High Angular Momentum Core States and Impurity Effects in the Mixed State of 
d-Wave Superconductors

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The local quasiparticle spectra around the vortex core of a d-wave superconductor in the mixed state is studied by solving the lattice Bogoliubov-de Gennes equations self-consistently. It is shown that in addition to the zero-energy states, there also exist core states of high angular momentum. A nonmagnetic unitary impurity sitting at the core center is nondestructive to these core states and the zero-energy resonant state induced by itself is still visible in the local quasiparticle spectrum. The calculated imaging shows a fourfold “star” shape of the local density of states whose orientation is energy dependent. It is also found that, although the zero-energy states are extended, the core states of finite energy level could be localized.

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In the Abrikosov vortex state (also called mixed state or Schubnikov phase) of type-II superconductors, the magnetic flux penetrates into the system in quantized units \( \Phi_0 = \hbar c/2e \). In the region of vortex core, the superconducting order parameter (or pair potential) is considerably suppressed from its zero-field value \( \Delta_0 \), going to zero at the vortex core center at a distance of several coherence lengths \( \xi_0 \). This reduction of the order parameter can affect various physical properties of the superconductor, for example, the nature of local electronic states around the Fermi energy. The vortex core problem of an s-wave superconductor was first studied in the classic papers of Caroli, de Gennes, and Matricon [1]. By solving approximately the Bogoliubov-de Gennes equations for an isolated vortex line in the limit of \( \kappa = \lambda/\xi_0 \gg 1 \), where \( \lambda \) is the magnetic penetration depth, these authors showed the existence of the low-lying bound quasiparticle states inside an s-wave vortex core. Later on, Bardeen et al. [2] extended the calculation to all values of \( \kappa \) by determining the pairing potential and magnetic field with a variational expression for the free energy, and the qualitative conclusion is similar to that of Caroli et al.. Recent theoretical attempts [3, 4, 5, 6, 7, 8] at understanding the electronic states of vortex lines in type-II superconductors was revived by STM experiments on NbSe2 [9], which not only showed a strong enhancement of the zero-bias tunneling conductance as a manifestation of the presence of bound states in the vortex core, but also provided images of vortex. For an s-wave superconductor, the energy gap open at the Fermi surface is a constant. One can naively think that, the spatial variation of the pair potential is analogous to a potential well carved with four notches along the nodal directions, so that quasiparticles can leak through the notches. It was shown for the first time by Wang and MacDonald [10] that there appears a single broad peak at zero energy in the local density of states (LDOS) at the center of a pure d-wave vortex core so that the quasiparticle states are virtually bound. Recently, the split-peak structure around zero bias in the local differential tunneling conductance at the vortex core center in YBa2Cu3O7−δ [11] and Bi2Sr2CaCu2O8+δ [12, 13] has been observed by scanning tunneling microscopy (STM). These experimental observations stimulated intensified study of the quasiparticles in the vortex core of high-\( T_c \) cuprates [14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25], leading to a variety of scenarios for the explanation of experimental data. No consensus on the mechanism has emerged. However, on the other hand, additional features of quasiparticle states of a pure d-wave vortex have not been well addressed even in the framework of BCS-type description. Specifically, nearly all of the theoretical and experimental works on the quasiparticle states of d-wave vortices focus on the LDOS directly on the core center, whether there exists high angular momentum core states have not been paid much attention. Furthermore, the imaging of the tunneling conductance of a d-wave vortex, as in the impurity case [26], has not been experimentally available. In this paper, we present a complete study of the electronic structure around one of the d-wave vortices forming the Abrikosov square lattice by solving self-consistently the Bogoliubov-de Gennes (BdG) equations within a tight-binding model, and new features are exposed for the first time.

The electronic structure of a d-wave superconductor can be described by the quasiparticle wavefunctions...
\[
\begin{pmatrix}
u_i^n \\
u_i^\alpha \end{pmatrix}
\]
which satisfy the BdG equations
\[
\sum_j \left( \begin{array}{cc}
\mathcal{H}_{ij} & \Delta_{ij} \\
\Delta^\ast_{ij} & -\mathcal{H}_{ij}^\ast 
\end{array} \right) \begin{pmatrix}
u_j^n \\
u_j^\alpha \end{pmatrix} = E_n \begin{pmatrix}
u_i^n \\
u_i^\alpha \end{pmatrix},
\]
(1)

Here the summation is over the nearest neighbor sites. The single particle Hamiltonian reads \(\mathcal{H}_{ij} = -te^{i\phi_j} \delta_{i+r,j} + (U_i - \mu)\delta_{ij}\) where \(t\) is the hopping integral, \(\mu\) is the chemical potential, \(U_i\) is the single particle potential describing, if any, the effects of impurities, defects, or crystal field, and \(r = \pm \hat{e}_x, \pm \hat{e}_y\) are the unit vectors along the crystalline \(x\) and \(y\) axes, respectively. In the mixed state, the magnetic field effect is included through the Peierls phase factor \(\varphi_{ij} = \frac{\pi a^2}{\hbar} A(r) \cdot dr\). By assuming the superconductor under consideration is in the extreme type-II limit where \(\kappa\) goes to infinity so that the screening effect from the supercurrent is negligible. The vector potential \(A\) can then be approximated by the solution \(\nabla \times A = H\hat{z}\) where \(H\) is the magnetic field externally applied along the \(c\) axis. The enclosed flux density within each plaquette is given by \(\sum \varphi_{ij} = \frac{\pi H a^2}{\hbar}\). Notice that the quasiparticle energy is measured with respect to the Fermi energy. \(\Delta_{ij}\) is the spin-singlet \(d\)-wave bond pair potential, which is subject to the self-consistency condition:
\[
\Delta_{ij} = \frac{V}{2} \sum_{n,E_n>0} (u_i^n v_j^n + v_i^n u_j^n) \tanh \left( \frac{E_n}{2k_B T} \right),
\]
(2)
with \(V\) the strength of nearest neighbor effective attraction between electrons. 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 \(T_{mn} r = r + \mathbf{R}\) where the translation vector \(\mathbf{R} = mN_x \hat{e}_x + nN_y \hat{e}_y\) with \(N_x\) and \(N_y\) the linear dimension of the unit cell of the vortex lattice. To ensure different \(T_{mn}\) 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 \(\Delta(T_{mn} \mathbf{R}) = e^{i\chi(r, \mathbf{R})} \Delta(r)\) where the phase accumulated by the order parameter upon the translation is \(\chi(r, \mathbf{R}) = \frac{\pi e^2}{\hbar c} A(r) \cdot r - 4\pi n_m n_n\). From this property, we can obtain the magnetic Bloch theorem for the wavefunction of the BdG equations:
\[
\begin{pmatrix}
u_k(T_{mn} \mathbf{R}) \\
u_k^\ast(T_{mn} \mathbf{R})
\end{pmatrix} = e^{ik \mathbf{R}} \begin{pmatrix} e^{i\chi(r, \mathbf{R})/2} \nu_k(\mathbf{R}) \\
- e^{-i\chi(r, \mathbf{R})/2} \nu_k^\ast(\mathbf{R}) \end{pmatrix}.
\]
(3)

Here \(\mathbf{R}\) is the position vector defined within a given unit cell and \(\mathbf{R} = \frac{2\pi l_{x,y}}{M_x N_x} \hat{e}_x + \frac{2\pi l_{x,y}}{M_y N_y} \hat{e}_y\) 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 dimension of the vortex lattice. The single particle Hamiltonian reads
\[
\sum_{k,F} \left[ \begin{array}{cc}
\mathcal{H}_k(F) & \mathcal{H}_{k,F} \\
\mathcal{H}_{k,F}^\ast & -\mathcal{H}_k^\ast(F) 
\end{array} \right] \begin{pmatrix}
u_k(F) \\
u_k^\ast(F) \end{pmatrix} = E_k \begin{pmatrix}
u_k(F) \\
u_k^\ast(F) \end{pmatrix},
\]
(4)

are the linear dimension of the whole system. We use exact diagonalization method to solve the BdG equation (3) self-consistently. The thermally broadened local density of states is then evaluated according to
\[
\rho(E) = -\frac{2}{N_k} \sum_{k,n} \left| u_{k,n}^\ast \right|^2 f'(E_k^N - E) + \left| v_{k,n}^\ast \right|^2 f'(E_k^N + E),
\]
where a prefactor comes from the spin degeneracy, and \(f'(E)\) is the derivative of the Fermi distribution function \(f(E) = 1/[\exp(E/k_BT) + 1]\) with respect to the energy \(E\), \(N_c = M_x \times M_y\) is the number of magnetic unit cells, \(\rho_0(E)\) is proportional to the local differential tunneling conductance at low temperatures which could be measured by STM experiments \([21]\).

In the following calculation, we take \(V = 1.2\), and the filling factor 0.85 by adjusting the chemical potential. The temperature is chosen to be \(T = 0.01\). Without loss of generality, we consider the unit cell of size \(N_x \times N_y = 42 \times 21\), and the number of the unit cells \(N_c = 21 \times 42\). This choice will give us a square vortex lattice. The numerical calculation shows as expected that each unit cell accommodates two superconducting vortices each carrying a flux quantum \(\Phi_0\). The spatial vari-
vation of the $d$-wave order parameter is similar to Fig. 1 of Ref. [10]. It decreases continuously to zero from the its bulk value as the vortex core center is approached in the length scale $\xi_0 = h v_F / 2\Delta_{\text{max}} \approx 5$, with the depleated region extending farther in the diagonal direction of the square lattice. Here $\Delta_{\text{max}} \approx 0.38$ is the gap edge defined as the energy position at which the bulk DOS becomes maxima, and $v_F$ is the Fermi velocity. For the given model parameter, the induced extended $s$-wave order parameter around the vortex is so small that its effect on the LDOS should be negligible. In Fig. 1 we plot the LDOS as a function of energy at various distance from the vortex core in a $d$-wave superconductor. The solid line in each panel represents the result of a clean system, while the dashed line for the case that a unitary impurity ($U_0 = 100$) sits at the vortex core center. For comparison, we have also displayed the bulk LDOS (the dotted lines) in the absence of magnetic field and impurities. We choose the core center as the coordinate origin $(0,0)$. For the given unit cell size, the site $(10,0)$ is the midpoint of two nearest neighboring vortices along the $x$ direction. Notice that the three curves in the right-bottom panel almost coincide with each other, indicating that the LDOS spectrum at the midpt has recovered the bulk DOS. The asymmetry of the LDOS spectrum with respect to the Fermi energy comes from the breaking of the particle-hole symmetry. In the absence of the unitary impurity, the LDOS at the core center $i = (0,0)$ shows a single resonant peak around the Fermi energy. Although the spectrum at the center does not exhibit a split-peak structure, the suppression of the coherent peak at the gap edge $\Delta_{\text{max}}$ seems to be consistent with the experimental observations. At this point, we also calculate the LDOS at the core center with various values of the bulk order parameter and find that the broad zero-energy peak always shows up, which leads us to conclude that the quasiparticle excitations along the nodal direction on the Fermi surface should be the origin. At a finite distance away from the core center, the single peak in the LDOS at the core center continuously evolves into two peaks, which are located at $\pm \delta E(i)$. The spacing between these two peaks, i.e., $2\delta E(i)$ increases with the distance away from the core center. In addition, the amplitude of these peaks decreases with the distance from the core center and finally they merge into the continuum of scattering state with $E > E_{\text{max}}$. We remark that, since the induced extended $s$-wave order parameter is almost negligible, this origin for the obtained split peaks should be excluded. Considering the distance dependence of these subgap peaks in the LDOS, we believe instead that they result from the core states with a high angular momentum. The effect of a nonmagnetic impurity in the unitary limit is twofold: First, it plays the role of a pinning center. We introduce such an impurity into the unit cell randomly. It is found that when this impurity has a distance from the vortex core center within the range of a coherence length, the vortex will be dragged onto the impurity site. The order parameter profile of the pinned vortex is quite similar to that of a clean case. Out of this range, the pinning effect is rather weak. Second, it is both theoretically and experimentally well established that a nonmagnetic impurity itself will induce resonant states in a $d$-wave superconductor in contrast to its counterpart in a conventional $s$-wave superconductor. For the convenience of discussion, we consider the lattice as a bipartite, i.e., those sites $i = (ix, iy)$ with index having even $(-1)^{ix+iy}$ form sublattice $A$, which contains the core center, while those with index having odd $(-1)^{ix+iy}$ form sublattice $B$. The panels in the left column of Fig. 1 display the LDOS at the sites belonging to $A$, and the panels in the right column show the LDOS at the sites belong to $B$. When such an impurity pins the vortex, the LDOS spectrum at the core center vanishes due to the strong potential scattering from the impurity [See the dashed line as shown in the panel of Fig. 1 corresponding to the site $(0,0)$]. However, the intensity of the single zero-energy peak in the LDOS at the nearest neighbor site of the core center is strongly enhanced. This enhancement comes from the additional contribution of the near-zero-energy resonant state induced directly by the impurity itself. As the measured point is away from the core center, the LDOS exhibits no central peak (near the Fermi energy) at the sites belonging to the sublattice $A$. In particular, the density of states at zero energy is more depressed on these sites as compared to the impurity free case. Nevertheless, the LDOS on the sites belonging to the sublattice $B$ has a zero-energy peak, the intensity of which decays with the increased distance away from the core center. This pattern of the LDOS around the zero energy is solely caused by the impurity-induced resonant state, which has an oscillation behavior [28, 31]. Also interestingly, it can be seen that the location of the LDOS peaks associated with the high angular momentum core states is quite insensitive to the impurity scattering. In this sense, we can say that the unitary impurity is nondestructive to the vortex from the point of view of core states. The above effect of the single nonmagnetic unitary impurity on the electronic structure of a $d$-wave vortex is dramatically different from its effect in the case of an $s$-wave vortex. Since there is no resonant states induced around this impurity in an $s$-wave superconductor, it drives the energy position of the low-level core states away from the Fermi energy, and simultaneously the intensity of the corresponding peaks in the LDOS becomes weaker with the impurity strength [23]. To take a closer inspection of the nature of the electronic structure around a $d$-wave vortex, we calculate the spatial distribution of the LDOS around the vortex core at the fixed energy $E_1 = 0$ and $E_2 = 0.15$. $E_1$ is the peak position of the LDOS at the core center, $E_2$ is that at the site $(2,1)$. For the clean case, we find strong anisotropy of
the spatial distribution of the LDOS, which has a fourfold "star" shape. At zero energy ($E_1 = 0$), the magnitude of the LDOS has tails extending along the diagonals of the square lattice, and decays rapidly along the CuO$_2$ bonds. This behavior can be understood as follows: When the energy gap vanishes along the nodal directions, the quasiclassical orbital of these low-lying quasiparticle states is not closed. Therefore, the zero-energy states are extended along these directions and consequently, in contrast to the $s$-wave case, they are not truly bound core states. However, at a finite energy ($E_2 = 0.15$), the situation is reversed and the LDOS decays more slowly along the CuO$_2$ bonds than along the diagonals of the square lattice, that is, the "star" shape is rotated by almost $\pi/4$. In particular, the decay even along the bonds is so short ranged that the core states at this energy is approximately localized. This energy-dependent orientation of the "star" shape around a $d$-wave vortex arises from the $d$-wave pairing symmetry itself, which is in striking contrast to the $s$-wave case, the shape rotation was explained by introducing a perturbation term. When the impurity is added on the core center, the above conclusion is not changed except that the LDOS directly at the impurity site and the "star" becomes more extended.

To summarize, we have presented a study of the quasiparticle states around the vortex core of a $d$-wave superconductor in the mixed state. We have shown that, in addition to the zero-energy core states, there also exist core states with high angular momentum. It has also been found that a nonmagnetic impurity is not destructive to these core states, and the impurity-induced near-zero energy resonant state can still be visible in the LDOS. The calculated images demonstrate that all core states are not truly localized. So far, it seems that all theoretical and experimental studies focused on the local electronic structure at the vortex core center, on which much controversy just arises. The test of the existence of the high angular momentum core states, as well as the effects of the single atomic impurity, is now accessible to the experiments. Currently, the STM is the technique of choice that allows the observation of vortex states. It has recently been improved in both the spatial (atomic scale) and energy (sub-meV) resolution. We suggest that the STM tip be scanned horizontally in the region of several lattice constants around the vortex core center to observe the predicted changes in intensity and energy position of peaks. If the above predictions are indeed experimentally observed, it will help us to understand the delicate nature of the electronic structure of high-$T_c$ vortices.

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**FIG. 2:** The spatial distribution of the LDOS around a $d$-wave vortex at the energy $E_1 = 0$ (top row) and $E_2 = 0.15$ (bottom row). The left column shows the results in the clean case. Those with a nonmagnetic unitary impurity sitting at the core center are displayed on the right column. The measured size is $21 \times 21$. The other parameter values are the same as Fig. 4.

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