One-dimensional Surface Bound States in d-wave Superconductors

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We present an exact quantum theory for the bound states in the vicinity of an edge or a line of impurities in a $d_{x^2-y^2}$ superconductor. For a (110)-surface we show that a finite dispersion of the one dimensional band of bound states leads to a two peak structure in the density of states (DOS). We study the effect of an applied magnetic field and a subdominant $id_{xy}$ order parameter on the DOS and discuss the implications of our results for tunneling experiments.

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The existence of a zero bias conductance peak (ZBCP), observed by in-plane tunneling spectroscopy on YBa$_2$Cu$_3$O$_7$ (YBCO) thin films [1-4] has been interpreted as a signature of unconventional superconductivity. In the framework of the quasiclassical approximation, it was first shown by Hu [5] and subsequently studied in more details in Refs. [6,7] that in superconductors with $d_{x^2-y^2}$ symmetry the ZBCP arises from a one-dimensional dispersionless band of surface bound states. Recently Covington et al. discovered the splitting of the ZBCP into two peaks not only in the presence of an applied field, $H$, but also for $H = 0$ below $T_c = 8$ K [8]. Within the quasiclassical approach, the splitting for $H = 0$ was ascribed to a spontaneously broken time reversal symmetry (BTRS) on the surface of YBCO and the generation of a subleading superconducting order parameter with $id_{xy}$ or $is$ symmetry [7]. While in conventional superconductors corrections to the bound state energy beyond the quasiclassical approximation are too small to be observed experimentally, the corrections in high temperature superconductors (HTSC) are of the order of $\Delta_E^2/E_F \approx 3$ meV and thus comparable to the experimentally observed peak splitting. This necessitates a fully microscopic treatment of the problem before a conclusion about the nature of the splitting for $H = 0$ can be reached.

In this Letter we present a microscopic theory which goes beyond the quasiclassical approximation and allows us to capture properties of the ZBCP that eluded earlier investigations. By developing a scattering matrix formalism for one-dimensional (1D) defects, appropriate to describe surfaces or lines of impurities, we show that the band of bound states has a finite dispersion that leads to a two-peak structure in the density of states (DOS), even in the absence of a BTRS. We predict the existence of Friedel oscillations associated with the bound states and show that their spatial dependence varies strongly with the so-called acceptance angle of the measurements. In the presence of a supercurrent or magnetic field the DOS exhibits a four-peak structure for small acceptance angles, but only two peaks with increased frequency splitting for large acceptance angles. We show that the onset of a subdominant order parameter with $id_{xy}$ symmetry leads to a sharpening of the two-peak structure in the DOS, but does not induce any qualitatively new features. Finally, we compare our results with the in-plane tunneling experiments on YBCO [6] and comment on the extensions of our formalism to treat surface bound states in systems with other non-trivial order parameters.

We begin by presenting an exact scattering theory which describes the emergence of a bound state in the vicinity of an interface, e.g., a line of impurities or a surface along the (110) direction, in a $d_{x^2-y^2}$ superconductor. The scattering of the electrons off the interface is described by $U(r) = U\sum_{\mathbf{R}_i}\delta(\mathbf{r}-\mathbf{R}_i)$, where the sum runs over all $\mathbf{R}_i = (x, mx)$. The Green’s function in the presence of this potential is given by

$$\hat{G}(\mathbf{r}, \mathbf{r'}, \omega) = \hat{G}_0(\mathbf{r}-\mathbf{r}, \omega) + \sum_{s,s'}\hat{G}_0(\mathbf{r}-\mathbf{s}, \omega)\hat{T}(\mathbf{s}, \mathbf{s'}, \omega)\hat{G}_0(\mathbf{s'}-\mathbf{r'}, \omega),$$

(1)

where the fourier transform of the scattering $\hat{T}$-matrix only depends on the momentum parallel to the line, $q_{||}$:

$$\hat{T}(q_{||}, \omega) = [1 - U\hat{T}_3\int dp \frac{dp}{2\pi} \hat{G}_0(\mathbf{p}, \omega)]^{-1}U\hat{T}_3.$$  

(2)

$\hat{\tau}_\alpha$ are the Pauli matrices, and the prime restricts the integration to those momenta in the first Brillouin zone (BZ) for which $p_x + mp_y - q_{||} = 2\pi n$, with $n$ integer. For the Green’s function of the clean system one has

$$\hat{G}_0(\mathbf{k}, \omega) = [\omega\hat{\tau}_0 - \epsilon_\mathbf{k}\hat{\tau}_3 - \Delta_\mathbf{k}^{(0)}\hat{\tau}_1]^{-1},$$

(3)

where $\Delta_\mathbf{k}^{(0)} = \Delta_0(\cos k_x - \cos k_y)/2$ is the $d_{x^2-y^2}$ superconducting gap. For the normal state we use a quasi-particle dispersion, representative for the HTSC

$$\epsilon_\mathbf{k} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$$

(4)

with $t = 300$ meV, $t'/t = -0.3$, $\mu/t = -0.99$ and $\Delta_0 = 25$ meV [11].

In the following we consider for definiteness a surface along the (110) direction (with $U = \infty$). The induced surface bound states represent quasiparticles that are localized in the direction perpendicular to the surface, but
have a well defined momentum parallel to it. The dispersion, \( \omega_s(q) \), of these bound states is determined by the poles of the \( T \)-matrix and thus follows from the condition

\[
\int_{\omega_0}^{\omega_0 + \omega_s} d\omega \frac{\epsilon_p}{\omega_0^2 - \epsilon_p^2 - \Delta_p^2} = \pm \int_{\omega_0}^{\omega_0 + \omega_s} d\omega \frac{\omega_s}{\omega_0^2 - \epsilon_p^2 - \Delta_p^2} .
\]

(5)

For a (110)-surface, the integration is restricted to a line of momenta parallel to the (110)-direction (dashed line in the inset of Fig. 1). For small \( q \) the integrals in Eq. (5) can be expanded by standard means, and one finds that the dispersion is quadratic in \( q \) if the Fermi surface (FS) is particle-hole symmetric and linear in \( q \) when this symmetry is absent (as is the case for the FS shown in Fig. 1). In Fig. 1 we present the dispersion of the bound states, obtained from the full numerical solution of Eq. (5), together with the gap edge of the particle-hole continuum.

The coloring indicates the magnitude of \( n(r, \omega) \), the one for a single impurity problem \( [11] \).

In Fig. 2 we plot\( n(r, \omega) \) obtained numerically for \( \Lambda = 1/\sqrt{2} \) and \( \sqrt{2} \). In both cases, the DOS exhibits a two-peak structure and Friedel oscillations (FO) whose spatial dependence is described by \( N(r, \omega) \sim e^{ik_{r,F}r} e^{-r/\xi} \). Both \( k_0 \) and \( \xi \) vary with frequency and through \( \omega_s(q) \) implicitly depend on \( q \). For \( \Lambda = \sqrt{2} \), there exist only two bound states with wave-vector \( q \) for any frequency \( \omega < \omega_s(\Lambda) \) and one has \( k_0(\omega_s) = 2k_{F,\perp}(\omega_s) = \sqrt{2}(k_F^x - k_F^y) \) (see Fig. 3). Moreover, since \( k_0 \) increases with increasing \( |q| \), the wavelength of the FO decreases with increasing \( |\omega| \), as can clearly be seen in Fig. 3a. The lengthscale \( \xi \) for the exponential decay of the FO into the bulk is set by \( \xi = \nu_{F,\perp}/\sqrt{\Delta^2 - \omega_0^2} \geq 1 \), where \( \Delta \) is the superconducting gap at the respective FS crossing. For \( \Lambda = \sqrt{2} \), where we integrate over all \( q \), the FO below and above 4 meV are qualitatively different. For \( \omega \lesssim 4 \) meV there exist four bound states, two close to \( q_0 \) and \( q_π \) (see Fig. 3a), whose superposition
The Doppler-shift varies much more strongly along the lines of integration which preserves the two-peak structure in the DOS, increases the frequency splitting between the two peaks, and leads to a filling-in of the gap between the peaks. Thus, we predict that only for small acceptance angles can a four-peak structure be resolved.

We now turn to the effect of a subdominant order parameter with $d_{xy}$ symmetry and gap $\Delta_{xy}^{(1)} \equiv \Delta_1 \sin k_x \sin k_y$ on the DOS. In Fig. 4 we plot $N(\omega, r_\perp)$ for a superconducting gap with $d_{x^2-y^2}$ (solid line) and $d_{x^2-y^2} + id_{xy}$ symmetry (dashed line). For the latter, we assume that the total superconducting gap is given by $\Delta^{(0)} + i\Delta_{xy}^{(1)}$ with $\Delta_1/\Delta_0 = 0.1$ [5–7]. The DOS at small $\omega$ increases linearly with energy for the $d_{x^2-y^2}$ case and exhibits as expected a gap for the $d_{x^2-y^2} + id_{xy}$ case. Note, that the onset of an $id_{xy}$ component shifts the two peaks to only slightly higher frequencies.

We next comment on the differences between our scattering matrix approach and earlier quasiclassical approaches within the Bogolyubov-deGennes formalism. In the latter, one considers only quasiparticles with a well defined momentum on the Fermi surface, such that for a (110)-surface the incident and reflected quasiparticles experience a superconducting gap of equal magnitude and opposite sign, which leads to a zero energy bound states for all $q_{||}$ [5–7]. This result is exact for $q_{||} = 0$, since here $\Delta(k) = 0$ but for any finite $q_{||}$, the scattering between states away from the FS introduces corrections to the quasiclassical energy. Hence, within our scattering matrix formalism, the quasiclassical results are recovered by restricting the integration in Eq. [5–7] to the Fermi surface which yields $\omega_s = 0$ for all $q_{||}$. The appearance of a dispersing band of bound states is thus a pure quantum effect [5–7], which cannot be obtained by a quasiclassical approximation.

Experiments of [8] on YBCO materials show a single peak above $T_s = 8$ K $\ll T_c$, and the emergence of a
two-peak structure at lower temperatures. This and the small increase in the overall width of the ZBCP was attributed to the appearance of a subleading order parameter \((id_{xy} \text{ or } is)\) below \(T_a\). However, the observed broadening of the ZBCP below \(T_a\) is much smaller than the splitting between the peaks. This is expected if the peak splitting arises not from the appearance of a BTRS, but from the finite bound state dispersion discussed above. A subleading order parameter may sharpen the two-peak structure at lower temperatures and suppress the low energy part of the spectrum but is not predominantly responsible for the peak splitting. Moreover, recent experiments on \(\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{O}_{8+\delta}\) [17], which find that the width of the ZBCP does not increase with the emergence of a two-peak structure in the DOS, are difficult to explain within the BTRS scenario. Currently, experiments using electron-spin resonance [16] and phase sensitive measurements [17] are under way to determine whether a BTRS exists on the surface of HTSC. In addition, detailed measurements of the low energy part of the DOS also provide important information since the DOS for a \(d_{x^2-y^2}\) superconductor is linear at low frequencies, whereas that for \(d+id\) or \(d+is\) order parameters is fully gapped. Another interesting feature of the experiments [8] is that only two peaks are observed in an applied magnetic field, which shift to higher energies with increasing field. One possible explanation of this result is that the acceptance angle of the experiment (see Fig. 3b) is large, in which case the regime of smaller acceptance angles can be accessed in tunneling experiments by using stronger barriers between the superconducting and normal materials. In this limit, we predict that an applied magnetic field induces a four-peak structure in the DOS (Fig. 3b). An alternative explanation is that the acceptance angle is small but that the magnetic field generates a large \(id\) (or \(is\)) component at the boundary that pushes the peaks to higher energies (Fig. 3). Each of the original peaks should then be split into two, however such splitting may be too small to be observed experimentally. The latter scenario is consistent with a strong decrease in the DOS at zero energy with increasing magnetic field [9].

Finally, the bound states discussed above provide an interesting new class of one dimensional fermions whose dispersion can be changed continuously by applying a magnetic field (or supercurrent), with the possibility of making all fermions chiral [13]. Moreover, the formalism presented above can be generalized to study surface bound states in systems with other non-trivial order parameters, such as \(d\)-density or spin density wave states suggested recently [19]. We find that a zero energy bound states also exists for a \(d\)-density wave state in the vicinity of a (110) surface. This bound state can be observed in tunneling experiments and may thus prove to be an important feature of the underdoped cuprates; an account of our results will appear elsewhere [18].

In summary we present an exact scattering theory for bound states which are induced close to lines of impurities or surfaces in a \(d_{x^2-y^2}\) superconductors. We find that these bound states disperse linearly with momentum \(q\), a dispersion that gives rise to a two-peak structure in the density of states. For small acceptance angles, we predict that an applied magnetic field leads to a splitting of the two peaks into four, while for a large acceptance angle, there exist only two peaks. Our results are consistent with recent in-plane tunneling experiments on YBCO and provide important insight into their interpretation. We present detailed predictions for the spatial dependence of the Friedel oscillations in the DOS that may be measured by the STM experiments near the surfaces, grain boundaries, or lines of impurities.

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