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Electronic states of high-T_c cuprate in the anomalous metallic regime

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Abstract

By use of the d–p model for cuprate, we investigate the density of states. One of the advantages in our method is to use the retarded propagator matrix which is defined by several composite particles, for example, pure fermion, dressed fermion with local spin fluctuation, and one with global fluctuation between nearest neighbour Cu sites. The shapes of the density of states rapidly change by doping and temperature because the propagator includes new poles and some mean fields which easily change by those external parameters. The competition between the composite states with spin fluctuation may originate from the spin gap formation observed in high-T_c cuprate.

Keywords: High-T_c cuprate; Equation of motion method; Composite operator; Intersite spin correlation

1. Introduction

The most realistic model for cuprate superconductors is the d–p model, where the effect of the Coulomb repulsion is included in the operator algebra of quasi-particles when the model Hamiltonian is written in bi-liner form. The equation of motion technique [1,2] is one of the powerful tools to treat such systems which do not satisfy the standard fermionic anticommutation relation. In this paper, we carry out a careful and systematic expansion of higher order hierarchy, and make it clear how doped holes and spin fluctuation form bound states. Additionally, we show that the appearance of such composite states and the antiferromagnetic spin correlation very strongly controls the shape of the density of states. The competition between the dressed fermion with local spin fluctuation and one with global fluctuation may relate to the spin gap formation observed in high-T_c cuprate.

2. Formulation

Let us consider the d–p model given by

$$H = \int \mathrm{d}^2x \big(\epsilon_p p^\dagger \cdot p + \epsilon_\xi \xi^\dagger \cdot \xi + t(\xi^\dagger \cdot q + q^\dagger \cdot \xi)\big), \qquad (1)$$

where $p = p(x)$ is the annihilation operator of p-hole and $\xi_\sigma = d_\sigma(1 - n_{-\sigma})$ the restricted d-hole operator which fills only the singly occupied state, $q = \alpha(-\mathrm{i}\nabla)p$ with $\alpha(\mathbf{k}) = \sqrt{1 - \alpha'(\mathbf{k})}$, and $\alpha'(\mathbf{k}) = (1/2)(\cos k_x a + \cos k_y a)$.

As the basis vector of the equation of motion, we introduce the following set of quasi-particles

$$\psi = \begin{pmatrix} p \\ \xi \\ \sigma^\mu \delta n_\mu q \\ \xi^\dagger \cdot qq \\ \sigma^\mu (q^\dagger \sigma_\mu q + \delta n_\mu \alpha'(-\mathrm{i}\nabla))\xi \end{pmatrix}, \qquad (2)$$

where $\sigma^\mu \delta n_\mu = \sigma \cdot \mathbf{n} - \delta n$, $n_\mu = \xi^\dagger \sigma_\mu \xi$, $n_0 = n$, and $\mathbf{n} = (n_1, n_2, n_3)$. The coherent peaks near the Fermi level are mainly created by the states ψ_3 (hole doped case) and ψ_5 (electron doped case).

The Fourier transformation of the retarded propagator matrix of ψ is expressed by

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$$S(k) = I(\mathbf{k})\frac{1}{k_0 I(\mathbf{k}) - M(\mathbf{k}) - \delta M(k)}I(\mathbf{k}), \tag{3}$$

where $k = (k_0, \mathbf{k})$, $I = \langle\{\psi, \psi^\dagger\}\rangle$, $M = \langle\{\mathrm{i}\frac{\partial}{\partial t}\psi, \psi^\dagger\}\rangle$, and $\delta M = \langle R\mathrm{i}\frac{\partial}{\partial t}\psi\left(\mathrm{i}\frac{\partial}{\partial t'}\psi\right)^\dagger\rangle_I$ with the symbol I indicating the irreducible part. The spectral weight I and the level energy matrix M include the $\chi'_s = \langle \mathbf{n}\cdot\mathbf{n}\rangle$ with $\mathbf{n}' = \alpha'(-\mathrm{i}\nabla)\mathbf{n}$. This order parameter gives a criterion about the singlet formation and is one of the most important quantities in numerical simulation. The higher order operators form the irreducible parts of the lower ones, for example, we have

$$\left(\mathrm{i}\frac{\partial}{\partial t} - \epsilon_p\right)\psi_3 = \langle n\rangle\xi - 4\psi_4 - \psi_5. \tag{4}$$

In this case, the correction $\delta M_{33}(k)$ completely vanishes.

In the dynamical correction $\delta M(k)$, we consider the following type of retarded function:

$$\delta M_\phi(x - x') = \langle R\phi(x)\phi^\dagger(x')\rangle_I, \tag{5}$$

where

$$\phi(x) \sim \int \mathrm{d}y^2\alpha'(x - y)m_i(x, y)\sigma_i q(y), \tag{6}$$

$$m_i(x, y) = i\epsilon_{ijl}n_j(x)n_l(y). \tag{7}$$

We treat this function by loop decomposition. The detail will be discussed elsewhere. The next section will be devoted to the result of the numerical calculation.

3. Result

We perform self-consistent calculation to determine some mean fields in I and M, for example $a = \langle qq^\dagger\rangle$, $b = \langle\xi q^\dagger\rangle$, $a_s = \langle n_i\sigma_i qq^\dagger\rangle$ and so on. In Fig. 1, the calculated densities of states for holes are shown. The model parameters are set as $t = 1$ (eV), $\Delta = \epsilon_p - \epsilon_\xi = 1.2t$ and $T = 0.05t$. The hole doping rate is 10%. The Fermi level is chosen as the origin of the energy. When the intersite spin correlation χ'_s is neglected, the result is given by Fig. 2. By the effect of the intersite spin correlation, the ingap state near the Fermi level becomes double peak structure. The appearance of the center peak around ϵ_p directly combines with the introduction of the composite state ϕ. The relative spin flip between neighbouring Cu ions m_i plays important role in this calculation. The reason is very simple in the equation of motion scheme. The structure of the equation of motion for ϕ is quite resemble to that for ψ_3, and the coupling constant between them is also very strong. The order of the magnitude of pseudogap between these spectra is expected to be of order J. However the magnitude is overestimated in the present numerical calculation.

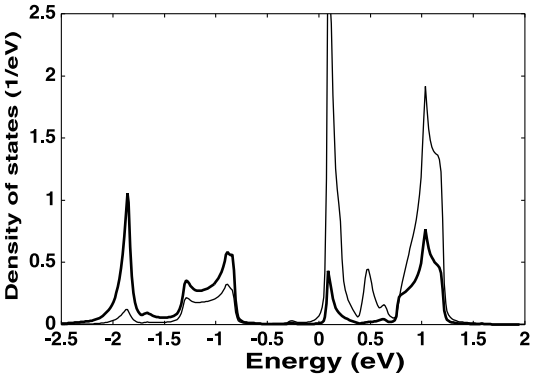

Fig. 1. The densities of states are illustrated. The fine solid line is for d-hole and the bold line is for p-hole.

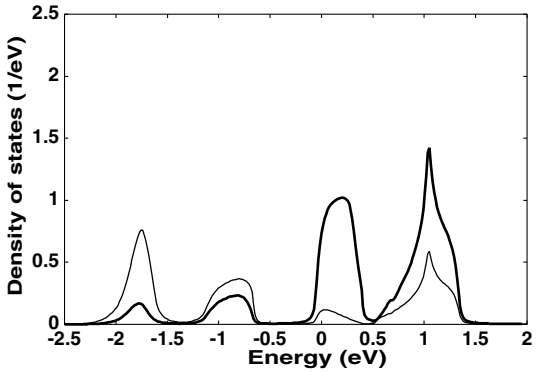

Fig. 2. The densities of states for p and d holes without intersite effect.

In this paper, we have shown that the double peak structure near the Fermi level in the density of states is constructed by the composite operator ϕ and the intersite effect plays dominant role in this system. More careful treatment of ϕ and higher order terms of M may improve the approximation.

References

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