Electronic states around a vortex core in high-$T_c$ superconductors based on the $t$-$J$ model

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Electronic states around vortex cores in high-$T_c$ superconductors are studied using the two-dimensional $t$-$J$ model in order to treat the $d$-wave superconductivity with short coherence length and the antiferromagnetic (AF) instability within the same framework. We focus on the disappearance of the large zero-energy peak in the local density of states observed in high-$T_c$ superconductors. When the system is near the optimum doping, we find that the local AF correlation develops inside the vortex cores. However, the detailed doping dependence calculations confirm that the experimentally observed reduction of the zero-energy peak is more reasonably attributed to the smallness of the core size rather than to the AF correlation developed inside the core. The correlation between the spatial dependence of the core states and the core radius is discussed.

There are several experimental results in high-$T_c$ superconductors which have not been explained in the conventional BCS $d_{x^2-y^2}$-wave superconductivity. The electronic structure inside the vortex core is one of the most interesting issues among them. The conventional theory for $d$-wave vortices based on Bogoliubov-de Gennes (BdG) mean-field theory predicts a large and broad peak at the Fermi energy in the local density of states (LDOS), so-called zero-energy peak (ZEP), at the vortex core. However, scanning tunneling spectroscopy (STS) spectrum in one of the high-$T_c$ materials, BSCCO, giving directly the LDOS around the vortex core, shows only a small-double peak structure at energies $\pm 7$ meV. A similar situation was also observed in YBCO compounds.

To resolve this discrepancy, there have been proposed several theoretical attempts, that is, a $d_{x^2-y^2} + s$ state, a $d_{x^2-y^2} + id_{xy}$ state, an antiferromagnetic (AF) vortex core, a staggered flux state, and a vortex core with small $k_F \xi_0$ where $k_F$ is the Fermi wave number and $\xi_0$ is the coherence length. These theories are, in greater or lesser degree, based on strongly correlated effects. Among them, we consider the AF vortex core and the effects of small $k_F \xi_0$ (the small vortex core) because they have some experimental grounds mentioned below.

The AF vortex core was first predicted using a phenomenological Ginzburg-Landau theory assuming the SO(5) symmetry. Later this possibility was confirmed in a microscopic calculation assuming the $t$-$J$ model, it was shown that the AF core is stabilized near the doping rate $\delta \sim 0.1$, where the system is close to the AF instability. Simultaneously it was observed that the electron density approaches half-filling inside the AF core. After these calculations, there are several experimental studies suggesting the existence of the enhancement of AF correlations or AF vortex core, such as neutron scattering experiments in LSCO compounds near optimal doping, $\mu$SR experiments in underdoped or near-optimally doped YBCO. Therefore it seems natural that the AF vortex core is also realized in the BSCCO sample which is optimum doped or slightly overdoped, and that the absence of the large ZEP is due to the mean-field AF gap (or Mott gap) developed inside the core.

Actually some theoretical studies for the AF vortex core have predicted the LDOS without the ZEP or at least, large-double peak structure.

The double peak structure is also found in the small vortex cores (small $k_F \xi_0$) by using the BdG equations for continuum $d$-wave model. In fact, the STM/S data has revealed that a radius for the vortex core in BSCCO is on the order of 10˚A, which is consistent with the short coherence length. Therefore, the small vortex core is also a possible explanation for the absence of the ZEP, but the lattice effects, which play an important role when $k_F \xi_0$ is small, need to be clarified.

Motivated by these backgrounds, in this paper we perform a detailed study on the electronic states around vortex cores in high-$T_c$ superconductors, taking account of the discrete lattice effects, smallness of the vortex core, and the AF instability. To investigate their effects within the same framework, we use the $t$-$J$ model which has a phase diagram consistent with experiments and enables us to study the reasonable doping dependence. We find that the reduction of ZEP is more reasonably attributed to the smallness of the core size rather than to the AF correlation developed inside the core. It is remarkable that a simple-minded picture of AF core does not play important roles in the suppression of LDOS.

The Hamiltonian of the $t$-$J$ model is written as

$$\mathcal{H} = - \sum_{(i,j), \sigma} P_G (t_{ij} c_{i\alpha}^\dagger c_{j\sigma} + \text{h.c.}) P_G$$
\[ + J \sum_{i,j} S_i \cdot S_j - \mu \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} \]  

in the standard notation where \((i,j)\) means the summation over nearest-neighbor pairs. The Gutzwiller’s projection operator \(P_G\) is defined as \(P_G = \Pi_s (1 - n_i \uparrow n_i \downarrow)\). The uniform magnetic field is introduced in terms of Peierls phase of the hopping term as \(t_{ij} = t \exp \left( \frac{\hbar}{2m} J^I \cdot A \cdot dr \right)\). The BdG equation based on the extended Gutzwiller approximation is

\[
\begin{pmatrix} H_{ij} \delta_{ij} & F_{ij}^* \delta_{ij} \\ F_{ji}^* \delta_{ij} & -H_{ji} \delta_{ij} \end{pmatrix} \begin{pmatrix} \nu_i^\alpha \\ \nu_i^\dot{\alpha} \end{pmatrix} = E^\alpha \begin{pmatrix} \nu_i^\alpha \\ \nu_i^\dot{\alpha} \end{pmatrix},
\]

with

\[
H^\sigma_{ij} = -\sum_{\tau} \left( t^H_{ij} + J^H_{ij} \chi_{ji} \right) \delta_{ij, i+\tau} + \sigma \delta_{ij} \sum_{\tau} h^H_{i, i+\tau} - \mu \delta_{ij},
\]

\[
F_{ij}^* = -\sum_{\tau} J^H_{ij} \chi_{ij} \delta_{ij, i+\tau},
\]

where \(i + \tau\) represents the nearest neighbor sites of the site \(i\), and \(\sigma = \pm 1\). The renormalized parameters \(t^H_{ij}\), \(J^H_{ij}\) and \(h^H_{ij}\) are determined from cluster calculations which reproduce the variational Monte Carlo results. They have the following forms:

\[
t^H_{ij} = g_t(i,j) t_{ij}, \quad J^H_{ij} = \frac{1}{2} \tilde{g}_{zy}^s(i,j) J + \frac{1}{4} g_{z}^s(i,j) J,
\]

\[
h^H_{ij} = \frac{1}{2} \tilde{g}_{\sigma}^s(i,j) J m_j + \frac{\partial \langle H_{ij} \rangle}{\partial m_i},
\]

where \(g_t(i,j), \tilde{g}_{z}^s(i,j)\) and \(g_{z}^s(i,j)\) depend on the local expectation values \(\chi_{ij} = \langle c^{\dagger}_{i\uparrow} c_{j\downarrow} \rangle\), \(\delta_{ij} = \langle c^{\dagger}_{i\sigma} c_{j\sigma} \rangle\), and \(m_i = \frac{1}{2} (n_{i\uparrow} - n_{i\downarrow})\). For example,

\[
g_{z}^s(i,j) = \left( \frac{2(1 - \delta_{ij})}{1 - \delta_{ij} + 4m_{ij}} \right)^2 \cdot a_{ij}^{-1},
\]

where \(\delta_{ij} (m_{ij})\) is an average of hole density (AF moment) for the corresponding bond and \(a_{ij}\) is a factor close to one which depends on \(\Delta_{ij}, \chi_{ij}, \delta_{ij}\) and \(m_{ij}\). These somewhat complicated renormalized parameters are necessary for treating the AF and d-wave superconductivity in the same framework. If one uses simple slave-boson mean-field theories, the AF order parameter is overestimated and one cannot discuss the AF vortex core because the AF order exists even in the bulk. In the present method, AF order does not exist away from the core for \(\delta \geq 0.10\), which is consistent with the numerical results.

To make the Peierls phase compatible with vortex lattice symmetry, we need a magnetic unit cell with \(2N \times N\) sites including two vortices. In this case, by the appropriate choice of gauge, the order parameter \(\Delta_{ij}\) has a translational symmetry with respect to the magnetic unit cell. Here we take \(N = 22-26\). We solve numerically the BdG equation and carry out an iteration until \(\Delta_{ij}, \chi_{ij}, \delta_{ij}\) are determined self-consistently. We take \(J/t = 0.3\) and examine the various values of the doping rates \(\delta = 0.10-0.15\), that is, from near optimum doped to overdoped region.

![FIG. 1: (a) Spatial dependence of the amplitude of d-wave (upper) and s-wave (lower) components of the superconducting order parameter around the vortex core. The doping rate is \(\delta = 0.15\). (b) The hole density \(n_i^\uparrow\). (c) The LDOS obtained at the vortex core center (the thick line) and obtained without the magnetic field (the thin line).](image)

First, let us look at the results for the overdoped region. Figure 4 shows the superconducting order parameters, the hole density, and the LDOS obtained around the vortex core for \(\delta = 0.15\). We can see the common features found in several theoretical studies within the weak-coupling d-wave superconductivity, that is, fairly large vortex cores, slightly induced s-wave component, the increase of the hole density inside the core, and the ZEP in the LDOS. We note that the local AF order inside the core does not exist in this case.

The situation drastically changes when the system approaches the optimum doping. Figure 2 shows the results for \(\delta = 0.11\) in the same manner as in Fig. 1. Similar results for \(\delta = 0.10\) have been shown before, but here much larger system-size is achieved. From Fig. 2 we can see that the size of the vortex core is fairly small, that is, the core having a radius of about 3 lattice spacings is realized. The magnitude of the induced s-wave component is also small as in the case of \(\delta = 0.15\). Figure 2(b) shows the spatial dependences of the local AF moment \(|m_i|\) and of the hole density \(n_i^\uparrow\). It is found that AF correlation develops and the hole density decreases inside the vortex.
FIG. 2: (a) Spatial dependence of the amplitude of $d$-wave (upper) and $s$-wave (lower) components of the superconducting order parameter around the vortex core. The doping rate is $\delta = 0.11$. (b) The hole density $n_h$ (upper) and local antiferromagnetic moment (lower). (c) The LDOS obtained at the vortex core center (the thick line) and obtained without the magnetic field (the thin line).

core, in sharp contrast with the $\delta = 0.15$ case shown in Fig. 1. We should note here that the AF moment extends outside the core, which is consistent with experiments.

The LDOS obtained at the center of the vortex core is shown in Fig. 2(c). We can see that the LDOS shows neither the ZEP nor an explicit double-peak structure. To clarify the effect of the local AF moment on the LDOS, we solve the BdG equations without AF order parameter for the same doping rate $\delta = 0.11$, as shown in Fig. 3. The LDOS obtained here (Fig. 3(b)) is quite similar to that shown in Fig. 2(c), but at this time, a small peak can be found at $E \sim 0$. This peak is regarded as a trace of the ZEP. The only effect of the presence of AF order parameter is to annihilate the small peak at $E \sim 0$.

We have confirmed that the spatial dependence of the amplitude of $d$- and $s$-wave components, and the hole density (Fig. 3(a)) are quite similar to those shown in Fig. 2(a) and (b).

From this comparison, we speculate as follows. The overall reduction of the spectral weight inside the vortex core already occurs without AF order parameters. Therefore this reduction is not due to the presence of the AF moment but due to the smallness of the core. For this doping rate ($\delta = 0.11$), the hole density inside the core decreases. This causes the appearance of the AF vortex core found in Fig. 2(b), but the effect of the AF core is subsidiary for the LDOS.

FIG. 4: The LDOS as a function of energy $E/t$ and distance $r/a$ from the vortex core center, where $a$ is the lattice constant. The range of the energy is $-0.3 \leq E/t \leq 0.3$.

In order to clarify the origin of the reduced spectral weight of ZEP due to the smallness of the core, we study the spatial dependence of the LDOS for several hole dopings. Figure 4 shows the LDOS at $\delta = 0.15, 0.12$ and 0.11 as a function of energy $E/t$ and distance $r/a$ from the vortex core center, with $a$ being the lattice constant. Here the distance dependence is plotted from the vortex core center ($r = 0$) along the $(1,0)$ direction of the square lattice. First we look at the result for $\delta = 0.15$ shown in Fig. 4(a). As $r/a$ increases from 0, the ZEP first becomes broader and smaller, then split into two peaks for $r/a \geq 3$. This kind of behavior of the LDOS, that is, the splitting of the ZEP away from the vortex core center, has been reported for $s$-wave vortex cores by Gygi and
They have shown that, in the s-wave case, the two peaks found away from the vortex core center correspond to the electronic bound states (core states) having higher angular momentum $\mu$. The angular momentum is quantized such that $\mu = m + \frac{1}{2}$ where $m$ is an integer. For small $\mu$, the energy eigenvalues of the core states are known to have the approximate dispersion relation $E_\mu \sim \omega_0 \mu$ where $\omega_0$ is an energy quantum. In a semiclassical sense, the vortex core states have maximum amplitude at a distance $r \sim \mu/p_F$ from the vortex core center. Of course in d-wave superconductors, the angular momentum is not conserved in a strict sense because axial symmetry is broken. Quite recently, however, it has been pointed out that there is an alternative quantum number in d-wave superconductors which corresponds to the angular momentum. Therefore the distance dependence of the splitting amplitude of ZEP shown in Fig. 4 indicates the dispersion relation of the core states: i.e., $E_\mu \sim \omega_0 \mu$. At $\delta = 0.12$ shown in Fig. 4(b), the splitting of the ZEP exists even at $r/a = 1$, that is, the ZEP can be seen only at the vortex core center. Note that the AF moment is not induced for this case. Comparing the results in Figs. 4(a) and (b), we find that the slope of the dispersion relation becomes greater as the doping rate $\delta$ decreases. This greater slope corresponds to larger $\omega_0$ or larger interlevel spacing of the core states, which is probably caused by the decrease of the core size. As the doping rate decreases further ($\delta = 0.11$), the LDOS around $E \sim 0$ is significantly reduced as shown in Fig. 4(c).

Finally let us comment on the effects of the next-nearest-neighbor hopping $t'$. The critical value of $\delta$ where the AF core appears depends on the value of $t'$ which re-enforces our viewpoint. For some values of $t'$, the AF core is realized even when the size of the vortex core is not so small. In this case, the spectral weight of the ZEP is not reduced owing to the large size of the vortex core, and there appears a large double peak structure in the LDOS caused by the presence of the AF moment. This, however, does not explain the reduction of the spectral weight inside the vortex observed in YBCO or BSCCO.

In summary, we have investigated the electronic states around vortex cores in high-$T_c$ superconductors based on the t-J model. The induced local AF moment and the LDOS without ZEP are found inside the vortex cores. However, the origin of the absence of ZEP is mainly due to the smallness of the vortex core sizes, which can be understood within the conventional BdG theory with short coherence length. We find that the doping dependence is very important and thus it is quite interesting to study the overdoped region or low-$T_c$ superconductors experimentally, in which the vortex core size is large and the ZEP with the spatial dependence as shown in Fig. 4(a) will be observed.

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[31] We notice that the sudden change of the LDOS is due to the appearance of staggered flux state inside the core which is caused by the smallness of the core and reduction of the hole density. This is consistent with the recent work by P. A. Lee (private communication).