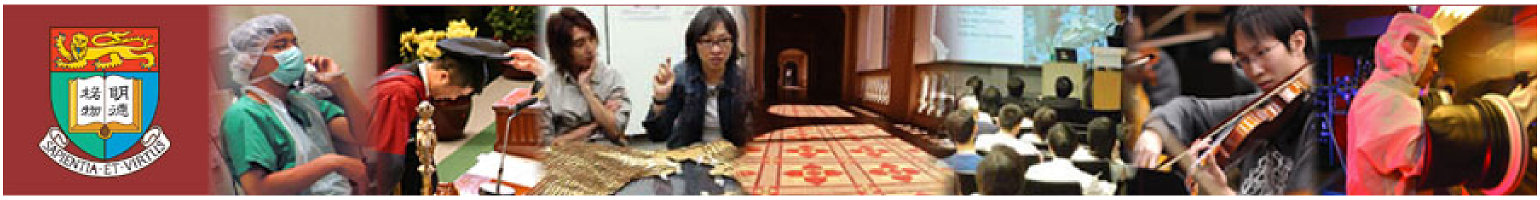

Impurity and interface bound states in $d_{x^2-y^2}+id_{xy}$ and p_x+ip_y superconductors

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Motivated by recent discoveries of novel superconductors such as $Na_xCoO_2 \cdot yH_2O$ and Sr_2RuO_4, we analyze features of quasiparticle scattering due to impurities and interfaces for possible gapful $d_{x^2-y^2}+id_{xy}$ and p_x+ip_y Cooper pairing. A bound state appears near a local impurity, and a band of bound states form near an interface. We obtained analytically the bound-state energy, and calculated the space and energy dependent local density of states resolvable by high-resolution scanning tunnelling microscopy. For comparison we also sketch results of impurity and interface states if the pairing is nodal *p* or *d* wave.

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Recently, Takada *et al.* discovered a novel superconductor $Na_xCoO_2 \cdot yH_2O$ ($x=0.35$) with a superconducting transition temperature $T_c=5K$.[1] A few features of this material bear strong connection to cuprates: (1) It has a layered structure. (2) As Cu^{2+} in cuprates, Co^{4+} atom is in a spin-1/2 state according to first-principles calculation of Singh.[2] Combined with the fact that the cobalt triangular lattice is frustrating to antiferromagnetic ordering, the new material offers a likely situation for the physics of Anderson's resonating valence bond (RVB) theory.[3] Soon after the discovery, theories based on RVB physics[4–7] and renormalization group analysis[8] predicted $d+id'$-wave pairing ($d=d_{x^2-y^2}$ and $d'=d_{xy}$), while other theories suggest p_x+ip_y-wave pairing derived from the weak ferromagnetic instability,[9] in close analogy to the case of Sr_2RuO_4.[10] Identifying the pairing symmetry would be a necessary step toward the understanding of the new superconductor. In this paper, we propose tunnelling measurements of impurity and interface states that are sensitive to both the gap amplitude and the internal phase of the gap function. Such measurements have played invaluable roles in high-temperature superconductors in the context of nodal *d*-wave pairing.[11,12] Our main results are as follows. As a consequence of the full gap as well as the internal phase degrees of freedom of $d+id'$ and p_x+ip_y Cooper pairs, a bound state appears at any nonzero scattering intensity near a local impurity and a band of bound states form near an interface. The bound-state energy is near the gap edge at weak scattering strength, and it approaches zero energy (the Fermi level) at increasing scattering strengths. We also calculated the energy and space dependent local density of states (LDOS), whose rich features are directly resolvable by future scanning tunnel microscope (STM) and can help identify the pairing symmetry in the new superconductors. For comparison, we also mention briefly the results of impurity and interface states for nodal *p*- and *d*-wave pairing.

As usual the elastic scattering problem is best described in terms of the retarded *T*-matrix formulation,

$$G(i,j)=G_0(i,j)+\sum_{a,b} G_0(i,a)T(a,b)G_0(b,j), \qquad (1)$$

where a,b denotes the position of the impurities and all other notations are standard. We suppressed the energy dependence in Green's functions, as it is conserved in elastic scattering. The *T* matrix is given by

$$(T^{-1})(a,b)=(V^{-1})(a,b)-G_0(a,b), \qquad (2)$$

where $V(a,b)$ is the general impurity potential that may be off-diagonal. In our case, G, G_0 and T are further 2×2 matrices in the particle-hole Nambu space. The scattering problem is solved once G_0 is known. The LDOS at site *i* is given by

$$N(i,\omega)=-\mathrm{Im}[G_{11}(i,i;\omega)+G_{22}(i,i;-\omega)]/\pi \qquad (3)$$

with the energy argument ω restored. A peak in $N(i,\omega)$ appears if either $G_{11}(i,i;\omega)$ or $G_{22}(i,i;-\omega)$ diverges. This corresponds to a bound/resonance state if $\mathrm{Det}[T^{-1}(\pm\omega)]=0$ occurs at real/complex energy ω, behaving as an eigenstate/virtual state with finite lifetime. Due to the mixing of particle and hole in the presence of pairing, it is possible that there are two peaks in $N(i,\omega)$ but $\mathrm{Det}(T^{-1})=0$ is satisfied at only one energy, or vice versa. In the following discussion, we always count the bound/resonance states according to the peaks seen in the total density of states $N(i,\omega)$.

Let us write the gap function as , in the momentum space, $\Delta_{\mathbf{k}}=\Delta e^{il\theta_{\mathbf{k}}}$ where Δ is the gap amplitude, $\theta_{\mathbf{k}}$ is the azimuthal angle of the vector $\mathbf{k}$ and $l=0,\pm1,\pm2$ for gapful *s*-, *p*-, and *d*-wave pairing, respectively. We include the case of *s*-wave pairing for comparison. The above pairing function is of simplified form, suitable near the normal-state Fermi surface, and suffices for qualitative discussion of low-energy quasiparticle states. Then $G_0(i,j)=G_0(\mathbf{r})$ (with $\mathbf{r}=\mathbf{r}_i-\mathbf{r}_j$) is given by

$$G_0(\mathbf{r})=\int \frac{d^2\mathbf{k}}{(2\pi)^2}\frac{\omega_+\sigma_0+\epsilon_k\sigma_3+\Delta\sum_\nu e^{i\nu l\theta_{\mathbf{k}}}\sigma_\nu}{\omega_+^2-\epsilon_k^2-\Delta^2}e^{i\mathbf{k}\cdot\mathbf{r}}$$
$$=\frac{\pi N_0\left(\omega_+J_0(k_Fr)\sigma_0+\Delta J_l(k_Fr)\sum_\nu e^{i\nu l\theta_{\mathbf{r}}}\sigma_\nu\right)}{\sqrt{\Delta^2-\omega_+^2}}, \qquad (4)$$

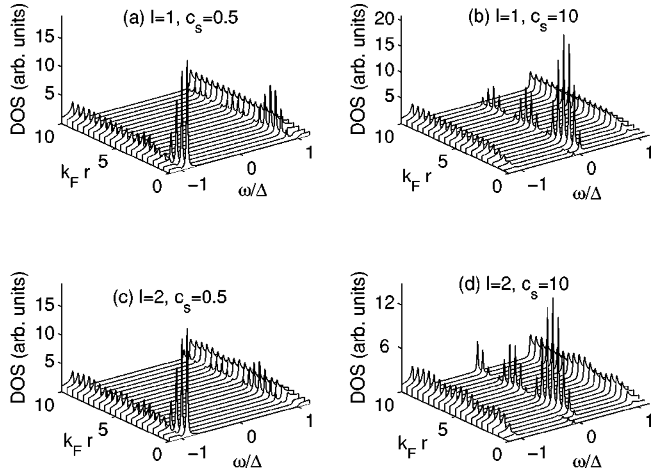

FIG. 1. Density of states as a function of energy ω and the radial distance r off a scalar impurity. See the text for details.

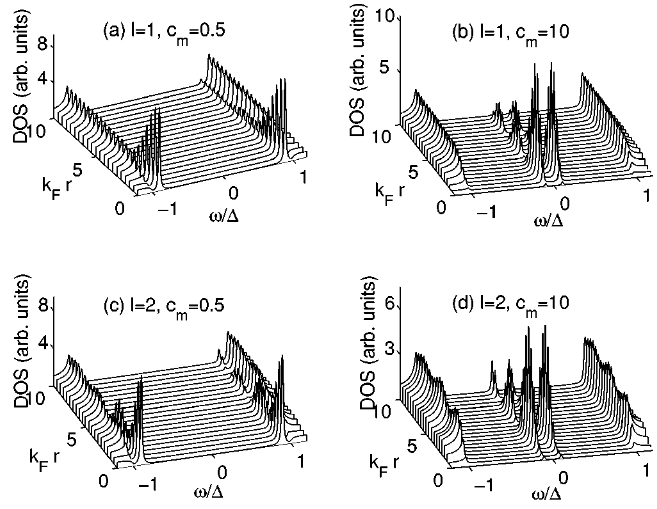

FIG. 2. The same plot as Fig. 1 but for a magnetic impurity.

where $\omega_+ = \omega + i0^+$, $\nu = \pm$, ϵ_k is the normal-state energy dispersion, σ_0 is the 2×2 unit matrix, $\sigma_{1,2,3}$ are the Pauli matrices, $\sigma_\pm = (\sigma_1 \pm i\sigma_2)/2$, and $J_l(u) = \int_0^{2\pi} d\theta \cos(l\theta)\exp(iu\cos\theta)/2\pi$ is the Bessel function. In arriving at the above results, we have assumed a cylindrical Fermi surface with Fermi vectors of magnitude k_F, and constant density of states N_0 near the Fermi level. We emphasize that a particle-hole asymmetry is present in the normal state DOS of Na_xCoO_2. We shall comment on such effects without going into details in the following qualitative discussions.

I. SCATTERING FROM A LOCAL IMPURITY

In this case we set the impurity site at the origin, i.e., $a = b = 0$, and drop these indices in $V = V_m\sigma_0 + V_s\sigma_3$ and $T^{-1} = V^{-1} - G_0(0,0)$, where $V_{m,s}$ is the strength of (classical) magnetic/scalar potential. With G_0 in Eq. (4) at hand, the T matrix is now given by

$$T^{-1} = V^{-1} + \frac{\pi N_0}{\sqrt{\Delta^2 - (\omega_+)^2}}(\omega_+\sigma_0 + \Delta\,\delta_{0l}\sigma_1). \qquad (5)$$

One sees that $\mathrm{Im}(T^{-1}) \to 0$ in the subgap regime $\omega^2 < \Delta^2$, so that a true *bound* state could be generated since the condition $\mathrm{Det}(T^{-1}) = 0$ could be satisfied at real ω.[13] This should be contrasted to the resonant impurity state in the case of nodal d-wave pairing for which the condition is met in general at complex ω.[14] The condition is governed by the dimensionless scattering strengths $c_{m,s} = \pi N_0 V_{m,s}$. A few cases are classified as follows.

For p- and d-wave pairing, the off-diagonal σ_1-component in T^{-1} is zero. This is not an accidental result from the adopted approximation, but rather a rigorous result from the pairing symmetry, which forbids the on-site pairing amplitude [related to the anomalous part of $G_0(0)$] to be finite. Consequently, both scalar and magnetic impurities can generate bound states. (1) For a scalar impurity, $\mathrm{Det}(T^{-1}) = 0$ is satisfied at

$$\omega_b = \pm|\Delta|/\sqrt{1 + c_s^2}. \qquad (6)$$

In general this implies two peaks in the LDOS according to Eq. (3). However, depending on the ratio ω_b^2/Δ^2 one of the peaks may dominate over the other, with an associated change in the spatial dependence of the LDOS. We present a few examples of the energy and space dependent LDOS in Fig. 1 for Cooper pairing with $l = 1,2$. For the weak impurity case $c_s = 0.5$ in Figs. 1(a) and 1(c), ω_b is near the gap edge, the dominant peak is at the energy with opposite sign to c_s, and the corresponding DOS right at the impurity site is maximal. In contrast, for the strong impurity case $c_s = 10$ in Figs. 1(b) and 1(d), ω_b is approaching the Fermi level (zero energy), the dominant DOS peak energy has the same sign as that of c_s, and the corresponding DOS is vanishing right at the impurity site. Note that the cusplike feature at $\omega = \pm\Delta$ away from the impurity is just a feature of the bulk DOS $\mathcal{N}(\omega)$. (2) For a magnetic impurity, $\mathrm{Det}(T^{-1}) = 0$ is satisfied at

$$\omega_b = -\mathrm{sign}(c_m)|\Delta|/\sqrt{1 + c_m^2}. \qquad (7)$$

Since $T^{-1} \propto \sigma_0$ in this case, there are actually two peaks in DOS, according to Eq. (3), located symmetrically with respect to the Fermi level. Examples are shown in Fig. 2, in comparison to Fig. 1. By inspection, we see that except for the symmetrical peaks, Fig. 2 are basically similar to Fig. 1. On the other hand, in both scalar and magnetic impurity cases the difference between $l = 1$ and $l = 2$ is mild. This would pose difficulty for STM to resolve this quantum number. Fortunately this can be resolved easily by other means such as spin susceptibility measurements from the fact that singlet pairing ($l = 2$ here) forms a gap for spin excitations while triplet pairing ($l = 1$ here) does not.

It is pertinent at this stage to comment on the effect of particle-hole asymmetry in the normal state Fermi surface. As can be seen from the derivation of G_0, this would introduce a σ_3 component in $G_0(0,0)$, which effectively acts as an excess energy-dependent scalar potential in T^{-1}. There-

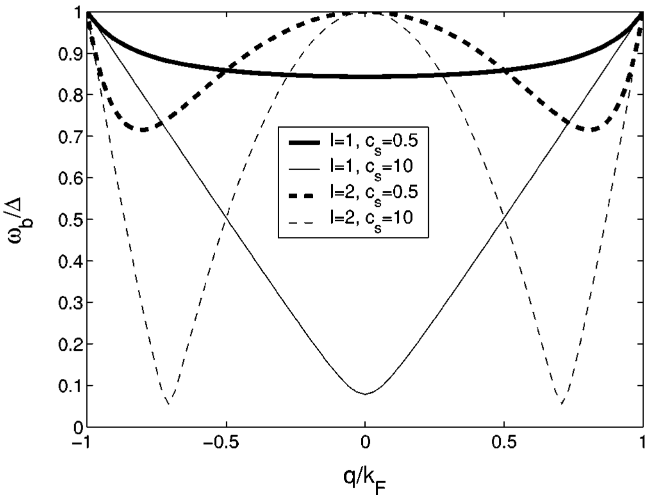

FIG. 3. Dispersion of the positive bound-state energy as a function of the wave vector along the interface. See the text for details.

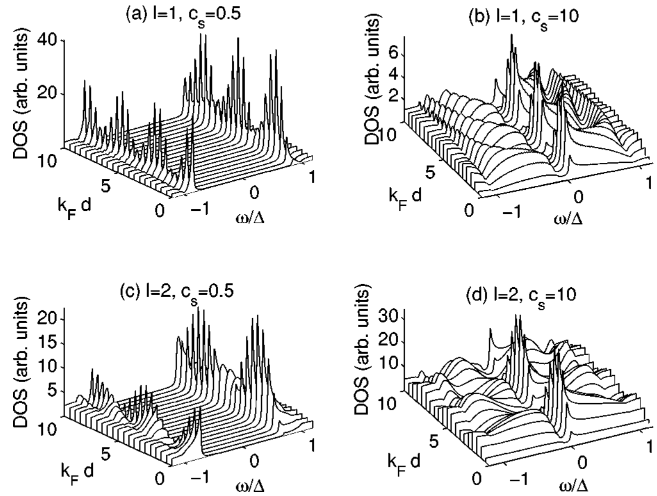

FIG. 4. Density of states as a function of energy ω and the distance d off an interface. See the text for details.

fore, the effect is to modify the bound-state energy, and to break the symmetry of the bound-state energies in the case of magnetic scattering.

II. SCATTERING FROM AN INTERFACE

We shall model an interface by an extended line of impurities. This could be fabricated by chemical erosion. It is to our advantage in that the T-matrix formalism can still be applied. Since the unperturbed system at hand has rotational symmetry, the interface states should not depend on the surface normal direction $\hat{n}$, which we fix to be $\hat{n}=\hat{y}$ for definiteness. Due to the remaining translation symmetry along the x axis, we can do partial Fourier transforms of Eqs. (1), (2), and (4) with respect to x to find the reduced T-matrix equations at the x direction wave vector q as

$$g(y_i,y_j)=g_0(y_i-y_j)+g_0(y_i)tg_0(-y_j), \tag{8}$$

$$g_0(y)\sim\frac{2\pi N_0\left[\omega_+\cos py\sigma_0+\Delta\sum_\nu \cos(py+\nu l\theta_q)\sigma_\nu\right]}{-p\sqrt{\Delta^2-\omega_+^2}}, \tag{9}$$

$$t^{-1}=v^{-1}+\frac{2\pi N_0}{p\sqrt{\Delta^2-\omega_+^2}}(\omega_+\sigma_0+\Delta\cos l\theta_q\sigma_1), \tag{10}$$

where $v=V_m\sigma_0+V_s\sigma_3$ is the same as the form of a single impurity, $p=\sqrt{k_F^2-q^2}=k_F|\sin\theta_q|$ and $\theta_q=\arccos(q/k_F)$. The conserved momentum q is suppressed in the arguments of g, g_0 and t^{-1} for brevity. The problem is reduced to an effective single impurity scattering in one dimension. With the implicit ω and q arguments restored, the partial DOS is given by $N(\omega,y;q)=-\mathrm{Im}[g_{11}(\omega,y;q)+g_{22}(-\omega,y;q)]/\pi$, and the total density of states is $N(\omega,\mathbf{r})=\int dqN(\omega,y;q)/2\pi$, which is independent of x due to the translation symmetry. (The integration over q should be cutoff at $\pm k_F$.) Again $\mathrm{Det}(t^{-1})=0$ would predict a bound state.

Although the above formulation is versatile to deal with any value of $V_{m,s}$, we shall consider only the more likely scalar interface with $V_m=0$. It is easy from the above equations that bound states occur at energies given by

$$\omega_b=\pm\Delta\sqrt{\frac{4c_s^2\cos^2 l\theta_q+k_F^2\sin^2\theta_q}{4c_s^2+k_F^2\sin^2\theta_q}}, \tag{11}$$

which clearly form two bands. (Note that we have taken the lattice constant to be unity so that k_F is dimensionless.) It is also clear that no subgap bound states exist for s-wave pairing $(l=0)$.

The dispersion of the positive bound-state energy is plot in Fig. 3 for weak ($c_s=0.5$, thick lines) and strong ($c_s=10$, thin lines) interface with p wave ($l=1$, solid lines) and d-wave ($l=2$, dashed lines) pairings. Here we have set $k_F=\pi/2$ for calculation. One sees that the energy disperses near the gap edge for weak scattering interfaces, and it tends to cover the whole subgap regime for strong interface scattering. Furthermore, the difference between p- and d-wave pairing is reflected in the number of minima, being identical to l, in the dispersion.

The spatial dependence of the LDOS near the interface can be calculated from the above theory. Examples are shown in Fig. 4. Consistent with the above bound-state energy dispersion, the subgap states are near the gap edge (or tend to cover the whole gap regime) for a weak (or strong) scattering interface, distributed more or less symmetrically (or asymmetrically) with respect to the Fermi level. In the limit of unitary scattering $c_s\to\infty$ (not shown here) the LDOS becomes symmetrical in energy again. An interesting feature in Figs. 4(b) and 4(d) is that the peaks or bumps in energy oscillate with increasing distance from the interface, forming wavelike pattern in the energy-distance space. Moreover, the peaks at lowest absolute energies in Fig. 4 can be related to the dips in the dispersion relations in Fig. 3. This is because the dips corresponds to a large contribution to the density of states. It is also clear from Fig. 4 that the spatial profile decays much more slowly than the single impurity cases in Figs. 1 and 2.

We note that Matsumoto and Sigrist[16] have addressed the quasiparticle states near a sample surface and a topological domain wall (with a π phase shift in the pairing gap) for p_x+ip_y-wave pairing in terms of quasiclassical theory. They found that subgap states appear near the domain wall but not the surface. Our interface is actually a nontopological domain wall but with potential scattering.

III. THE CASE OF NODAL *p*- AND *d*-WAVE PAIRING

Along similar lines to that sketched above, we have also considered the impurity and interface states for nodal *p*- and *d*-wave pairing for comparison. The gap function may be written as $\Delta_{\mathbf{k}}=\Delta\sin l\theta_{\mathbf{k}}$ or $\Delta_{\mathbf{k}}=\Delta\cos l\theta_{\mathbf{k}}$, depending on whether one of the nodal or antinodal directions is along the *x*-axis. Note that there are only one nodal and one antinodal direction for *p*-wave pairing. Due to limited space we sketch the results without going into details.

For the local impurity case, we found resonant energies at $\omega_r\sim\pm\pi\Delta/[lc_{m,s}\ln(4lc_{m,s}/\pi)]$ for a scalar/magnetic impurity. This reduces to the known result in the case of nodal *d*-wave pairing ($l=2$).[14] The new features for the case of nodal *p*-wave pairing is that that LDOS pattern near the impurity is *twofold* symmetric, forming stripelike features extending along the antinodal direction, which should be compared to the fourfold symmetric pattern in the case of nodal *d*-wave pairing.[14,15,17,18]

On the other hand, the interface states depend on the interface orientation: (1) If the (scalar scattering) interface is along one of the nodal directions, say $\hat{x}$, there are bound states at energies $\omega_b=\pm\Delta|k_F\sin\theta_q\sin l\theta_q|/\sqrt{4c_s^2+k_F^2\sin^2\theta_q}$. The definition of θ_q is the same as in Sec. II. All these energies approach zero in the unitary limit $c_s\to\infty$. The abundance of zero-energy states is due to the fact that in this limit quasiparticles reflect spectacularly from the interface, experiencing a sign change of the gap. The same physics is nicely described in Refs. 19,20 in other contexts. (2) Finally if the interface is along one of the antinodal directions, redefined also as $\hat{x}$, there are resonant states exactly at $\omega_r=\pm\Delta\cos l\theta_q$ irrespectively of the scattering strength. In fact this is equivalent to the case of *s*-wave pairing but with a *q*-dependent gap amplitude.

IV. DISCUSSION

We have only shown results for the cases $l=\pm1,\pm2$ that are relevant in the new superconductors, but the theory is clearly general for any integer value of *l*. There are some details missing in the theory, however. First, it does not take into account possible anisotropy in the normal-state Fermi surface. For example, in Na_xCoO_2, the Fermi surface has a rounded hexagonal structure.[2] Such anisotropy may cause corresponding anisotropic LDOS pattern around impurities. Second, Eq. (4) is obtained by fixing the momentum on the Fermi surface while integrating over energy. This possibly leaves out an excess decay of G_0 in space with the length scale $\xi=v_F/\Delta$. Apart from such details, our qualitative analytical results are robust.

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