Impurity resonance peaks in the vortex core of cuprate superconductors with induced spin density wave order

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(Received 20 August 2009; published 3 November 2009)

Considering the competing spin density wave (SDW) and d-wave superconductivity interactions, we investigate the effects of a nonmagnetic impurity on the vortex-core state of cuprate superconductors within the Bogoliubov–de Gennes formalism. We illustrate that the local SDW order is induced by the impurity on top of the magnetic field induced SDW order. The local density of states of a pinned vortex core exhibit a resonance peak at negative energy, which is drastically different from the double-peak structure observed in an unpinned vortex core. This resonance peak is insensitive to the impurity-scattering strength. Consequently, the impurity resonance peak may be used to identify the nature of vortex-core state of cuprate superconductors.

DOI: 10.1103/PhysRevB.80.172502   PACS number(s): 74.20.−z, 74.25.Jb, 74.25.Op

High-T_c cuprates, as type-II superconductors, possess the vortex state as one of the magnetic properties when the applied magnetic field is greater than a critical value (H_{c1}) but less than the upper limit (H_{c2}).[1] The scanning tunneling microscopy (STM) experiments on these materials reveal rich and intriguing features of the vortex-core states.[2–5] In the local differential conductance at the vortex-core center of $YBa_2Cu_3O_{7-\delta}$ (YBCO), the vortex states with double peaks are observed.[2,3] Two less prominent peaks in the vortex-core states have also been detected in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO).[4] The spacing between the STM tip and the CuO_2 layer where the vortex core resides is two atomic layers (BiO layer and SrO layer) in BSCCO while the spacing is monatomic BaO layer in YBCO. Furthermore, highly anisotropic BSCCO allows vortices to move even at low temperature. For less anisotropic YBCO, the vortex motion could be ignored. However the STM spectra are inconsistent with a model calculation assuming a pure superconducting $d_{x^2-y^2}$-wave symmetry in which a single peak near the zero bias at the vortex-core center is predicted.[6] A theoretical attempt to resolve such a disagreement employed a mixed $d_{x^2-y^2}+id_{xy}$-wave order parameter.[7]

The competing order scenario has been applied to understand the two peaks feature of vortex-core states.[8–11] The concept is motivated by several important experimental findings; for example, neutron-scattering experiment on the optimally doped $La_{2-x}Sr_2CuO_4$,[12] a quasiparticle-state pattern near the cores in BSCCO,[13] and a high-field nuclear magnetic-resonance imaging experiment on near-optimally doped YBCO.[14] All these experiments indicate that an antiferromagnetic or spin density wave (SDW) order may show up in the vortex state. In the presence of the magnetic field induced SDW order, the original zero-bias peak can be split into two peaks due to the lifting of spin degeneracy.[9–11] Numerical results show that local SDW order can be induced not only by the magnetic field[10] but also by vacancy, strong impurity, or finite disorder.[15–17]

It is now widely accepted that impurities may provide excellent probes of the still poorly understood ground state of the cuprates.[18] Meanwhile impurities play an important role in the vortex state such as a pinning effect. One may invoke the pinning effect to make the Bogoliubov–de Gennes (BdG) formulation applicable to electronic structures of the vortex core without considering, if any, complication due to the vortex motion mentioned earlier. Since the competing SDW order is apparently important around the vortex cores and strong impurities, thorough studies on the impurity effect on the vortex state with the induced SDW order are necessary to understand the cross relations between impurities and vortex cores in high-T_c superconductors. In this paper, we investigate the impurity effect on vortex cores including the induced SDW order by using the BdG formalism. We propose the impurity resonance peaks as a decisive methodology to explore the nature of the vortex-core state.

We start with a widely used effective model Hamiltonian,

$$H = -\sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i,\sigma} (U n_{i\bar{\sigma}} + V^{imp}_i - \mu) c^\dagger_{i\sigma} c_{i\sigma} + \sum_{i,j} (\Delta_{ij} c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} + \text{H.c.}), \tag{1}$$

where the operator $c^\dagger_{i\sigma}$ creates an electron with a spin σ at a site i. The hopping amplitude is written as $t_{i,j} = t_{ij,0} \exp[i(\pi/\Phi_0)\int_{\mathbf{r}_j}^{\mathbf{r}_i} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r}]$ in the presence of a magnetic field, where $\Phi_0 = \pi/e$ is the superconducting flux quantum and $\mathbf{A}$ is the vector potential. For the nearest-neighbor hopping, $t_{ij,0} = t_0$ while $t_{ij,0} = t'$ for the next-nearest-neighbor hopping. As for other parameters, U is the on-site Coulomb repulsion, V^{imp}_i is an impurity potential at the ith site, and μ is the chemical potential. The d-wave bond order parameter is defined as $\Delta_{ij} = V_{DSC}\langle c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow}\rangle/2$ while the SDW order parameters are determined by $\Delta^{SDW}_i = U\langle c^\dagger_{i\uparrow} c_{i\uparrow} - c^\dagger_{i\downarrow} c_{i\downarrow}\rangle$. These order parameters will be obtained self-consistently by solving the BdG equations,

$$\sum_j \begin{pmatrix} \mathcal{H}_{ij,\sigma} & \Delta_{ij} \\ \Delta^*_{ij} & -\mathcal{H}^*_{ij,\bar{\sigma}} \end{pmatrix} \begin{pmatrix} u^n_{j,\sigma} \\ v^n_{j,\bar{\sigma}} \end{pmatrix} = E_n \begin{pmatrix} u^n_{i,\sigma} \\ v^n_{i,\bar{\sigma}} \end{pmatrix}, \tag{2}$$

where $\mathcal{H}_{ij,\sigma} = -t_{ij} + (U n_{i\bar{\sigma}} + V^{imp}_i - \mu)\delta_{i,j}$ and

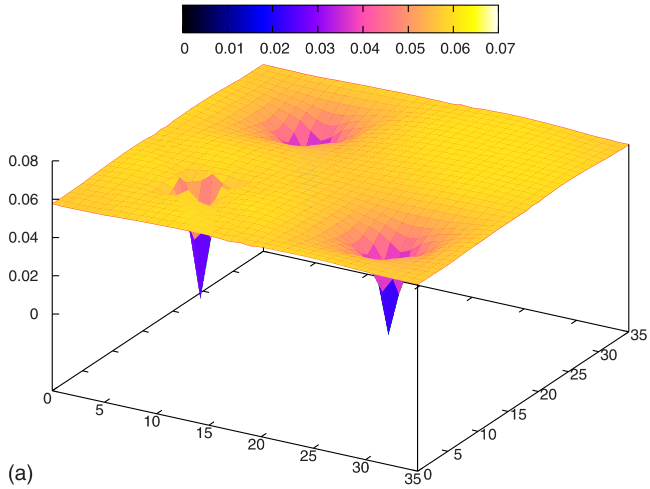

FIG. 1. (Color online). Spatial variations in the superconducting order parameter for $V_{DSC}=1.0$, $V^{imp}=100$, $t'=0$, and $U=2.2$. Two vortices are located at (9,27) and (27,9). An impurity is at (9,9) in (a) while it resides at (9,27) in (b).

$$n_{i\uparrow} = \sum_n |u^n_{i,\uparrow}|^2 f(E_n), \tag{3}$$

$$n_{i\downarrow} = \sum_n |v^n_{i,\downarrow}|^2 [1 - f(E_n)], \tag{4}$$

$$\Delta_{ij} = \frac{V_{DSC}}{4} \sum_n [u^n_{i\uparrow} v^{n*}_{j\downarrow} + v^{n*}_{i\downarrow} u^n_{j\uparrow}] \tanh\left(\frac{E_n}{2T}\right) \tag{5}$$

with the Fermi distribution function $f(E_n)$. The local d-wave order parameter at site i is given by $\Delta^d_i = \frac{1}{4}\Sigma_j \bar{\Delta}_{ij}[\delta_{j,i+\hat{x}} + \delta_{j,i-\hat{x}} - \delta_{j,i+\hat{y}} - \delta_{j,i-\hat{y}}]$, where $\bar{\Delta}_{ij} = \Delta_{ij} \exp[i(\pi/\Phi_0)\int_{\mathbf{r}_j}^{(\mathbf{r}_i+\mathbf{r}_j)/2} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r}]$. The self-consistency is achieved by iterations. In the numerical calculations, we set the hopping amplitude t and lattice constant a as units, the d-wave pairing potential $V_{DSC}=1.0$. We use the symmetric gauge for the magnetic field and a $N \times N = 36 \times 36$ square lattice is chosen. The averaged electron density is fixed at $\bar{n} \simeq 0.85$. Note that parameters are chosen in such a way that the system is a purely d-wave superconductor in the absence of magnetic field and impurity.

In Fig. 1, we plot the spatial profile of the d-wave order parameters in the presence of an strong impurity with $V^{imp}=100$ away from the vortex cores [Fig. 1(a)] as well as inside a core [Fig. 1(b)]. The SDW order is induced as shown in Fig. 2 and will be explained below. The superconducting order parameters are significantly suppressed in the vortex cores at (9,27) and (27,9). At the same time, the impurity at (9,9) in Fig. 1(a) also reduces the order parameters. It is clearly illustrated that the vortex suppression is different from its counterpart due to the impurity. Since the distance between the impurity and either of vortex cores is much larger than the critical distance[19] in Fig. 1(a), the impurity has no effect on the cores. If the impurity-vortex-core distance is less than the critical value, the impurity would drag the core near it as demonstrated before.[19] Our results clearly confirm such pinning effects. In Fig. 1(b), on the other hand, an impurity locates at (9,27), which is the center of a vortex

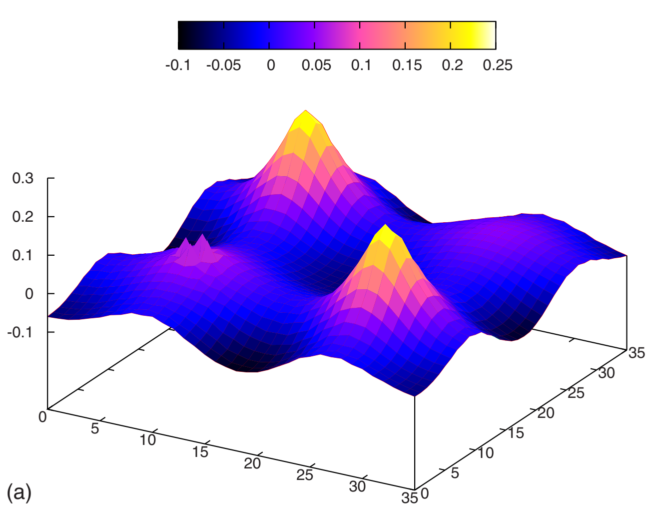

FIG. 2. (Color online). The spatial distribution of the staggered magnetization. All the parameters and the impurity location are same as in Fig. 1.

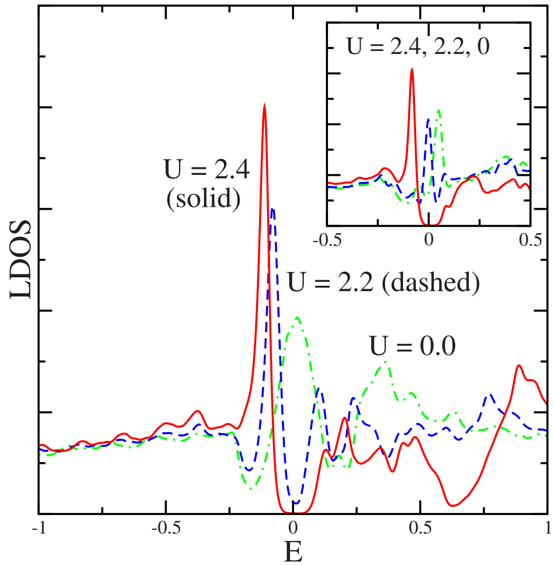

FIG. 3. (Color online). The LDOS at the nearest-neighbor site of the impurity inside a vortex core as in Fig. 1(b). The on-site repulsion U are chosen as 2.4 (solid line), 2.2 (dashed line), and 0 (dot-dashed line). We choose $V_{DSC}=1.0$, $t'=0$, and $V^{imp}=100$. The inset shows the resonance peak of an impurity away from the core for the same parameters.

core; therefore, this vortex is pinned by the impurity and it would be called a *pinned vortex*.

It is already known that the local suppression of the d-wave superconducting order due to the presence of vortex cores or impurities may lead to the local induction of the SDW order because of the competing nature between these two orders. Figure 2 shows the spatial distribution of the staggered magnetization defined as $M_i^s=(-1)^i\Delta_i^{SDW}/U$ corresponding to Fig. 1. On top of the magnetic field induced SDW order around vortex cores, the strong impurity induces the local SDW order around the impurity site (9,9) in Fig. 2(a) and impurity site (9,27) in Fig. 2(b), respectively. It would be understandable that due to the additional impurity effect the induced SDW order is stronger in the pinned vortex core as shown in Fig. 2(a) than in the unpinned core as exhibited in Fig. 2(b).

Next we study the local density-of-states (LDOS) spectrum of the system. The supercell method[20,21] is employed in order to calculate the LDOS. If the lattice size is $N\times N$ as a unit cell and the number of unit cells is $M\times M$, then the total size is $NM\times NM$. Introducing quasimomenta $k_{x(y)}=2\pi n_{x(y)}/(NM)$, where $n_{x(y)}=0,1,\ldots,M-1$, the LDOS, $\rho_i(E)$, is calculated as follows:

$$\rho_i(E)=-\frac{1}{M^2}\sum_{\mathbf{k},n}[|u_{\mathbf{k}i}^n|^2 f'(E_{\mathbf{k}-}^n)+|v_{\mathbf{k}i}^n|^2 f'(E_{\mathbf{k}+}^n)], \qquad (6)$$

where f' is the derivative of the Fermi distribution function and $E_{\mathbf{k}\pm}^n=E_{\mathbf{k}}^n\pm E$. Even for moderately strong impurity potentials, the LDOS at the impurity site is significantly suppressed while the resonance peak shows up at its nearest-neighbor sites. Here we will not consider the detailed STM

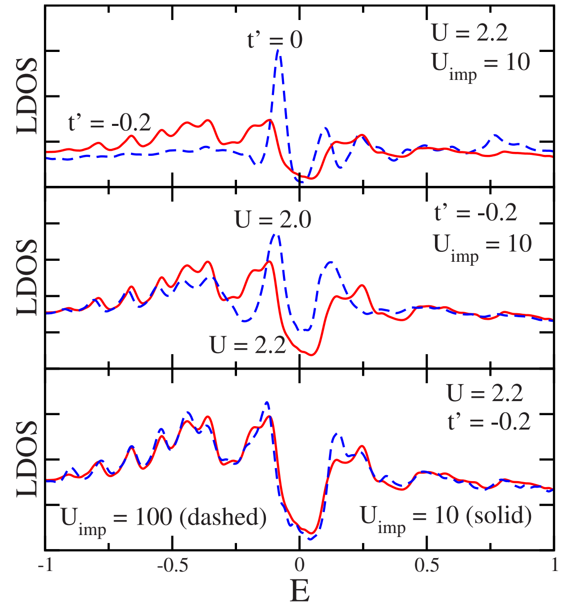

FIG. 4. (Color online). The LDOS of a pinned vortex in the presence of the next-nearest-neighbor hopping. The top panel describes the LDOS for $t'=0$ (dashed line) and $t'=-0.2$ (solid line) with $U=2.2$ and $V^{imp}=10$. The middle panel shows how LDOS changes for different values of $U=2$ (dashed) line and 2.2 (solid line) when $t'=-0.2$ and $V^{imp}=10$. The bottom panel demonstrates that the LDOS with $V^{imp}=10$ (solid line) is not much different from one with $V^{imp}=100$ (dashed line) even when $t'=-0.2$.

tunneling processes[22,23] such as the blocking or filtering effects for simplification.

In the main panel of Fig. 3, we present the LDOS spectrum at the nearest-neighbor site of the impurity inside the vortex core. The on-site Coulomb repulsion is chosen to be $U=2.4$ (red solid line), 2.2 (blue dashed line), and 0 (green dot-dashed line) while other coupling parameter values are same as in Fig. 1. The resonance peak is zero biased and relatively widespread for $U=0$ while the location of the peak is shifted to a negative energy when U becomes finite. Examining further the holelike resonance peak in the pinned vortex core for $V_{imp}=-100$ or ± 10 with $U=2.2$, we obtained qualitatively same resonance structure as in the present figure. We also obtained, in the absence of the induced SDW order, the zero-biased peak in the pinned vortex core regardless of V^{imp}. This indicates that the induced SDW order gives rise to the holelike peak in the pinned vortex core. The inset illustrates the resonance peak of an impurity away from the core. For zero field, the locally induced SDW order[16] splits the resonance peak into two neighboring peaks. However, this splitting disappears in the vortex state as shown in the inset. One can understand this in terms of the effect of Doppler shift, which induces a broadening of the resonance peak.[24] It is worth to mention that the LDOS at the impurity site has been studied for weak scattering potential.[25]

Finally, we will study the effect of band structure by varying the next-nearest-neighbor hopping t'. As illustrated in Fig. 4, the top panel compares the LDOS of the pinned vortex for $t'=0$ and $t'=-0.2$ while U and V^{imp} are fixed. The dashed curve is similar with the LDOS for $V^{imp}=100$ in

Fig. 3 as we mentioned earlier. This implies that the impurity potential of $V^{imp}=10$ is strong enough to induce a local SDW order. When $t'=-0.2$, the dominant peak otherwise appearing at a negative energy is substantially suppressed and two weak peaks show up. We also illustrate in the middle panel how LDOS changes for different values of $U=2.0$ and 2.2 when $t'=-0.2$ and $V^{imp}=10$. Since the SDW order with $U=2$ is a bit smaller than one with $U=2.2$, the distance between two weak peaks is narrower for $U=2$. The bottom panel shows that the LDOS with $V^{imp}=10$ is not much different from one with $V^{imp}=100$ even in the presence of the next-nearest-neighbor hopping.

In summary, we examine the effects of single nonmagnetic impurity on a vortex state of high-T_c superconductors. It is illustrated that the local SDW order is induced by the impurity on top of the field-induced SDW order in the vortex state. When a strong impurity is away from the vortex core, we always obtain the zero-bias resonance peak at the nearest-neighbor sites of the impurity regardless t' equals to 0 or not. When a vortex core is pinned at a strong impurity site, the structure of the resonances at the neighbor sites of the impurity depends critically on the values of t'. For $t'=0$, the resonance peak is still there and always shifts to slightly negative energy no matter the impurity potential is positive or negative, and this feature is insensitive to the strength of the impurity. But for $t'=-0.2$ which is a more reasonable parameter when fitting the Fermi surface of hole-doped cuprate superconductors, the resonance peak disappears and splits into two broader peaks around the zero bias. The impurity resonance peak of a pinned vortex core may serve as an interesting methodology to probe the vortex-core state of high-T_c superconductors.

We acknowledge S. H. Pan and Z. D. Wang for valuable discussions. This work was supported by the Robert A. Welch Foundation under Grant No. E-1146 and the Texas Center for Superconductivity at the University of Houston through the State of Texas, the National Natural Science Foundation of China and the State Key Programs of China (Grant No. 2009CB929204). Y.C. acknowledges the program for Special Appointment (Eastern Scholar) at Shanghai Institutions of Higher Learning and Shanghai Municipal Government.

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