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Bound states and vortex core shrinking effects in iron-based superconductors

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ABSTRACT

Quasiparticle bound states and vortex core contraction effects in iron-based superconductors are studied by solving the Bogoliubov de Gennes (BdG) equations self-consistently including pair coupling effects. We find that the appearance of quasiparticle bound states in the vortex core is controlled not only by the pair coupling effects but also by the inter-orbit coupling strength. We also point out that the rapid vortex core contraction is controlled by quasiparticle interference effects. We suggest that these results deserve more attention in analysis of vortex quasiparticle bound states and vortex core contraction effects found in scanning tunneling microscopy (STM) experiments for different iron-based superconductors.

Understanding of the symmetry of the gap functions in iron-based superconductors is one of the major tasks in strongly correlated physics today. As an important clue to identify the symmetry of the pairing state, determination of the properties of quasiparticle excitations is essential. In conventional *s*-wave superconductors, theory predicts that quasiparticles in the vortex core consist of a bound state [1]. The bound state appears as a zero bias peak in the local density of states (LDOSs) which splits into two symmetric peaks and eventually merges into the coherence peaks on moving away from the vortex center. This prediction was confirmed by STM experiments on $NbSe_2$ [2]. In iron-based superconductors, a nodeless $s_{x^2y^2}$ wave pairing has been proposed based on various experiments and theoretical works. It is natural to believe that the bound state will appear in the vortex core. The STM experiment in stoichiometric *FeSe* reveals evidences for the bound state in the vortex core [3]. The hole-doped *Ba*122 shows a zero bias peak in the LDOS at the vortex center, which splits and merges with the coherence peaks away from the vortex [4]. *LiFeAs* also shows a vortex core peak in the LDOS [5]. These results seem to be consistent with the prediction. However, Yin et al. find that electron-doped *Ba*122 shows no bound state in the vortex core [6]. As these compounds have the similar crystal structure, energy bands and Fermi surfaces, we can naturally expect that these compounds should have the similar magnetic properties and superconductivities. But the appearance or disappearance of the bound state in the vortex core of these compounds indicates more complicated electronic interactions in these materials than those initially predicted. The discrepancy between theories and experiments needs further theoretical studies on the bound states in the vortex core.

On the other hand, there is another confusing observation in STM experiments. Hanaguri et al. observed vortex cores shrink rapidly with lowering temperature in *LiFeAs* [5]. The explanation of the vortex core shrinking effect is still controversial. Hanaguri et al. think that this unusual temperature effect can be explained by so-called Ktamer–Pesch (KP) effect [7]. In this paper, we will give a different explanation to the vortex core shrinking effect. In order to solve these questions, we investigate the bound state and the vortex core shrinking effect by considering the pair coupling effect and the inter-orbit coupling effect in vortex cores. We find that the appearance of the bound state in vortex cores is controlled by the strength of the inter-orbit coupling and the quasiparticle interference effect. By directly numerical calculation on the self-consistent BdG equation in two-orbit model with a magnetic field, we also point out that the shrinking of vortex cores is due to an increasing overlap of the wave functions of quasiparticles in the neighbor orbits. The extended wave functions of pairing states of the neighbor orbits interfere with each other. This effect partly restores the destroyed pairing states in vortex cores. It corresponds to a reduction in the size of the vortex core. This important result gives a clear account of the confusing vortex core contraction effect observed in experiments in many iron-based superconductors.

The quasiparticle interference effect due to impurity scattering was also explored in iron-based superconductors as it can directly probe the pairing symmetry. Teague et al. use Fourier transformed tunneling conductance in STM experiment to study the quasiparticle scattering interference (QPI) in $Ba(Fe_{1-x}Co_x)_2As_2$ [8]. They find that dominant QPI occurs at three wave-vectors: $\mathbf{q_1} = (2\pi,0)/(0,2\pi)$; $\mathbf{q_2} = (\pi,0)/(0,\pi)$; and $\mathbf{q_3} = (\pi,\pi)$. They think that the appearance of $\mathbf{q_3}$ wave-vector might be due to a larger density of *Co* – atoms which may behave like magnetic impurities. In this paper, we find that the strength of the inter-orbit coupling will increase

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the quasiparticle interaction between the electron pockets (or hole) pocket. So the appearance of $\mathbf{q_3}$ wave-vector might be due to the different strength of the inter-orbit coupling.

We start with an effective two-orbital model that includes only the iron d_{xz} and d_{yz} orbits [9–11]. The Hamiltonian is defined on two dimensional square lattice: $H = H_0 + H_{1I} + H_{2I}$. H_0 is an effective tight-binding Hamiltonian on the two-dimensional lattice with a pairing interaction V between two electrons on the next nearest neighbor sites for s-wave superconductors, $H_0 = -\sum_{i,j,\alpha,\beta,\alpha} e^{i\varphi_{ij}} t_{i,j,\alpha,\beta} c^+_{i,\alpha,\sigma} c_{j,\beta,\sigma} + \sum_{i,j,\alpha,\beta}\left[\Delta_{ij} c^\dagger_{i\uparrow,\alpha} c^\dagger_{j\downarrow,\beta} + h.c.\right] - \mu\sum_{i,\alpha,\sigma} c^+_{i,\alpha,\sigma} c_{i,\alpha,\sigma}$. The intra- ($t_{ij,\alpha\alpha}$) and inter-orbital ($t_{ij,\ \alpha\neq\beta}$) hopping integrals with the subscripts α, β (α, (β) labels d_{xz} and d_{yz} orbits) describe the electron effective hopping integrals between sites i and j of the Fe ions on the square lattice. $c^+_{i,\alpha,\sigma}(c_{i,\alpha,\sigma})$ creates (annihilates) an α orbital electron with spin σ at the site i, and μ is the chemical potential. The phase factor $\varphi_{ij} = \frac{\pi}{\phi_0}\int_{r_j}^{r_i} \mathbf{A}(\mathbf{r})\cdot d\mathbf{r}$, where $\mathbf{A} = (hy,0,0)$. h is magnetic field. The second term H_{1I} is the Coulomb interactions including intra-orbital, inter-orbital, and spin-flip and pair-hopping interactions. $H_{1I} = U\sum_{i,\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + \sum_{i,\alpha\langle\beta,\sigma}[U' n_{i\alpha\alpha} n_{i\beta-\sigma} + (U'-J) n_{i\alpha\alpha} n_{i\beta\sigma}] + J\sum_{i,\alpha\langle\beta,\sigma}\left(c^+_{i\alpha\uparrow} c^+_{i\beta\downarrow} c_{i\alpha\downarrow} c_{i\beta\uparrow} + c^+_{i\alpha\uparrow} c^+_{i\alpha\downarrow} c_{i\beta\downarrow} c_{i\beta\uparrow} + H.c.\right)$. The third term $H_{2I} = \sum_{(ij\alpha\beta)} \lambda \Delta^\alpha_{ij} \Delta^\beta_{ij}$ is responsible for pair coupling where λ is pair coupling constant. After the mean field approximation for this Hamiltonian, the model hamiltonian can be diagonalized and we obtain the following BdG equations:

$$\sum_{j\alpha}\begin{pmatrix} H_{i\alpha,j\beta,\sigma} & \Delta_{i\alpha,j\beta} \\ \Delta^*_{i\alpha,j\beta} & -H^*_{i\alpha,j\beta,\bar{\sigma}} \end{pmatrix}\begin{pmatrix} u^n_{j\alpha\sigma} \\ v^n_{j\alpha\bar{\sigma}} \end{pmatrix} = E_n\begin{pmatrix} u^n_{i\beta\sigma} \\ v^n_{i\beta\bar{\sigma}} \end{pmatrix}, \tag{1}$$

where $u^n_{j\alpha\sigma}$, $v^n_{j\alpha\bar{\sigma}}$ are the Bogoliubov quasiparticle amplitudes on the j-th site with corresponding eigenvalues E_n. The obtained equations are solved by numerical iterations starting with a random set of initial conditions. In the following, we set t_1 as an energy unit. We use the following parameters in our calculation: ($t_1 = -1.0$, $t_2 = 1.3$, $t_3 = -0.9$, $J = 1.0$, $U = 3.5$, $U' = 1.5$). The doping is $\delta = -0.2$ in following calculations. The band dispersions can be written as: $E_\pm(k) = \varepsilon_+(k) \pm \sqrt{\varepsilon^2_-(k) + \varepsilon^2_{xy}(xy)} - \mu$, $\varepsilon_\pm(k) = \frac{1}{2}[\varepsilon_x(k) \pm \varepsilon_y(k)]$, $\varepsilon_x(k) = -2t_1\cos k_x - 2t_2\cos k_y - 4t_3\cos k_x\cos k_y$, $\varepsilon_y(k) = -2t_2\cos k_x - 2t_1\cos k_y - 4t_3\cos k_x\cos k_y$, $\varepsilon_{xy}(k) = -4t_4\sin k_x\sin k_y$. These dispersions catch the main characteristics of the local-density approximation energy band calculations.

The superconducting order parameter and the local electron density $n(\mathbf{r}_i)$ satisfy the self-consistent conditions,

$$\Delta_{i\alpha,j\beta} = \frac{V}{4}\sum_n\left(u^n_{i\alpha\uparrow} v^{n*}_{j\beta\downarrow} + u^n_{j\beta\uparrow} v^{n*}_{i\alpha\downarrow}\right)\tanh\left(\frac{E_n}{2k_BT}\right), \tag{2}$$

$$n_\alpha(\mathbf{r}_i) = \sum_n |u^n_{i\alpha\uparrow}|^2 f(E_n) + \sum_n |v^n_{i\alpha\downarrow}|^2[1 - f(E_n)], \tag{3}$$

where $f(E) = 1/[e^{E/k_BT} + 1]$ is the Fermi distribution function. The $s_{x^2y^2}$-wave pairing potential at site i is given by $\Delta_i = (\Delta_{i,i+\hat{\mathbf{e}}_x+\hat{\mathbf{e}}_y} + \Delta_{i,i-\hat{\mathbf{e}}_x+\hat{\mathbf{e}}_y} + \Delta_{i,i+\hat{\mathbf{e}}_y-\hat{\mathbf{e}}_x} + \Delta_{i,i-\hat{\mathbf{e}}_y-\hat{\mathbf{e}}_x})/4$. Here $\hat{\mathbf{e}}_{x,y}$ denotes the unit vector along x, y direction. In the present work, we consider the pairing between the same orbital of the next nearest neighbor site. We calculate the LDOS at the core of vortices when a magnetic field is applied. For the calculation we use unite cell of size $N_x \times N_y = 20a \times 40a$ with periodic boundary condition. The $M_x \times M_y = 10 \times 10$ supercell is used to calculate the LDOS. By taking the strength of magnetic field, $h = 2\phi_0/N_xN_y$, such that the flux enclosed by each unit cell is twice ϕ_0, the equation is solved with the aid of the magnetic Bloch theorem:

$$\begin{pmatrix} u_{\mathbf{k},\sigma}(\mathcal{T}_{mn}\vec{\mathbf{r}}) \\ v_{\mathbf{k},\sigma}(\mathcal{T}_{mn}\vec{\mathbf{r}}) \end{pmatrix} = e^{i\mathbf{k}\cdot\vec{\mathbf{R}}}\begin{pmatrix} e^{i\chi(\mathbf{r},\vec{\mathbf{R}})/2} u_{\mathbf{k}\sigma}(\vec{\mathbf{r}}) \\ e^{-i\chi(\mathbf{r},\vec{\mathbf{R}})/2} v_{\mathbf{k}\sigma}(\vec{\mathbf{r}}) \end{pmatrix}, \tag{4}$$

here $\vec{\mathbf{r}}$ is the position vector defined within a given unit cell, and the vector $\vec{\mathbf{R}} = mN_x\hat{e}_x + nN_y\hat{e}_y \cdot \mathbf{k} = \frac{2\pi l_x}{M_xN_x}\hat{\mathbf{e}}_x + \frac{2\pi l_y}{M_yN_y}\hat{\mathbf{e}}_y$ with $l_{x,y} = 0,1,\ldots,M_{x,y}-1$ are the wave vectors. M_xN_x and M_yN_y are the linear dimensions of the whole single-layer system, and the phase $\chi(\vec{\mathbf{r}},\vec{\mathbf{R}}) = \frac{2\pi}{\varphi_0}A(\vec{\mathbf{R}})\cdot\vec{\mathbf{r}} - 4mn\pi$. The LDOS is given by

$$\rho(r_i, E) = -\frac{1}{M_xM_y}\sum_{n,k,\alpha,\sigma}\left[|u^{n,k}_{i\alpha\uparrow}|^2 f'(E^{n,k} - E) + |v^{n,k}_{i\alpha\downarrow}|^2 f'(E^{n,k} + E)\right], \tag{5}$$

where $f'(E)$ is the derivative of the Fermi distribution function. The $\rho(r_i,E)$ is proportional to the local differential tunneling conductance which could be measured by STM experiments [12].

In Fig. 1, we show the spatial variation of the vortex structure for different pair coupling strength. Spatial variation of the $s_{x^2y^2}$-wave order parameter is similar to the results of previous researches [13–16]: it decreases continuously to zero from its bulk value as the vortex core center is approached. From the figure we can see that the vortex core region occupies a smaller part of a unit cell of the vortex lattice with increasing the pair coupling strength. Fig. 1c is the core radius variation of the vortex with different temperatures. The vortex core shrinks with decreasing the temperature. This is consistent with the experiments [5]. There is no gap magnitude increase as t_4 changes from -0.85 to -1.2 without the magnetic field. So we do not think that the appearance of bound states in the vortex is due to the enhancing of superconducting gap. In fact, we increase the gap magnitude at $t_4 = -0.85$ by enhancing the pairing coupling constant V and find no bound states in the vortex. Instead, we clarify that the appearance of bound states in the vortex is due to the increasing the quasiparticle interference effect. The extended wave functions of the pairing states of the d_{xz} and d_{yz} orbits are close enough to interfere with each other (in fact they are in the same atoms). The interference effect increases as t_4 increases. This effect partly restores the destroyed pairing states in the vortex cores. With temperature decreased, more and more quasiparticles become condensing. So the interference effect grows stronger with decreasing the temperature. The sensitivity of the core radius variation of the vortex on the effect of the inter-orbit coupling is also investigated. Fig. 1d is the core radius variation of the vortex with different inter-orbit coupling strength. The vortex cores shrink with increasing the inter-orbit coupling strength. The strong inter-orbit coupling enhances the quasiparticle interference effect between different orbits.

In the following, we will investigate the bound state in the vortex core for the iron-based superconductors. We firstly compute the inter-orbit coupling $t_4 = -0.85$ (small) and pairing coupling strength $\lambda = 0.1$ case. We find that the zero bias peak in the vortex core is too weak to be seen. Then we fix $t_4 = -0.85$ and increase the pair coupling strength. We find that the zero bias peak becomes stronger. These results are not strange because the strong pair coupling enhances the quasiparticle interference effect. However, we find that the appearance of the zero bias peak in iron-based superconductors is also related to the strength of inter-orbit coupling. For inter-orbit coupling $t_4 = -0.85$ and pair coupling $\lambda = 0.0$, the spatial profiles of the LDOS near the vortex core are plotted in Fig. 2a. Interestingly, the vortex charges show no zero bias peak in the vortex core in the LDOS. With increasing the t_4, the zero bias peak appears slowly. It grows stronger as t_4 becomes larger. When $t_4 = -1.2$, the LDOS shows an apparent bound state in Fig. 2c. This variation of the LDOS inside the vortex core is consistent with many experiment observations [3–6]. From these results, we emphasize that the appearance of the bound state in the iron-based superconductors is controlled not only by the pair coupling effect but also by the inter-orbit coupling strength.

The inter-orbit coupling effect also has effect on the QPI in iron-based superconductors. In order to show their relations, we discuss the nonmagnetic impurity effect on $s_{x^2y^2}$-wave superconductivity.