Effects of impurities on the magnetic property in copper oxides

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Abstract

We study effects of the nonmagnetic impurities on the magnetic property in the CuO_2 plane of copper oxides. We calculate the spin susceptibility in the normal state, for the CuO_2 plane with nonmagnetic impurities substituted for Cu atoms, on the basis of the d-p model. We take account of the impurity scattering and the Coulomb interaction at each Cu site within the single-site coherent potential approximation and the fluctuation-exchange approximation, respectively. Our result implies that the nonmagnetic impurities suppress the antiferromagnetic spin fluctuations which mediate the superconductivity in high-temperature superconductors.

Key words: spin susceptibility ; impurity ; d-p model ; Green's function methods

Many copper oxides are well-known as high-temperature superconductors (HTSC). They share layered perovskite structures and contain two-dimensional CuO_2 planes in which superconductivity appears below T_c. Regarding HTSC, evidence has accumulated for an anisotropic energy gap most likely of $d_{x^2-y^2}$ symmetry. The effects of the Coulomb-enhanced spin fluctuations are believed to play an essential role in HTSC.

For $d_{x^2-y^2}$ pairing, nonmagnetic impurities in the CuO_2 planes, such as Zn impurity atoms substituted for Cu atoms, destroy the superconductivity and are shown to be pair breakers, producing a finite lifetime for quasiparticles near the nodes and a finite density of states at low energies [1]. It is also known that resonant impurity scattering leads to important effects for the penetration depth [2] and the NMR response [3].

In this paper, we investigate both of effects of Coulomb correlations and the impurity scattering, on the spin susceptibility, within the fluctuation exchange approximation (FLEX) [4] and the single-site coherent potential approximation (CPA) [5] respectively. In order to describe the CuO_2 plane of copper oxides, we adopt the d-p Hamiltonian as follows:

$$
\begin{aligned}
H = &\sum_{\boldsymbol{k},\sigma} \left(d^\dagger_{\boldsymbol{k},\sigma}\ p^{x\dagger}_{\boldsymbol{k},\sigma}\ p^{y\dagger}_{\boldsymbol{k},\sigma} \right) \\
&\times \begin{pmatrix} \epsilon_d & \zeta^x_{\boldsymbol{k}} & \zeta^y_{\boldsymbol{k}} \\ (\zeta^x_{\boldsymbol{k}})^* & \epsilon_p & 0 \\ (\zeta^y_{\boldsymbol{k}})^* & 0 & \epsilon_p \end{pmatrix} \begin{pmatrix} d_{\boldsymbol{k},\sigma} \\ p^x_{\boldsymbol{k},\sigma} \\ p^y_{\boldsymbol{k},\sigma} \end{pmatrix} \\
&+ \frac{U}{N} \sum_{\boldsymbol{k},\boldsymbol{k}'} \sum_{\boldsymbol{q}(\neq 0)} d^\dagger_{\boldsymbol{k}+\boldsymbol{q},\uparrow} d^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\downarrow} d_{\boldsymbol{k}',\downarrow} d_{\boldsymbol{k},\uparrow} \\
&+ \sum_{i,\sigma} u_i d^\dagger_{i,\sigma} d_{i,\sigma}
\end{aligned}
\tag{1}
$$

where $\zeta^{x(y)}_{\boldsymbol{k}} = 2it \sin \frac{k_{x(y)}}{2}$. $u_i = u$, when an impurity is present at $\boldsymbol{r}_i$. We measure the site energy of $d(p)$-orbital $\epsilon_{d(p)}$ from the Fermi level, which is set to zero. The Green's function of d-electron is given by

$$G_d(k) = \frac{i\epsilon_n - \epsilon_p}{(i\epsilon_n - \epsilon_d - \Sigma(k))(i\epsilon_n - \epsilon_p) - V^2_{\boldsymbol{k}}} \tag{2}$$

$$\Sigma(k) = \Sigma^{FLEX}(k) + \Sigma^{CPA}(i\epsilon_n) \tag{3}$$

$$V^2_{\boldsymbol{k}} = 2t^2(2 - \cos k_x - \cos k_y). \tag{4}$$

The self-energy within FLEX is given as follows:

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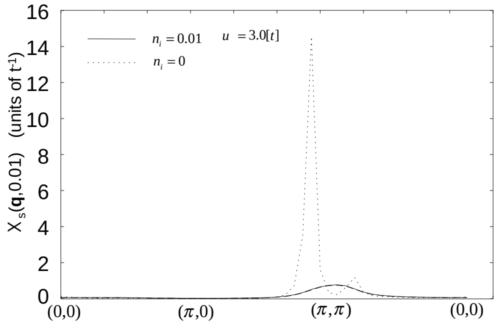

Fig. 1. $\chi_s(\boldsymbol{q}, 0.01)$ at the various concentrations of the impurity, at $T = 0.0047[t]$, for $U = 4.2[t]$, $\epsilon_d = -1.7030[t]$ and $\epsilon_p = -1.9030[t]$.

$$\Sigma^{\rm FLEX}(k) = \frac{1}{N}\sum_k V(k-k')G_d(k') \quad (5)$$

$$V(q) = \frac{3}{2}\frac{U^2\chi(q)}{1-U\chi(q)} + \frac{1}{2}\frac{U^2\chi(q)}{1+U\chi(q)} - U^2\chi(q) \quad (6)$$

$$\chi(q) = -\frac{T}{N}\sum_k G_d(k)G_d(k+q). \quad (7)$$

where $G_d(k)$ is the Green's function of d-electron. The self-consistent equation for the coherent potential $\Sigma^{\rm CPA}$ is

$$n_i \frac{u - \Sigma^{\rm CPA}(i\epsilon_n)}{1 + (\Sigma^{\rm CPA}(i\epsilon_n) - u)\, G_d(i\epsilon_n)} - (1-n_i)\, \frac{\Sigma^{\rm CPA}(i\epsilon_n)}{1 + \Sigma^{\rm CPA}(i\epsilon_n) G_d(i\epsilon_n)} = 0 \quad (8)$$

where n_i is the concentration of the impurity and $G_d(i\epsilon_n) = \frac{1}{N}\sum_{\boldsymbol{k}} G_d(k)$. We solve eqs. 5, 6, 7 and 8, numerically with the Dyson quation, and get G_d that satisfies them. In these calculations, the vertex correction is neglected consistently. From the self-consistent solution, we calculate the spin susceptibility $\chi_s(\boldsymbol{k}, \omega)$ defined by

$$\chi_s(\boldsymbol{q}, \omega) = \frac{\chi(\boldsymbol{q}, \omega)}{1 - U\chi(\boldsymbol{q}, \omega)}. \quad (9)$$

We show the q-dependence of the imaginary part of χ_s at $T = 0.0047[t]$ in Fig. 1. In the case of $n_i = 0$, we see the peak near (π, π). In the case of $n_i \neq 0$, the peak is suppressed. The result implies that impurities suppress the antiferromagnetic spin fluctuations which mediate the superconductivity in HTSC.

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