Quasiparticle States at a \(d\)-Wave Vortex Core in High-\(T_c\) Superconductors: Induction of Local Spin Density Wave Order

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The local density of states (LDOS) at one of the vortex lattice cores in a high \(T_c\) superconductor is studied by using a self-consistent mean field theory including interactions for both antiferromagnetism (AF) and \(d\)-wave superconductivity (DSC). The parameters are chosen in such a way that in an optimally doped sample the AF order is completely suppressed while DSC prevails. In the mixed state, we show that the local AF-like SDW order appears near the vortex core and acts as an effective local magnetic field on the quasiparticles. As a result, the LDOS at the core exhibits a double-peak structure near the Fermi level that is in good agreement with the STM observations on YBCO and BSCCO. The presence of local AF order near the vortex core is also consistent with the recent neutron scattering experiment on LSCO.

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The quasiparticle states at the vortex core in the mixed state of a superconductor have been one of the major interest in condensed matter physics. For an \(s\)-wave superconductor, the energy gap opened at the Fermi surface is a constant and it was predicted long time ago by Caroli et al. \[1\] that there should exist the low-lying bound quasiparticle states inside an \(s\)-wave vortex core. This prediction was later confirmed by detailed numerical computations \[2,3\] and by STM experiments on NbSe\(_2\) \[4\] although a direct observation of the discrete levels is yet to be performed. However, for a \(d\)-wave pairing state as recently established in high-\(T_c\) cuprates, the situation becomes more complex, mostly due to the fact that the energy gap is closed at the nodal direction on the essentially cylindrical Fermi surface. In an earlier study by Wang and MacDonald based on a lattice model \[5\], it was shown that the local density of states (LDOS) at the \(d\)-wave vortex core exhibits a single broad peak at zero energy. Recent low temperature STM experiments on YBa\(_2\)Cu\(_3\)O\(_7\) (YBCO) \[6\](a) and Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_8\) (BSCCO) \[7\] both observed a double-peak structure around zero bias in the local differential tunneling conductance at the vortex core center, which identifies the widely split core states at energies \(\pm 5.5\) meV and \(\pm 7\) meV, respectively. The discrepancy between the theory and the experiment stimulated further theoretical studies \[8,9\] on the quasiparticles in the vortex core of high-\(T_c\) cuprates. Franz and Tésonović \[10\] proposed an explanation of the observed double-peak structure in terms of a mixed \(d_{x^2+y^2}+id_{xy}\) pairing state. Such a pairing state was previously suggested \[11\] to be realized through the field-induced second phase transition as motivated by the observation of a plateau in thermal conductivity \[12\]. The origin of this plateau is still hotly debated \[13\]. By pointing out that the parameter values are unrealistically chosen in Ref. \[10\] that the \(d_{x^2+y^2}+id_{xy}\) state even already exists in zero magnetic field, Yasui and Kita \[14\] applied the “Landau-level expansion method” to study the quasiparticles in \(d\)-wave vortex lattice based on the continuum model. They found that the double-peak structure may be considered as inherent to systems with short coherence length. Since the splitting sensitively depends on the field strength, the validity of this scenario still needs to be clarified theoretically and experimentally. On the other hand, the superconducting vortex with antiferromagnetic (AF) core was also predicted based on either the SO(5) theory \[15\] or the standard \(t-J\) model with spin-charge separation \[16\], which leads to a featureless LDOS and is in disagreement with the STM data on the optimally doped YBCO \[6\](a) and BSCCO \[7\]. Partly motivated by the observation of magnetic vortex cores in recent neutron scattering experiment by Lake \textit{et al.} \[17\] on optimally doped La\(_{2−x}\)Sr\(_x\)CuO\(_4\), we present in this Letter an alternative mechanism for the double-peak structure in the LDOS around zero energy. We show that due to electron correlations, the AF-like spin density wave (SDW) order can develop locally around the vortex core and vanish in the superconducting regions. The lift of the spin degeneracy leads to the splitting of the zero energy peak. The induced SDW order around the vortex core manifests the repulsive electron interaction responsible for the strong spin fluctuations in the underdoped region of high-\(T_c\) cuprates. In fact, the coexistence of superconducting (SC) and SDW orders has been theoretically studied \[18,19\], which shows a rich phase diagram with a classic AF order at half filling, striped phase at underdoping, and \(d\)-wave SC at optimal doping.

We start with a generalized Hubbard model defined on two dimensional (2D) lattice. By assuming that the on-site repulsion is solely responsible for the antiferromagnetism while the nearest neighbor attraction causes the \(d\)-wave superconductivity, we can construct an effective mean-field (MF) model \[20\] to study the vortex physics in the mixed state:
Here $c_{i\sigma}$ annihilates an electron of spin $\sigma$ at site $i$. The summation is over the nearest neighbor sites. $\mu$ is the chemical potential. $m_{i,\sigma} = U(c_{i\sigma}^\dagger c_{i\sigma})$ is the spin-dependent Hartree-Fock potential at site $i$, where $U$ is the strength of on-site repulsion. $\Delta_{ij} = \frac{1}{2}(c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow})$ is the spin-singlet $d$-wave pair potential, where $V$ is the strength of nearest neighbor effective electron-electron attraction. As a phenomenological model, we do not intend to address the microscopic mechanism for this attraction. In the mixed state, the magnetic field effect was included through the Peierls phase factor $\varphi_{ij} = \frac{2\pi}{\Phi_0} \int_{ij}^i A(r) \cdot dr$, where $\Phi_0 = \hbar c/2e$ is the superconducting flux quantum. By assuming the superconductor under consideration is in the extreme type-II limit where the Ginzburg-Landau parameter $\kappa = \lambda/\xi$ goes to infinity so that the screening effect from the supercurrent is negligible. Therefore, the vector potential $A$ can be approximated by the solution $\nabla \times A = Hz$ where $H$ is the magnetic field externally applied along the $c$ axis. The enclosed flux density within each plaquette is given by $\sum_{ij} \varphi_{ij} = \frac{2\pi H a^2}{\Phi_0}$. A similar mean-field Hamiltonian can also be arrived at within a $t$-$U$-$J$ model proposed recently [2].

We diagonalize the Hamiltonian Eq. [1] by solving the BdG equation:

$$\sum_j \begin{pmatrix} \mathcal{H}_{ij,\sigma} & \Delta_{ij}^* \\ \Delta_{ij} & -\mathcal{H}_{ij,\sigma}^* \end{pmatrix} \begin{pmatrix} u_{i\sigma} \cr v_{i\sigma} \end{pmatrix} = E_n \begin{pmatrix} u_{i\sigma} \cr v_{i\sigma} \end{pmatrix}, \eqno(2)$$

where $(u_{i\sigma}, v_{i\sigma})$ is the quasiparticle wavefunction corresponding to the eigenvalue $E_n$, the single particle Hamiltonian $\mathcal{H}_{ij,\sigma} = -t(c_{i\sigma}^\dagger c_{j\sigma}) + (m_{i,\sigma} - \mu)\delta_{ij}$. Notice that the quasiparticle energy is measured with respect to the Fermi energy. The self-consistent conditions read:

$$m_{i,\sigma} = U \sum_n |u_{i\sigma}^n|^2 f(E_n), \eqno(3)$$

and

$$\Delta_{ij} = \frac{V}{4} \sum_n (u_{i\uparrow}^n v_{j\downarrow}^n + v_{i\uparrow}^n u_{j\downarrow}^n) \tanh \left( \frac{E_n}{2k_B T} \right), \eqno(4)$$

where the Fermi distribution function $f(E) = 1/(e^{E/k_BT} + 1)$. Here the summation is also over those eigenstates with negative eigenvalues thanks to the symmetry property of the BdG equation: If $(u_{i\uparrow}^n, u_{i\downarrow}^n, v_{i\uparrow}^n, v_{i\downarrow}^n)^{\text{transpose}}$ is the eigenfunction of the $4 \times 4$ equation in the spin space with energy $E_n$, then $(v_{i\uparrow}^n, -u_{i\uparrow}^n, -v_{i\downarrow}^n, u_{i\downarrow}^n)^{\text{transpose}}$ up to a global phase factor is the eigenfunction with energy $-E_n$.

Hereafter we measure the length in units of the lattice constant $a$ and the energy in units of the hopping integral $t$. Within the Landau gauge the vector potential can be written as $A = (-Hy, 0, 0)$ where $y$ is the $y$-component of the position vector $r$. We introduce the magnetic translation operator $\mathcal{T}_{mnr} = r + R$ where the translation vector $R = m_N x_0 e_\lambda + n_N y_0 e_\eta$ with $N_x$ and $N_y$ the linear dimension of the unit cell of the vortex lattice. To ensure different $\mathcal{T}_{mn}$ to be commutable with each other, we have to take the strength of magnetic field so that the flux enclosed by each unit cell has a single-particle flux quantum, i.e. $2\Phi_0$. Therefore, the translation property of the superconducting order parameter is $\Delta(\mathcal{T}_{mn}) = e^{i\chi(r,R)} \Delta(r)$ where the phase accumulated by the order parameter upon the translation is $\chi(r,R) = \frac{2\pi}{\Phi_0} A(R) \cdot r - 4\pi n n_0$. From this property, we can obtain the magnetic Bloch theorem for the wavefunction of the BdG equations:

$$\begin{pmatrix} u_{k,\sigma}(\mathcal{T}_{mn} \hat{r}) \\ v_{k,\sigma}(\mathcal{T}_{mn} \hat{r}) \end{pmatrix} = e^{i\mathbf{k} \cdot \hat{r}} \begin{pmatrix} e^{i\chi(r,R)/2} u_{k,\sigma}(\hat{r}) \\ e^{-i\chi(r,R)/2} v_{k,\sigma}(\hat{r}) \end{pmatrix}. \eqno(5)$$

Here $\hat{r}$ is the position vector defined within a given unit cell and $k = \frac{2\pi}{M_x N_y} \frac{e}{\mathcal{I}_x} + \frac{2\pi}{M_y N_x} \frac{e}{\mathcal{I}_y}$ with $m_{x,y} = 0, 1, \ldots, M_{x,y} - 1$ are the wavevectors defined in the first Brillouin zone of the vortex lattice and $M_x N_x$ and $M_y N_y$ are the linear dimension of the whole system. The vortex carrying the flux quantum $hc/2e$ is the generic feature of the pairing theory for superconductivity. Therefore, it is not surprising that in the slave boson approach to the $t$-$J$ model, the vortex always carries $hc/2e$ flux quantum if the magnetic field is assumed [13] to act on electrons only through the spinon degrees of freedom.

As a model calculation, we take the following parameter values: The pairing interaction is $V = 1.0$, and the filling factor, which is defined as $n_f = \sum_{i,\sigma} (c_{i\sigma}^\dagger c_{i\sigma})/N_x N_y$ with the summation over one unit cell, is fixed to be 0.84 so that the chemical potential needs to be adjusted each time the on-site repulsion $U$ is varied. For our interest in the low energy quasiparticle states, we only consider the zero temperature limit. We have typically considered the unit cell of size $N_x \times N_y = 42 \times 21$, and the number of the unit cells $M_x \times M_y = 21 \times 42$. This choice will give us a square vortex lattice. We use exact diagonalization method to solve the BdG equation [12] self-consistently: To allow the inhomogeneity of all physical quantities, randomly distributed $\Delta_{ij}$ and $m_{i,\sigma}$ are taken as initial parameters; the newly obtained $\Delta_{ij}$ and $m_{i,\sigma}$ are then substituted back into the equation. The above procedure is repeated until the convergence with required accuracy is achieved. In the absence of magnetic field, we have reproduced the results reported in previous work [12] including an AF SDW order, a stripe phase, and a $d$-wave SC phase when the system is doped away from the undoped to the optimally doped region. In the present work, we are
mainly concerned with the electronic structure around the vortex core in the optimally doped region. In this region, the SDW order is strongly suppressed and the d-wave SC order is homogeneous in real space. However, when a magnetic field is applied to drive the system into the mixed state so that the d-wave order parameter is suppressed around the vortex core, we find that as the on-site repulsion is increased to about 1.5, the SDW order is nucleated around the vortex core. Typical results on the nature of the vortex core is displayed in Fig. 1 with the on-site repulsion $U = 2$. As shown in Fig. 1(a), each unit cell accommodates two superconducting vortices each carrying a flux quantum $\hbar c/2e$. The d-wave SC order parameter vanishes at the vortex core center and starts to increase at the scale of the coherence length $\xi_0$ to its bulk value which is about 0.1 for the chosen parameter values. Fig. 1(b) displays the spatial distribution of the staggered magnetization of the local SDW order as defined by $M_x = (-1)^i S_{x,i}^z$ with $S_{x,i}^z = n_{i\uparrow} - n_{i\downarrow}$. Clearly, the maxima strength of $M_x$ appears at the vortex core center and decays also with a scale of $\xi_0$ to zero into the superconducting region. More interestingly, the SDW order parameters has opposite polarity around two nearest neighbor vortices along the $x$ direction. We have compared the free energy between this configuration with that obtained by switching the orientation of the SDW order around one of the two nearest neighbor vortices, and found that the free energy for both configurations is very close but it is always lower in the former case. Therefore, the induction of the SDW order around the vortices reduces the four-fold rotational symmetry of the whole system to the two-fold, and the period of the translational symmetry of the vortex lattice along the $x$ is doubled. This result is understandable when we notice the zero-field result [23]: The homogeneous superconducting order in the optimally doped region derives from the melting of the strongly overlapped quasi-one dimensional (Q1D) superconducting stripes (i.e, soliton-like AF anti-phase domain boundaries, at which the AF SDW order changes sign). The development of the Q1D stripes breaks at the beginning the four-fold rotational symmetry of the system. Therefore, it seems that the development of the local SDW order around the vortices in the optimally doped region can be regarded as a duality of the development of the local SC order around the AF stripe in the underdoped region. On the other hand, the appearance of the SDW order around the vortex strongly affects the electron density $n_i = \sum_{\sigma} n_{i\sigma}$. As shown in Fig. 1(c), at the vortex core center, where the SDW amplitude reaches the maximum, the electron density is strongly enhanced and is very close to unity, which is characteristic of the bulk AF-like SDW order at the half filling. Therefore, the hole charge density is depleted in the vortex core center. The depletion of the hole charges near the vortex core center is compensated by the corresponding enhancement along $\pi/4$ and $3\pi/4$ directions with respect to the underlying crystal lattice, which correspond to the nodal directions on the Fermi surface. This kind of charge inhomogeneity is closely related to the development of the local SDW order around the vortex core due to the large on-site repulsion. Finally, with the chosen parameter values, we also find that when the on-site repulsion $U$ is increased to 3.5, the SC vortex state is collapsed and the SDW order becomes dominant. Our numerical analysis seems to be consistent with the recent result [23] of the magnetic field driven quantum phase transition from the SC state into a state with microscopic coexistence of SC and SDW orders to understand the recent neutron scattering experiments [49]. Notice that the quantum fluctuation of the SDW order parameter, which plays an important role in addressing correctly the spin excitations, has been neglected in the present model because our interest is in the quasiparticle states.

We now turn our attention to the quasiparticle state at the vortex core center. The local density of states is defined by

$$\rho_i(E) = -\frac{1}{M_x M_y} \sum_{k,n,\sigma} |u_{k,i,\sigma}|^2 f(E_{k}^n - E), \quad (6)$$

where $f(E)$ is the derivative of the Fermi distribution function. $\rho_i(E)$ is proportional to the local differential tunneling conductance which could be measured by STM experiments [23]. In Fig. 3 we plot the LDOS as a function of energy at the vortex core center for different values of on-site repulsion. For comparison, we have also displayed the LDOS at the midpoint between two nearest-neighbor vortices along the $x$ direction, which resembles that for the bulk system. The asymmetry line shape in $\rho_i(E)$ with respect to zero energy reflects the lack of particle-hole symmetry as the chemical potential $\mu$ deviates from zero for $n_f$ being less than the half filling ($n_f = 1$). As can be seen from Fig. 3(a), when $U = 0$ for which no local SDW order is induced, the LDOS at the core center shows a single resonant peak around the Fermi energy, which is similar to that reported by other authors [49]. When $U$ is sufficiently large that the local SDW order develops around the vortex core, the LDOS peak at zero energy is split into a double-peak structure (see Fig. 3(b)). The splitting comes from the fact: When the SDW order is localized around the vortex center, the spin-dependent potential, which can be rewritten as $n_{i\uparrow(\downarrow)} = U(n_{i\uparrow} \pm S_i^z)/2$, plays the role of a local magnetic field interacting with the electrons via the Zeeman coupling. When $U$ is increased, $S_i^z$ at the vortex core center is enhanced, and the combination of them enlarges the Zeeman interaction. As a consequence, the LDOS peak at zero energy is further split (see Fig. 3(c)). This splitting of the LDOS at the vortex core center is in good agreement with the STM experiments on the optimally doped YBCO and BSCCO. The induction of the
local AF order at the vortex core is consistent with recent neutron scattering experiment on LSCO [19].

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FIG. 1(a) Zhu et al.
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FIG. 2 Zhu et al.