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Impurity bound states and symmetry of the superconducting order parameter in Sr_2RuO_4

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Recent experiments on Sr_2RuO_4 have indicated the presence of linear nodes in the superconducting order parameter. Among the possible spin triplet states, two-dimensional (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 quasiparticle 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_2RuO_4 single crystals. This development has led 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 two-dimensional (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_2RuO_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 an 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 quasiparticle bound-state wave function around nonmagnetic impurities in unconventional superconductors with the anisotropic order parameters which have been proposed for Sr_2RuO_4. It has recently been observed in a series of scanning tunneling microscopy (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 fourfold 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.[12,13,14] 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 $\vec{\Delta}(\mathbf{k}) = \Delta \hat{z} \exp(\pm i\phi)$ the Bogoliubov–de Gennes equations have already been worked out.[16,17] In particular, when $\Delta(\mathbf{r}) = \Delta = \text{const}$,[15] one obtains

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

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

where μ 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

$$u(\mathbf{r}) = A \exp(-\gamma r) J_0(p_F r), \tag{3}$$

$$v(\mathbf{r}) = A\alpha \exp(-\gamma r) J_1(p_F r) \exp(i\phi), \tag{4}$$

where p_F is the Fermi momentum, $J_l(z)$ 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

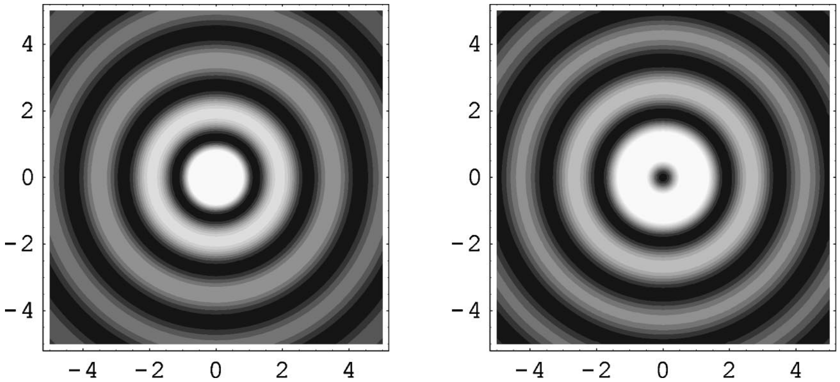

FIG. 1. Spatial variation of the local tunneling conductance, centered at a nonmagnetic impurity in a 2D p-wave superconductor with $\vec{\Delta}(\mathbf{k})=\Delta\hat{z}\exp(\pm i\phi)$. In the left figure, the dominant contribution $|u(\mathbf{r})|^2$ at the positive bound-state resonant frequency E_0 is shown. On the right-hand side, the dominant contribution $|v(\mathbf{r})|^2$ at the negative bound-state resonant frequency $-E_0$ is shown.

$$K\equiv\frac{\int_0^\infty drr\{[\partial_r\exp(-\gamma r)J_l(p_F r)]^2+[l\exp(-\gamma r)J_l(p_F r)/r]^2\}}{2m\int_0^\infty drr[\exp(-\gamma r)J_l(p_F r)]^2}-\mu\simeq\frac{\gamma^2}{2m}, \tag{5}$$

$$V\equiv\frac{\int_0^\infty drr\exp(-2\gamma r)J_0^2(p_F r)V(\mathbf{r})}{\int_0^\infty drr\exp(-2\gamma r)J_0^2(p_F r)}\simeq(2\pi\gamma p_F)\int_0^\infty drr\exp(-2\gamma r)J_0^2(p_F r)V(\mathbf{r}). \tag{6}$$

The squares of the wave functions $u(\mathbf{r})$ and $v(\mathbf{r})$ can be observed by scanning tunneling microscopy.[11] The tunneling current, $I(\mathbf{r},V)\propto\int dEA_S(\mathbf{r},E)A_N(\mathbf{r},E+eV)$, is a convolution of the local one-particle spectral function of the normal-state tip, $A_N(\mathbf{r},E)=\Sigma_k\delta(E-E_k)$, and that of the superconducting sample, $A_S(\mathbf{r},E)=\Sigma_k[|u(\mathbf{r})|^2\delta(E-E_k)+|v(\mathbf{r})|^2\delta(E+E_k)]$. The differential tunneling conductance is thus obtained by taking the partial derivative of $I(\mathbf{r},V)$ with respect to the applied voltage V,

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

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

In Figs. 1(a) and 1(b), we show $|u(\mathbf{r})|^2$ and $|v(\mathbf{r})|^2$, respectively. The Fermi wave vector $p_F\simeq 2.7/a$ was chosen to be consistent with band-structure calculations.[18] The patterns described by the squares of these wave functions are concentric circles without a trace of fourfold symmetry. If the underlying superconducting order parameter is indeed $\vec{\Delta}(\mathbf{k})=\Delta\hat{z}\exp(\pm i\phi)$ the patterns of the local tunneling current around nonmagnetic 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 $\vec{\Delta}(\mathbf{k})=\Delta\hat{z}\cos(2\phi)\exp(\pm i\phi)$. Following the above procedure, the corresponding Bogoliubov–de Gennes equations are then given by

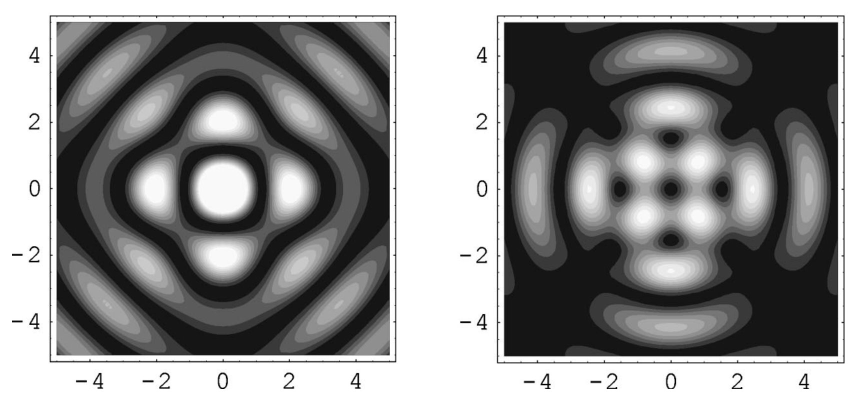

FIG. 2. Spatial variation of the local tunneling conductance, centered at a nonmagnetic impurity in a 2D f-wave superconductor with $\vec{\Delta}(\mathbf{k})=\Delta\hat{z}\cos(2\phi)\exp(\pm i\phi)$. On the left-hand side, the dominant contribution $|u(\mathbf{r})|^2$ at the positive bound-state resonant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

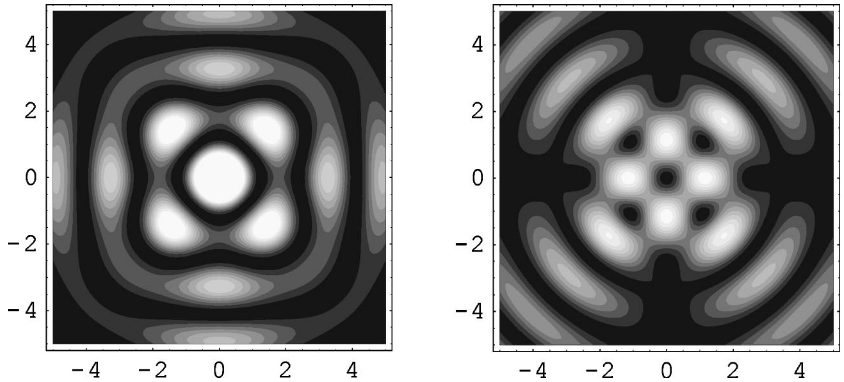

FIG. 3. Same as Fig. 2, but for strong impurity scattering.

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

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

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

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

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

In analogy to Ref. 13, we obtain

$$E=K-V-\frac{1}{\sqrt{2}}\Delta(\alpha+\delta),\qquad(12)$$

$$E\alpha=-K\alpha-\frac{1}{\sqrt{2}}\Delta\left(1+\frac{\beta}{\sqrt{2}}\right),\qquad(13)$$

$$E\beta=K\beta-\frac{1}{2}\Delta(\alpha+\delta),\qquad(14)$$

$$E\delta=-K\delta-\frac{1}{\sqrt{2}}\Delta\left(1+\frac{\beta}{\sqrt{2}}\right).\qquad(15)$$

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, $E\simeq 0$, and $V\simeq\Delta$. This gives $\beta\simeq -1/\sqrt{2}$. On the other hand, in the Born limit $E\simeq\Delta$ and $V\simeq 0$, which gives $\beta\simeq 1/\sqrt{2}$. In Figs. 2(a) and 2(b), we plot $|u(\mathbf{r})|^2$ and $|v(\mathbf{r})|^2$ 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 Figs. 3(a) and 3(b). It is observed that for 2D *f*-wave superconductors with $\vec{\Delta}(\mathbf{k})=\Delta\hat{z}\cos(2\phi)\exp(\pm i\phi)$, both $|u(\mathbf{r})|^2$ and $|v(\mathbf{r})|^2$ have a fourfold 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°. 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 quasiparticle bound-state wave functions around Zn impurities in Bi2212,[11,19] we have studied the analogous patterns of impurity bound states in Sr_2RuO_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 $\vec{\Delta}(\mathbf{k})=\Delta\hat{z}\exp(\pm i\phi)$, and (ii) gapless 2D *f*-wave (or $B_{1g}\times E_u$) superconductors with $\vec{\Delta}(\mathbf{k})=\Delta\hat{z}\cos(2\phi)\exp(\pm i\phi)$. While the tunneling conductance patterns of the fully gapped odd-parity 2D *p*-wave superconductor are featureless along the azimuthal direction, a clear fourfold symmetry in $|u(\mathbf{r})|^2$ and $|v(\mathbf{r})|^2$ is predicted for the 2D *f*-wave superconductor.

The experimentally observed in-plane anisotropy of the upper critical field H_{c2} in Sr_2RuO_4 is quite small (≈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 $\vec{\Delta}(\mathbf{k})=\Delta\hat{z}\cos(ck_z)\exp(\pm i\phi)$. 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 $u(\mathbf{r})$ and $v(\mathbf{r})$ clearly reflect the symmetry of $\Delta(\mathbf{r})$. 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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