Impurity Bound States and Symmetry of the Superconducting Order Parameter in Sr$_2$RuO$_4$

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Abstract

Recent experiments on Sr$_2$RuO$_4$ have indicated the presence of linear nodes in the superconducting order parameter. Among the possible spin triplet states, 2D p-wave superconductivity with $E_u$ symmetry appears to be inconsistent with the experiments, whereas the 2D f-wave order parameter with $B_{1g} \times E_u$ symmetry turns out to be a more likely candidate. Here it is shown how the quasi-particle bound state wave functions around a single impurity provide a clear signature of the symmetry of the underlying superconducting order parameter.
I. INTRODUCTION

In recent years, we have experienced a rapid improvement in the quality of Sr$_2$RuO$_4$ single crystals. This development has lead to a renewed discussion regarding the symmetry of the underlying superconducting order parameter. The data from specific heat measurements [1], NMR results on $T_1^{-1}$ [2], and magnetic penetration depth experiments [3] in very pure single crystals with $T_c \simeq 1.5$K suggest a linear nodal structure in the superconducting order parameter, similar to the $d_{x^2−y^2}$-wave superconductors [4]. Hence, the initially proposed fully gapped 2D $p$-wave superconductivity with $E_u$ symmetry [5] appears to be inconsistent with the experimentally observed nodal structure. On the other hand, the spin triplet nature of the superconductivity in Sr$_2$RuO$_4$ has clearly been established by muon rotation experiments [6] which probe a spontaneous spin polarization, and by the flat Knight shift seen in NMR [7].

Motivated by these recent experiments, several spin triplet order parameters with linear nodes have been proposed [8]. In particular, from a study of the thermal conductivity tensor in a planar magnetic field it has been suggested that the 2D $f$-wave order parameter with $B_{1g} \times E_u$ symmetry is a likely candidate [9]. Furthermore, recent measurements of the angular dependence of the upper critical field have detected a in-plane anisotropy consistent with a $B_{1g} \times E_u$ component to the order parameter [10].

The objective of this paper is to calculate the quasi-particle bound state wave function around non-magnetic impurities in unconventional superconductors with the anisotropic order parameters which have been proposed for Sr$_2$RuO$_4$. It has recently been observed in a series of STM imaging experiments that a Zn-impurity in the high-$T_c$ compound Bi2212 gives rise to such a bound state, leading to a distinct four-fold symmetric pattern in the local tunneling conductance around the impurity [11]. From the theoretical side it was shown that this type of bound state wave function can be interpreted in terms of the solutions of the Bogoliubov-de Gennes equations for $d_{x^2−y^2}$-wave superconductors [12,13]. Here we will perform an analogous analysis for the proposed 2D $p$-wave and $f$-wave order parameters.
II. BOUND STATE WAVE FUNCTIONS

A. 2D p-wave superconductors

For the initially proposed fully gapped odd-parity 2D p-wave superconductivity with an order parameter $\vec{\Delta}(\mathbf{k}) = \Delta z \exp(\pm i\phi)$ the Bogoliubov - de Gennes equations have already been worked out. In particular, when $\Delta(\mathbf{r}) = \Delta = \text{const}$. one obtains

\[ Eu(\mathbf{r}) = \left( -\frac{\nabla^2}{2m} - \mu - V(\mathbf{r}) \right) u(\mathbf{r}) + p_F^{-1} \Delta (i\partial_x - \partial_y) v(\mathbf{r}), \]

\[ Ev(\mathbf{r}) = - \left( -\frac{\nabla^2}{2m} - \mu - V(\mathbf{r}) \right) v(\mathbf{r}) + p_F^{-1} \Delta (i\partial_x + \partial_y) u(\mathbf{r}), \]

where $\mu$ is the chemical potential, and the impurity potential, centered at the site $\mathbf{r} = 0$, is approximated by $V(\mathbf{r}) = a\delta^2(\mathbf{r})$. For simplicity, only the 2D system is considered here.

A simple variational solution of Eqs. (1) and (2) is found to be

\[ u(\mathbf{r}) = A \exp(-\gamma r)J_0(p_F r), \]

\[ v(\mathbf{r}) = A\alpha \exp(-\gamma r)J_1(p_F r) \exp(i\phi), \]

where $p_F$ is the Fermi momentum, $J_i(z)$ are Bessel functions of the first kind, and $A$ is a global normalization factor. By inserting these variational wave functions $u(\mathbf{r})$ and $v(\mathbf{r})$ into the Bogoliubov - de Gennes equations, it follows that $E = -(V/2) \pm \sqrt{(K - V)^2 + \Delta^2}$ and $\alpha = \Delta/(E + K) \simeq 1$, where the kinetic $K$ and the potential $V$ contributions to the energy are defined by

\[ K \equiv \int_0^\infty dr r \left[ (\partial_x \exp(-\gamma r)J_i(p_F r))^2 + (l \exp(-\gamma r)J_i(p_F r)/r)^2 \right] - \mu \simeq \frac{\gamma^3}{mp_F}, \]

\[ V \equiv \int_0^\infty dr r \exp(-2\gamma r)J_0^2(p_F r)V(\mathbf{r}) \simeq (2\pi\gamma p_F) \int_0^\infty dr r \exp(-2\gamma r)J_0^2(p_F r)V(\mathbf{r}). \]

The squares of the wave functions $u(\mathbf{r})$ and $v(\mathbf{r})$ can be observed by scanning tunneling microscopy. The tunneling current, $I(\mathbf{r}, V) \propto \int dE A_S(\mathbf{r}, E)A_N(\mathbf{r}, E + eV)$, is a convolution of the local one-particle spectral function of the normal-state tip, $A_N(\mathbf{r}, E) = \sum_k \delta(E - E_k)$, and that of the superconducting sample, $A_S(\mathbf{r}, E) = \sum_k |u(\mathbf{r})|^2 \delta(E - E_k) + $
The differential tunneling conductance is thus obtained by taking the partial derivative of $I(r, V)$ with respect to the applied voltage $V$,

$$\frac{\partial I}{\partial V}(r, V) \propto \operatorname{sech}^2\left(\frac{eV - E_0}{2T}\right) |u(r)|^2 + \operatorname{sech}^2\left(\frac{eV + E_0}{2T}\right) |v(r)|^2. \tag{7}$$

At small temperatures, the local tunneling conductance around the impurity site is dominated by $|u(r)|^2$ for a fixed binding energy $E_0$ and by $|v(r)|^2$ for $-E_0$.

In Fig. 1(a) and (b), we show $|u(r)|^2$ and $|v(r)|^2$ respectively. The Fermi wave vector $p_F \simeq 2.7/a$ was chosen to be consistent with band structure calculations.\cite{17} The patterns described by the squares of these wave functions are concentric circles without a trace of four-fold symmetry. If the underlying superconducting order parameter is indeed $\vec{\Delta}(k) = \Delta \hat{z} \exp(\pm i\phi)$ the patterns of the local tunneling current around non-magnetic impurities should thus be featureless along the azimuthal direction in the 2D plane.

### B. 2D f-wave superconductors

Let us now consider 2D f-wave superconductors with an order parameter $\vec{\Delta}(k) = \Delta \hat{z} \cos(2\phi) \exp(\pm i\phi)$. Following the above procedure, the corresponding Bogoliubov - de Gennes equations are then given by

$$Eu(r) = \left(-\frac{\nabla^2}{2m} - \mu - V(r)\right) u(r) + p_F^{-3} \Delta (\partial_x^2 - \partial_y^2)(i\partial_x - \partial_y)v(r), \tag{8}$$

$$Ev(r) = -\left(-\frac{\nabla^2}{2m} - \mu - V(r)\right) v(r) + p_F^{-3} \Delta (\partial_x^2 - \partial_y^2)(i\partial_x + \partial_y)u(r). \tag{9}$$

Bound state solutions for this case are found to be of the form

$$u(r) = A \exp(-\gamma r)(J_0(p_Fr) + \beta J_4(p_Fr) \cos(4\phi)), \tag{10}$$

$$v(r) = A \exp(-\gamma r)(\alpha J_1(p_Fr) \exp(-i\phi) + \delta J_3(p_Fr) \exp(3i\phi)). \tag{11}$$

In analogy to Ref.\cite{13}, we obtain

$$E = K - V - \frac{1}{\sqrt{2}} \Delta(\alpha + \delta), \tag{12}$$
\[ E_\alpha = -K\alpha - \frac{1}{\sqrt{2}}\Delta(1 + \frac{\beta}{\sqrt{2}}), \quad (13) \]
\[ E_\beta = K\beta - \frac{1}{2}\Delta(\alpha + \delta), \quad (14) \]
\[ E_\delta = -K\delta - \frac{1}{\sqrt{2}}\Delta(1 + \frac{\beta}{\sqrt{2}}). \quad (15) \]

From Eqs. (12)-(15) we get \( \alpha = \delta = (V - K)/(\sqrt{2}\Delta) \) and \( \beta = (1 - V/(K - E))/\sqrt{2} \). For an impurity with a scattering strength in the unitary limit the energy of the bound state is expected to be very small, \( E \approx 0 \), and \( V \approx \Delta \). This gives \( \beta \approx -1/\sqrt{2} \). On the other hand, in the Born limit \( E \approx \Delta \) and \( V \approx 0 \), which gives \( \beta \approx 1/\sqrt{2} \). In Fig. 2(a) and (b), we plot \(|u(r)|^2\) and \(|v(r)|^2\) for \( \beta = 1/\sqrt{2} \), corresponding to weak scattering. In the limit of strong impurity scattering, \( \beta = -1/\sqrt{2} \), the patterns are changed as shown in Fig. 3(a) and (b). It is observed that for 2D f-wave superconductors with \( \vec{\Delta}(k) = \Delta \hat{z} \cos(2\phi) \exp(\pm i\phi) \), both \(|u(r)|^2\) and \(|v(r)|^2\) have a four-fold symmetry. Depending on the impurity scattering strength, they extend either in the directions of the Ru-O bonds or are tilted by an angle of 45 degrees. The STM imaging of impurity bound states can thus provide a clear signature of the order parameter symmetry for the underlying superconductivity.

**III. CONCLUDING REMARKS**

Stimulated by the successful scanning tunneling microscopy imaging of quasi-particle bound state wave functions around Zn-impurities in Bi2212 [11,18], we have studied the analogous patterns of impurity bound states in Sr\(_2\)RuO\(_4\). By applying the appropriate Bogoliubov - de Gennes equations, the characteristic patterns were distinguished for two proposed order parameters: (i) gapped 2D p-wave (or \( E_u \)) superconductors with \( \vec{\Delta}(k) = \Delta \hat{z} \exp(\pm i\phi) \), and (ii) gapless 2D f-wave (or \( B_{1g} \times E_u \)) superconductors with \( \vec{\Delta}(k) = \Delta \hat{z} \cos(2\phi) \exp(\pm i\phi) \). While the tunneling conductance patterns of the fully gapped odd-parity 2D p-wave superconductor are featureless along the azimuthal direction, a clear four-fold symmetry in \(|u(r)|^2\) and \(|v(r)|^2\) is predicted for the 2D f-wave superconductor.

The experimentally observed in-plane anisotropy of the upper critical field \( H_{c2} \) in
Sr$_2$RuO$_4$ is quite small ($\approx 3\%$). This may indicate that there is a combination of 2D f-wave and p-wave superconductivity in this compound. [10] Furthermore, a possible alternative to the plain 2D p-wave superconductivity considered above would be a 3D $A_{1g}\times E_u$ f-wave order parameter of the form $\tilde{\Delta}(k) = \Delta \hat{z} \cos(ck_z) \exp(\pm i\phi)$. The in-plane impurity bound state patterns for 2D $E_u$ and 3D $A_{1g}\times E_u$ are the same, and a directional probe along the $\hat{k}_z$-direction would be needed to distinguish between these two cases.

Our study suggests that the Bogoliubov - de Gennes formalism in the continuum limit is very useful in addressing the shape of impurity induced bound states. The corresponding bound state wave functions $u(r)$ and $v(r)$ clearly reflect the symmetry of $\Delta(r)$. Therefore the imaging of these wave functions provides unique insight into the underlying symmetry of the order parameter. A similar study of the vortex state is in progress.

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For the high-$T_c$ cuprates, it is known that their superconducting coherence length is rather short, $\xi \approx 10 - 20\text{Å}$. Therefore the impurity induced spatial dependence of the gap function $\Delta(\mathbf{r})$ was neglected in Ref. [13]. In contrast, for Sr$_2$RuO$_4$ $\xi \approx 1\mu m$. Hence a self-consistent treatment of the spatial variation in $\Delta(\mathbf{r})$ may be needed for a more quantitative account of the impurity problem in this material.

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FIG. 1. Spatial variation of the local tunneling conductance, centered at a non-magnetic impurity in a 2D p-wave superconductor with $\bar{\Delta}(k) = \Delta \hat{z} \exp(\pm i\phi)$. In the left figure, the dominant contribution $|u(r)|^2$ at the positive bound state resonant frequency $E_0$ is shown. On the right hand side, the dominant contribution $|v(r)|^2$ at the negative bound state resonant frequency $-E_0$ is shown.
FIG. 2. Spatial variation of the local tunneling conductance, centered at a non-magnetic impurity in a 2D f-wave superconductor with $\Delta(k) = \Delta \hat{z} \cos(2\phi) \exp(\pm i\phi)$. On the left hand side, the dominant contribution $|u(r)|^2$ at the positive bound state resonant frequency $E_0$ is shown. On the right hand side, the dominant contribution $|v(r)|^2$ at the negative bound state resonant frequency $-E_0$ is shown. The solution in this figure corresponds to the weak impurity scattering limit.

FIG. 3. Same as Fig. 2, but for strong impurity scattering.