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 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). In a zero-field optimally doped sample the AF order is completely suppressed while DSC prevails. In the mixed state, we show that the local AF-like spin density wave order appears near the vortex core and acts as an effective local magnetic field on electrons via Zeeman coupling. As a result, the LDOS at the core exhibits a double-peak structure near the Fermi level that is in good agreement with recent scanning tunneling microscopy observations.

The quasiparticle states at the vortex core in the mixed state of a superconductor have been one of the major interests in condensed matter physics. For an *s*-wave superconductor, the energy gap opened at the Fermi surface is a constant and it was predicted a 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 [2–4] and by scanning tunneling microscopy (STM) experiments on NbSe$_2$ [5]. 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 [6] 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$_{7-\delta}$ (YBCO) [7(a)] and Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO) [8] both observed a double-peak structure around zero bias in the local differential tunneling conductance at the vortex core center. The discrepancy between the theory and the experiment stimulated further theoretical studies [9–13] on the quasiparticles in the vortex core of high-T_c cuprates. Franz and Tešanović [11] 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 [14] to be realized through the field-induced second phase transition as motivated by the observation of a plateau in thermal conductivity [15]. The origin of this plateau is still hotly debated [16]. Alternatively, Yasui and Kita [13] pointed out 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. On the other hand, an insulating antiferromagnetic (AF) vortex core predicted based on either the SO(5) theory [17] or the standard *t*-*J* model with spin-charge separation [18] is inconsistent

with the STM observations. Partly motivated by the observation of magnetic vortex cores in a recent neutron scattering experiment by Lake *et al.* [19] on optimally doped La$_{2-x}$Sr$_x$CuO$_4$ (LSCO), we present in this Letter an alternative mechanism for the double-peak structure. 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 [20–23].

We start with a generalized Hubbard model defined on a 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 (DSC), we can construct an effective mean-field model [23] to study the vortex physics in the mixed state:

$$H = -t \sum_{ij,\sigma} c_{i\sigma}^\dagger c_{j\sigma} e^{i\varphi_{ij}} + \sum_{i,\sigma} (m_{i,\bar{\sigma}} - \mu) c_{i\sigma}^\dagger c_{i\sigma}$$
$$+ \sum_{ij} (\Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \Delta_{ij}^* c_{j\downarrow} c_{i\uparrow}). \quad (1)$$

Here $c_{i\sigma}$ annihilates an electron of spin σ at the *i*th site. The summation is over the nearest neighbor sites. μ is the chemical potential. $m_{i,\sigma} = U\langle c_{i\sigma}^\dagger c_{i\sigma} \rangle$ is the spin-dependent Hartree-Fock potential at the *i*th site, where U is the strength of on-site repulsion. $\Delta_{ij} = \frac{V}{2}\langle c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow} \rangle$ is the spin-singlet *d*-wave pair potential, where V is the strength of nearest neighbor attraction. In the mixed state, the magnetic field effect is included through the Peierls phase factor $\varphi_{ij} = \frac{\pi}{\Phi_0} \int_{\mathbf{r}_j}^{\mathbf{r}_i} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r}$, where $\Phi_0 = hc/2e$ is the superconducting flux quantum. By assuming the superconductor under consideration is in the extreme type-II

limit, the screening effect from the supercurrent is negligible. The vector potential $\mathbf{A}$ can then be approximated by the solution $\nabla \times \mathbf{A} = H\hat{\mathbf{z}}$, where H is the magnetic field externally applied along the c axis. The enclosed flux density within each plaquette is given by $\sum_\square \varphi_{ij} = \frac{\pi H a^2}{\Phi_0}$. A similar mean-field Hamiltonian can also be arrived at within a t-U-J model proposed recently [24].

We diagonalize the Hamiltonian Eq. (1) by solving the Bogoliubov–de Gennes (BdG) equation:

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

where $(u_{i\sigma}^n, v_{i\bar{\sigma}}^n)$ is the quasiparticle wave function corresponding to the eigenvalue E_n, and the single particle Hamiltonian $\mathcal{H}_{ij,\sigma} = -t e^{i\varphi_{ij}} \delta_{i+\delta,j} + (m_{i,\bar{\sigma}} - \mu)\delta_{ij}$ with the subscript $\delta = (\pm 1, 0)$ or $(0, \pm 1)$. Notice that the quasiparticle energy is measured with respect to the Fermi energy. The self-consistent conditions read $m_{i\sigma} = U \sum_n |u_{i\sigma}^n|^2 f(E_n)$, and $\Delta_{ij} = \frac{V}{4} \sum_n (u_{i\uparrow}^n v_{j\downarrow}^{n*} + v_{i\downarrow}^{n*} u_{j\uparrow}^n) \times \tanh(\frac{E_n}{2k_B T})$, where the Fermi distribution function $f(E) = 1/(e^{E/k_B T} + 1)$. 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 4×4 equation in the spin space with energy E_n, then $(v_{i\uparrow}^{n*}, -v_{i\downarrow}^{n*}, u_{i\uparrow}^{n*}, -u_{i\downarrow}^{n*})^{\text{transpose}}$ 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 $\mathbf{A} = (-Hy, 0, 0)$, where y is the y component of the position vector $\mathbf{r}$. We introduce the magnetic translation operator $\mathcal{T}_{mn}\mathbf{r} = \mathbf{r} + \mathbf{R}$, where the translation vector $\mathbf{R} = mN_x\hat{\mathbf{e}}_x + nN_y\hat{\mathbf{e}}_y$ with N_x and N_y the linear dimension of the unit cell of the vortex lattice. To ensure different $\mathcal{T}_{mn}$ are commutable with each other, we have to take the strength of the 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 $\Delta(\mathcal{T}_{mn}\mathbf{r}) = e^{i\chi(\mathbf{r},\mathbf{R})}\Delta(\mathbf{r})$, where the phase accumulated by the order parameter upon the translation is $\chi(\mathbf{r}, \mathbf{R}) = \frac{2\pi}{\Phi_0}\mathbf{A}(\mathbf{R}) \cdot \mathbf{r} - 4mn\pi$. From this property, we can obtain the magnetic Bloch theorem for the wave function of the BdG equations [12]:

$$\begin{pmatrix} u_{\mathbf{k},\sigma}(\mathcal{T}_{mn}\tilde{\mathbf{r}}) \\ v_{\mathbf{k},\sigma}(\mathcal{T}_{mn}\tilde{\mathbf{r}}) \end{pmatrix} = e^{i\mathbf{k}\cdot\mathbf{R}} \begin{pmatrix} e^{i\chi(\mathbf{r},\mathbf{R})/2} u_{\mathbf{k},\sigma}(\tilde{\mathbf{r}}) \\ e^{-i\chi(\mathbf{r},\mathbf{R})/2} v_{\mathbf{k},\sigma}(\tilde{\mathbf{r}}) \end{pmatrix}. \quad (3)$$

Here $\tilde{\mathbf{r}}$ is the position vector defined within a given unit cell, $\mathbf{k} = \frac{2\pi l_x}{M_x N_x}\hat{\mathbf{e}}_x + \frac{2\pi l_y}{M_y N_y}\hat{\mathbf{e}}_y$ with $l_{x,y} = 0, 1, \ldots, M_{x,y} - 1$ are the wave vectors defined in the first Brillouin zone of the vortex lattice, and $M_x N_x$ and $M_y N_y$ are the linear dimensions of the whole system.

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 $n_f = \sum_{i,\sigma}\langle c_{i\sigma}^\dagger c_{i\sigma}\rangle/N_x N_y$

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 consider only 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 $M_x \times M_y = 21 \times 42$. We use the exact diagonalization method to solve the BdG equation (2) self-consistently. In the absence of a magnetic field, we have reproduced the results reported in previous work [23] including an AF SDW order, a stripe phase, and a d-wave SC phase with the increased doping. In the optimally doped 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 $U_c = 1.5$, the SDW order is nucleated around the vortex core. Typical results on the nature of the vortex core are 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 $hc/2e$. The d-wave SC order parameter vanishes at the vortex core center and starts to increase at the scale of the coherence length ξ_0 to its bulk value. Figure 1(b) displays the spatial distribution of the staggered magnetization of the local SDW order as defined by $M_s = (-1)^i S_z^i$ with $S_z^i = n_{i,\uparrow} - n_{i,\downarrow}$. Clearly, the maximum strength of M_s appears at the vortex core center and decays also with a scale of ξ_0 to zero into the superconducting region. More interestingly, the SDW order parameters have 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 fourfold rotational symmetry of the whole system to the twofold, and the period of the translational symmetry of the vortex lattice along the x direction 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. The development of the Q1D stripes breaks the fourfold 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
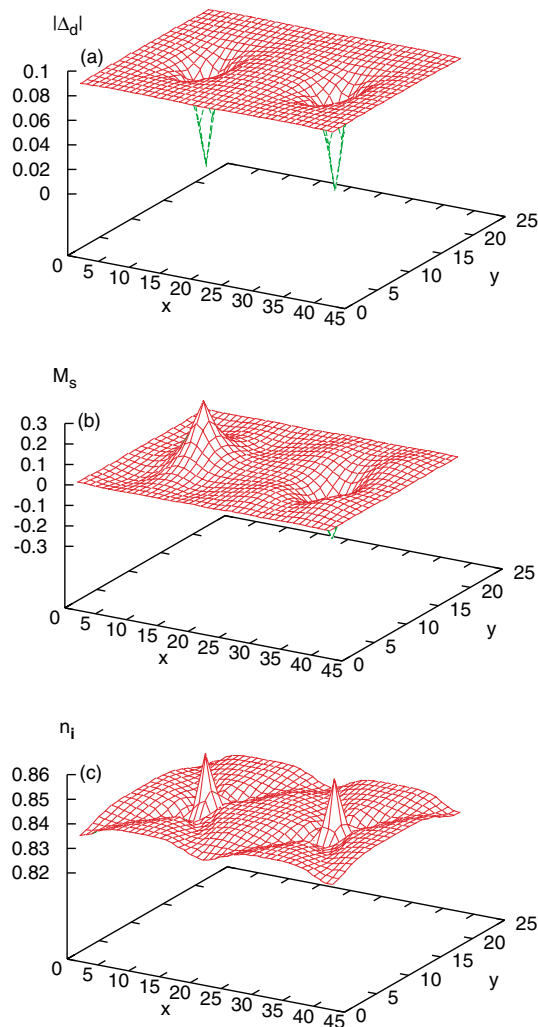
FIG. 1 (color). The amplitude distribution of the d-wave SC order parameter $|\Delta_d|$ (a), the staggered magnetization M_s (b), and the electron density n_i (c) in one magnetic unit cell obtained at the zero temperature. The size of the cell is 42×21. The strength of the on-site repulsion $U = 2$. The other parameter values: the d-wave pairing interaction $V = 1$; the filling factor $n_f = 0.84$.

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 argument [25] 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 [19]. Here we have restricted our study of the on-site interaction U within the Hartree-Fock mean-field approximation and the effect of quantum fluctuation has been neglected. For a fixed U, this fluctuation would lead to a reduction of the staggered magnetic moment induced around the vortex core center. As a result, the magnitude of splitting in the LDOS (as discussed below) could be overestimated in the present approximation. To compare with experiments, the true value of U then has to be at least bigger than the critical value U_c. So far the physical value of U in high-T_c cuprates is experimentally unavailable. However, the value of U from 2 up to 6 has been chosen by other authors in the models with the competition between the AF and DSC orderings [23,24]. On the other hand, the mean-field approximation is expected to describe reasonably the low-lying quasiparticle states, which is relevant to the STM experiments at low temperatures, particularly in view of the fact that the weak interlayer coupling in real cuprates may help to reduce the fluctuation effect.

The local density of states is defined by

$$\rho_i(E) = -\frac{1}{M_x M_y} \sum_{\mathbf{k},n,\sigma} |u_{\mathbf{k},i,\sigma}|^2 f'(E_{\mathbf{k}}^n - E), \quad (4)$$

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. In Fig. 2 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 μ deviates from zero for n_f being less than the half filling ($n_f = 1$). As can be seen from Fig. 2(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 [6]. 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. 2(b)]. The splitting comes from the fact that when the SDW order is localized around the vortex center, the spin-dependent potential, which can be rewritten as $m_{i,\uparrow(\downarrow)} = U(n_i \pm S_z^i)/2$, plays the role of a local magnetic field interacting with the electrons via the Zeeman coupling. When U is increased, S_z^i 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. 2(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. We have also found
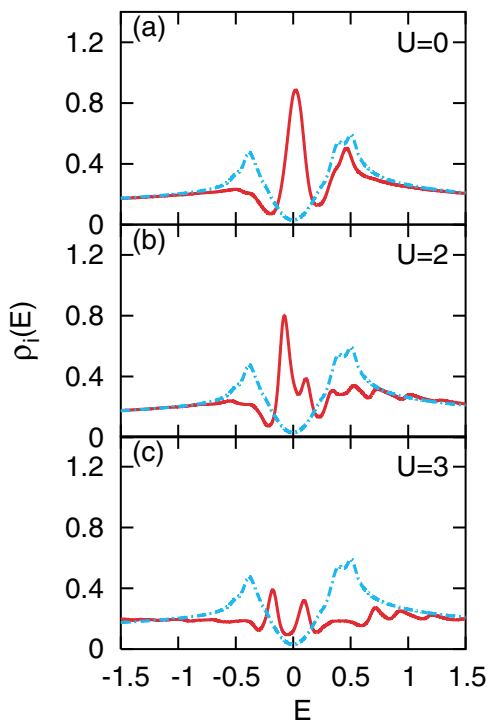
FIG. 2 (color).   The zero-temperature LDOS at the vortex core center (red solid line) with various strengths of on-site repulsion $U = 0$ (a), $U = 2$ (b), and $U = 3$ (c). Also displayed is the zero-temperature LDOS at the midpoint (green dot-dashed line) between two nearest neighbor vortices along the x direction. The other parameter values are the same as Fig. 1.

that the splitting is independent of the applied magnetic field because it is determined by the strength of the induced AF SDW order at the vortex core center. This field independence has been indeed indicated experimentally [26]. In addition, considering the experimental observation [27] that the pseudogap is seen in under-, optimally, and overdoped BSCCO samples while not in optimally and overdoped YBCO samples, we believe that the induction of the local AF order at the vortex core center plays a more important role in the splitting of the LDOS around zero energy in the optimally doped YBCO than in BSCCO samples. This induction is consistent with a recent neutron scattering experiment on LSCO [19].

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