, where μ is the chemical potential. The results on the single-layer and the bilayer CuO_2 models are compared with the neutron scattering data on Zn substituted $YBa_2Cu_3O_7$.

In pure $YBa_2Cu_3O_7$, the important feature of the $\mathbf{Q} = (\pi, \pi)$ neutron scattering intensity is a resonant peak which becomes observable only in the superconducting state [1]. The recent experiments by Fong *et al.* [2] have found that upon substituting 0.5% Zn impurities the resonant peak becomes observable in the normal state as a broadened peak centered at 40 meV. In the presence of dilute Zn impurities, significant amount of spectral weight develops in the peak already in the normal state. For instance, at 94°K, the amplitude of the neutron scattering intensity at 40 meV is about half of its value at 22°K.

Here, the effects of dilute nonmagnetic impurities on the neutron scattering spectral weight $\text{Im}\,\chi(\mathbf{Q}, \omega)$ will be calculated using the framework of the two-dimensional Hubbard model and the random-phase approximation for the magnetic susceptibility. This framework was introduced for calculating the NMR T_1^{-1} rates for pure $YBa_2Cu_3O_7$ in the normal state [3]. It will be shown that the scattering of the spin fluctuations by an impurity with momentum transfers near $2\mathbf{k}_F$, where $\mathbf{k}_F$ is the Fermi momentum, could lead to a peak in $\text{Im}\,\chi(\mathbf{Q}, \omega)$ above T_c. Here, results will be given for both the single-layer and the bilayer CuO_2 structures. Within the random-phase approximation, the peak occurs at $\omega_0 = 2|\mu|$, where μ is the chemical potential. The underlying reason for the peak within this model is a kinematic constraint against creating a particle-hole pair with center-of-mass momentum $\mathbf{q} = (\pi, \pi) - 2\mathbf{k}_F$ and energy $\omega > \omega_0$.

Within the presence of an impurity, the magnetic susceptibility is defined in terms of the Matsubara time τ as

$$\chi(\mathbf{q}, \mathbf{q}', \tau) = \langle T_\tau m^-(\mathbf{q}, \tau) m^+(\mathbf{q}', 0)\rangle, \qquad (1)$$

where $m^+(\mathbf{q}) = N^{-1/2} \sum_{\mathbf{p}} c^\dagger_{\mathbf{p}+\mathbf{q}\uparrow} c_{\mathbf{p}\downarrow}$, $m^-(\mathbf{q}) = (m^+(\mathbf{q}))^\dagger$, and T_τ is the τ-ordering operator. In this case, the RPA expression for the susceptibility in real ω space is given by

$$\chi(\mathbf{q}, \mathbf{q}', \omega) = \chi_0(\mathbf{q}, \mathbf{q}', \omega) + U \sum_{\mathbf{q}''} \chi_0(\mathbf{q}, \mathbf{q}'', \omega) \chi(\mathbf{q}'', \mathbf{q}', \omega), \qquad (2)$$

where $\chi_0(\mathbf{q}, \mathbf{q}', \omega)$ is the irreducible susceptibility dressed with the impurity scatterings, but not with the Coulomb correlations. Here, the diagonal $\mathbf{q} = \mathbf{q}'$ terms of $\chi_0(\mathbf{q}, \mathbf{q}', \omega)$ will be approximated by the Lindhard function of the pure system, $\chi_0^L(\mathbf{q}, \omega)$, since it is already known from previous calculations that the effect of impurity scattering on $\chi_0(\mathbf{q}, \mathbf{q}, \omega)$ is to cause a weak, smooth smearing [4]. The $\mathbf{q} \neq \mathbf{q}'$ off-diagonal terms of $\chi_0(\mathbf{q}, \mathbf{q}', \omega)$ will be calculated in the lowest order in the strength of the effective electron-impurity interaction as shown diagrammatically in Fig. 1(a). In addition, only the component of the effective electron-impurity interaction which transfers momentum $\mathbf{Q}^* = 2\mathbf{k}_F$,

$$V_0 \sum_{\mathbf{p}\sigma} (c^\dagger_{\mathbf{p}+\mathbf{Q}^*\sigma} c_{\mathbf{p}\sigma} + c^\dagger_{\mathbf{p}-\mathbf{Q}^*\sigma} c_{\mathbf{p}\sigma}), \qquad (3)$$

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will be taken into account. This is because, for other values of $\mathbf{Q}^*$, $\chi_0(\mathbf{Q}, \mathbf{q} = \mathbf{Q} - \mathbf{Q}^*, \omega)$ is a smooth function of ω and does not lead to any singular structure in χ. The resulting $\chi(\mathbf{Q}, \mathbf{Q}, \omega)$, denoted by $\chi(\mathbf{Q}, \omega)$, is plotted in Figs. 1(b) and (c) for the single-layer and the bilayer band structures, respectively.

In Fig. 1(b), $\mathrm{Im}\,\chi(\mathbf{Q} = (\pi, \pi), \omega)$ versus ω is shown for a single layer with the quasiparticle dispersion $\varepsilon_{\mathbf{p}} = -2t(\cos p_x + \cos p_y) - \mu$ and $\mathbf{k}_F$ chosen along $(1,1)$. In addition, here, the following model parameters were used: $U = 2t$, bandwidth $8t = 1$ eV, and filling $\langle n \rangle = 0.86$. This choice of the parameters was used in Ref. [3], and provided a good fit of the NMR T_1^{-1} rates. The calculation of $\mathrm{Im}\,\chi(\mathbf{Q}, \omega)$ was next carried out for a CuO_2 bilayer with the dispersion relation

$$\varepsilon_{\mathbf{p}} = -2t(\cos p_x + \cos p_y) \\ -2t_\perp \cos p_z (\cos p_x - \cos p_y)^2 - \mu, \qquad (4)$$

which was previously used in calculating $\mathrm{Im}\,\chi(\mathbf{Q}, \omega)$ for the d-wave superconducting state of pure $YBa_2Cu_3O_7$ [5]. Here $t_\perp = 0.1t$ was chosen as in Ref. [5], and for U, the bandwidth and μ the same values as in the single-layer case were used. The resulting $\mathrm{Im}\,\chi(\mathbf{Q}, \omega)$ at $\mathbf{Q} = (\pi, \pi, \pi)$ is shown in Fig. 1(c). In Figs. 1(b) and (c), the peaks at $\omega_0 = 0.55t$ would have diverged, if slightly larger values of V_0 were used. Here, the dashed curves are for $V_0 = 0$, corresponding to the pure systems. These results show how the $2\mathbf{k}_F$ impurity scatterings could induce a peak in $\mathrm{Im}\,\chi(\mathbf{Q}, \omega)$ above T_c within an itinerant model. The peak frequency of $\omega_0 = 0.55t$ corresponds to 66 meV, not far from the experimental value of 40 meV. Here, it is also noted that, in addition to the peak at ω_0, the impurity scatterings could induce spectral weight at low frequencies.

In summary, the effect of dilute nonmagnetic impurities on $\mathrm{Im}\,\chi(\mathbf{Q}, \omega)$ was studied in the normal state using the framework of the Hubbard model and the random-phase approximation. It has been pointed out that the $2\mathbf{k}_F$ scattering of the spin fluctuations by the impurities could induce a peak in $\mathrm{Im}\,\chi(\mathbf{Q}, \omega)$ in the normal state of $YBa_2Cu_3O_7$.

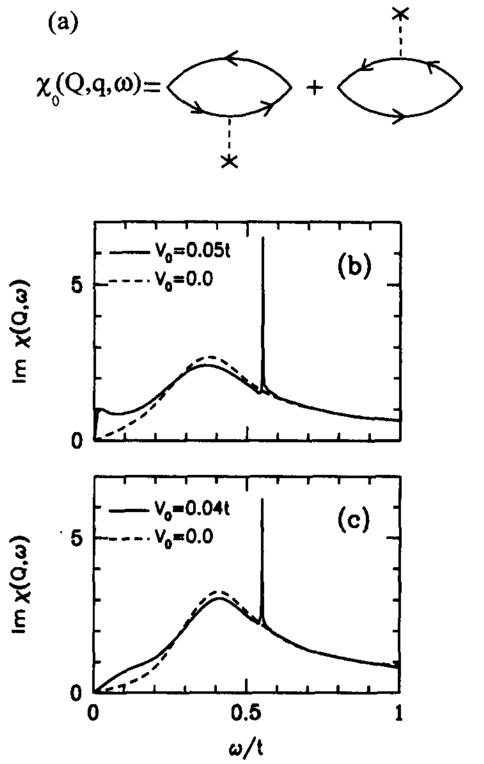

Figure 1. (a) Feynman diagrams representing the lowest-order terms of the irreducible off-diagonal susceptibility $\chi_0(\mathbf{Q}, \mathbf{q}, \omega)$. Frequency dependence of $\mathrm{Im}\,\chi(\mathbf{Q}, \omega)$ for (b) the single-layer and (c) the bilayer CuO_2 models showing the effects of the $2\mathbf{k}_F$ impurity scatterings.

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