Doppler Shift of the Andreev Bound States at the YBCO Surface

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The effect of applied magnetic field on the zero-bias conductance peak (ZBCP) observed in tunneling spectra of YBCO reveals the number of states is conserved; the splitting magnitude depends upon field orientation and hysteresis. Both the conservation and anisotropy are consistent with the ZBCP resulting from quasiparticle (QP) Andreev bound states at the YBCO surface with a Doppler shift arising from the scalar product between the QP velocity and superfluid momentum, $\mathbf{v}_F \cdot \mathbf{P}_S$. The hysteresis is consistent with the effects of strong vortex pinning on the surface screening currents.

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The zero-bias conductance peak (ZBCP) observed in tunnel junctions fabricated on high T_c [1] superconductors remains a topic of broad interest. Further attention to this subject was stimulated by the suggestion that the ZBCP observed in the in-plane tunneling spectra of $YBa_2Cu_3O_7$ (YBCO) is associated with zero-energy surface bound states that arise in the d-wave model of superconductivity [2] and rely on broken reflection symmetry of the unconventional order parameter at the surface [3]. Consider a specular (110)-oriented surface of a $d_{x^2-y^2}$ symmetry superconductor. The sign change of the order parameter causes an incoming quasiparticle (QP) to experience a strong Andreev reflection at the surface. A bound state results from the constructive interference of electronlike and holelike excitations which originate from such a reflection. This occurs for energies which fulfill the quantum condition on the total phase shift of the QP [4]. For a d-wave symmetry superconductor, the intrinsic π-phase shift of the condensate produces zero-energy bound states, in analogy to the vortex-core bound states where the superfluid circulation provides the π-phase shift [5]. Previous experiments that provide detailed dependence of the ZBCP on crystallographic orientation [1,6], barrier transparency [7], temperature [8], magnetic field [1,8], doping [9], and ion-induced damage [10] indicate that ZBCP does arise from surface-induced Andreev bound states (ABS).

Recently, to explain the magnetic field dependence of the ZBCP observed in YBCO/Pb and YBCO/I/Cu junctions [8], Fogelström, Rainer, and Sauls (FRS) [11] suggested that these surface states move from zero to finite energy in the presence of supercurrents. More precisely, at the surface the ABS interact with the superfluid producing two major effects. First, the ABS are shifted in energy by a Doppler-like term, $\mathbf{v}_F \cdot \mathbf{P}_S$, where $\mathbf{v}_F$ is the QP Fermi velocity and $\mathbf{P}_S$ is the field-induced superfluid momentum, which is revealed as a field-induced splitting of the ZBCP, as described below. Second, the low-temperature penetration depth increases as a result of counterflowing currents carried by the ABS [12].

A striking consequence of the FRS theory is the dependence of the magnitude of the Doppler shift upon the angle between the QP trajectory and the superfluid momentum. Therefore, if the QP's in YBCO are confined to the ab plane, the Doppler shift should present a strong anisotropy as a function of the orientation of an external magnetic field. In particular, it should be zero when the field is applied parallel to the ab plane and maximum when the field is perpendicular. Furthermore, as the magnitude of the bound state depends upon the magnitude of the bulk d-wave gap [11], the ABS, corresponding to larger Doppler shifts and hence to smaller angles, exhibit larger spectral weight. Experimentally, this leads to the observation of a distinct splitting of the ZBCP in the tunneling spectra [8] and allows a k-resolved spectroscopy of these surface states. In that earlier work, a systematic study of the directional dependence of the splitting as a function of the applied magnetic field was not done. The data reported in this Letter are the first that explicitly show that the quasiparticles in the ABS experience highly anisotropic transport properties, thus providing the key spectroscopic evidence for the ABS origin of the ZBCP, and eliminating other possibilities.

The principal result of this Letter is presented in Fig. 1. The QP density of states (DOS) of (110)-oriented YBCO thin films is measured on YBCO/Pb junctions at 1.5 K, as described below. An external magnetic field is applied parallel to the junction interface, and either parallel or perpendicular to the ab planes. For fields higher than the Pb critical field, the Pb is driven normal so that only the YBCO DOS is probed. Conductance data obtained at low applied field are independent of field orientation, as is seen in the data obtained on junction 2 at $H = 0.2$ T. Data obtained at higher fields exhibit a dependence on the angle between field and the normal to the ab plane, as exhibited by the conductance of junction 2, taken in an applied field of $H = 5$ T. When the field is perpendicular to the ab plane, $H_\perp$, the splitting of the ZBCP is significantly greater than that observed when the field is parallel to the ab plane, $H_\parallel$. We point out that the $H_\parallel$ data obtained in the configuration at 5 T is similar to that obtained at 0.2 T and is compatible with a small misalignment of H. This behavior is consistent with the

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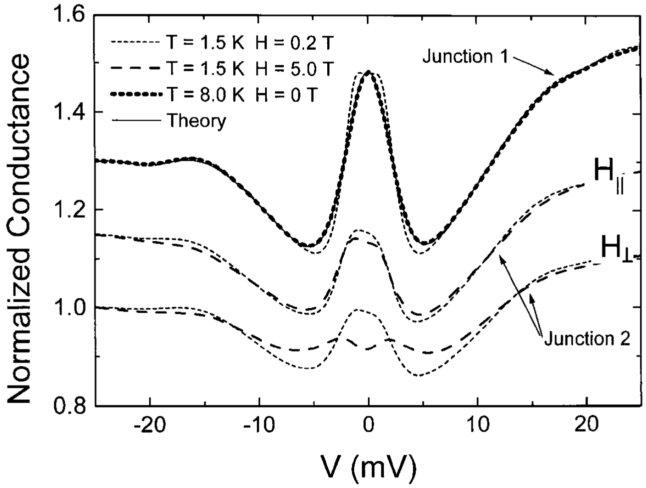

FIG. 1. The temperature dependence of the in-plane tunneling conductance of (110)-YBCO/Pb junctions as function of bias and magnetic field is shown. The field H is always applied parallel to the junction interface, and either parallel or perpendicular to the YBCO *ab* planes, as labeled. The theoretical curve (solid line) is calculated using the FRS theory [11], as described in the text. For junction 2, low-temperature spectra for low and high applied magnetic field are shown. Note the field-induced splitting in the ZBCP is strongly anisotropic with respect to the field orientation. Data obtained on junction 1 show reproducibility between junctions for data taken at low temperature and field ($T = 1.5$ K, $H = 0.2$ T). Zero-field data taken at a temperature above the T_c of Pb is also shown for junction 1.

anisotropy expected for the Doppler shift described by the FRS theory. Moreover, integration of the curves in Fig. 1 over the ± 25 meV range reveals that the tunneling spectra conserve 85%–90% of the QP states, indicating the YBCO DOS is being probed.

Thin films of (110)-oriented YBCO are grown by off-axis magnetron-sputter deposition [13]. The c axis is parallel to the sample edge within 1%, and x-ray diffraction reveals no secondary phase. The resistivity anisotropy, $\rho_c/\rho_{ab} \sim 50$ at $T = 100$ K [13] is in agreement with that reported for single crystals, suggesting that all the grain boundaries are aligned perpendicular to the c axis, as expected for (110)-oriented films [14]. An *ex situ* evaporation of 5000-Å-thick and 0.1-mm-wide Pb counterelectrodes naturally forms the insulating tunnel barrier [15] with typical surface resistances of order 0.02 Ω cm^2. The mean barrier height derived from the background tunneling conductance [16] is $\sim$0.3 V, which is approximately 100 times larger than the features discussed in this Letter. The tunneling cone, defined as the angle corresponding to half transmission probability, is $\theta_c \sim 15°$ [17], consistent with low barrier transparency [7]. Conductance data show junction leakage as low as 5% at $T = 1.5$ K, a well-defined Pb gap and phonons at the correct energies, ensuring that elastic tunneling is the main transport mechanism through the barrier. When the Pb is driven normal, the measured YBCO tunneling spectra (Fig. 1) are typical for those observed in junctions formed on all *ab*-plane oriented films [1,8,10], including a ZBCP of height approximately 30%–40% of the background conductance and full width at half maximum of $\sim$5 meV, a gaplike feature at $\sim$16 meV and a parabolic background conductance, which we attribute to the barrier shape [16].

Quantitative analysis of the data in Fig. 1 allows for an accounting of the magnitude of the ZBCP splitting, the shape of the tunneling spectra, and the temperature dependence. Here we focus on the ZBCP behavior when the magnetic field is perpendicular to the *ab* plane. In the FRS theory, the ABS contribution to the angle resolved DOS can be approximated by a Lorentzian centered at the energy of the bound state $E_B(\theta)$, as also pointed out by Walker [18].

As mentioned earlier, $E_B = \mathbf{v}_F \cdot \mathbf{P}_S = v_F P_S \cos\theta$ defines the Doppler shift, where θ is the angle between the ABS QP trajectories and the superfluid momentum. The ABS spectral weight is given by the d-wave gap function, where $\Delta_d(\theta) = \Delta_0 \sin(2\theta)$; the width is given by $\Gamma = \gamma[\Delta_0/\Delta_d(\theta)]$, where γ is a broadening parameter determined by surface defects and roughness [19,20]. Consequently, the lifetime of the ABS depends on the QP trajectory. The tunneling DOS is derived by integration of the angle resolved DOS multiplied by the tunneling probability distribution $W(\theta)$:

$$N_T(E) = \int_{-\theta_c}^{+\theta_c} \Delta_d(\theta) \frac{\Gamma^2(\theta)}{[E - E_B(\theta)]^2 + \Gamma^2(\theta)} W(\theta)\, d\theta \,.$$

Here we take $W(\theta) = 1$ for $|\theta| < \theta_c$, and 0 elsewhere.

In Fig. 2 the tunneling conductance of junction 2 obtained in applied fields of 0.2 to 5 T, normalized by the continuum at $H = 0.2$ T, is presented. Assuming that the tunneling conductance is proportional to the surface DOS, the data are fit using the formula above, leaving the product $v_F P_S$ and γ as fitting parameters. Corrections for thermal broadening produce negligible changes on the fits. We find $\gamma = 0.8 \pm 1$ meV, independent of the applied magnetic field. As seen in Fig. 2, there is an overall good fit of the theoretical curves with the data, with clear deviations near 5 and 18 meV. These deviations likely arise from crude approximations for the ABS lifetimes, tunneling parameters, including the size of the tunneling cone and magnitude of the surface roughness, and the disregard for the field-induced shift in the continuum [11,20]. Finally, we test the accurateness of our procedure by recovering the FRS results [11] for a larger tunneling cone as shown in inset (a) of Fig. 2. Here the parameters obtained from the fits, renormalized to the energy scale of Ref. [11], reproduce approximately the same ZBCP splitting, δ. Note that in the FRS theory, a larger tunneling cone allows a better resolution of the splitting. Since YBCO is orthorhombic, the bulk order parameter is likely to contain a small admixture of an s component, yielding $d + s$. The resulting small shift in the nodes

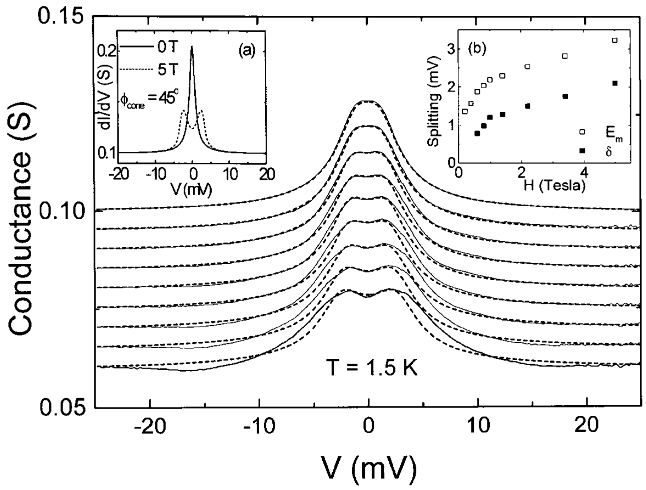

FIG. 2. The dependence of the zero-bias conductance peak for applied magnetic fields of $H = 0.2$, 0.4, 0.6, 0.8, 1.0, 2.2, 3.4, and 5.0 T is analyzed quantitatively. The curves are normalized, as described in the text, and shifted for clarity. The dotted lines represent the best fits obtained from the FRS theory, leaving $v_F P_S$ and γ as fitting parameters. The low-energy spectra predicted by the theory for a larger tunneling cone are recovered in inset (a). In inset (b) the maximum Doppler shift $E_m = v_F P_S \cos(\pi/2 - \theta_c)$ and the ZBCP splitting δ are both shown as a function of applied field H.

from the (110) direction is insignificant in comparison to the Doppler-shift anisotropy, which is determined by the *ab*-plane vs c-axis Fermi velocities.

Let us now focus on the $v_F P_S$ parameter itself. The field dependence of the maximum Doppler shift $E_m = v_F P_S \cos(\pi/2 - \theta_c)$ corresponds to the higher angle QP trajectories probed by tunneling, where $\theta_c \sim 15°$ is the maximum in the tunneling cone angle. As shown in Fig. 2, inset (b), with increasing field, the screening increases and produces larger Doppler shifts, consistent with earlier measurements [1,8]. An upper bound for E_m is set by the depairing current, and hence, we expect E_m to be smaller than $\Delta_0 v_F P_S \cos(\pi/2 - \theta_c) \sim 3.5$ meV, where Δ_0 is the d-wave gap maximum as always verified. Because of the integral in the tunneling conductance, δ is smaller than E_m, by a constant offset of roughly 1 meV. The energy scale of E_m is a factor of 10 larger than what is expected for a Zeeman splitting in the ZBCP [8]. We also observe that E_m at small field is consistently nonzero, although comparable with γ. The finite value of E_m in zero field and low temperature is consistent with a superconducting state with broken time-reversal symmetry (BTRS) [8].

If E_m at zero field is set by the spontaneously induced supercurrents, it should decrease with increasing temperature and disappear for $T > T_s$, where T_s is the transition temperature from the BTRS state. To investigate this point, we extended the modeling of the ZBCP in zero applied field to account for thermal population effects: The DOS is convolved with the derivative of the Fermi function at the appropriate temperature. In Fig. 1 (junction 1), we fit the spectrum taken at $T = 8$ K with the formula introduced above for the DOS, but with a reduced $v_F P_S$ value. The other fitting parameters are those obtained from the curve at low temperature, $T = 1.5$ K, and $H = 0.2$ T. The magnitude of the ZBCP and the shape of the continuum are also taken into account to reproduce the behavior at higher bias. A striking agreement between the data (dots) and the fit (solid line) is found for $E_m = 0.8$ meV. We note that the temperature dependence of the tunneling conductance conserves the number of QP states, as also found for the field dependence, and E_m is finite at 8 K. The broadening of the ABS, γ, is the same order of magnitude, so a value for T_s cannot be derived. However, these data suggest that the splitting of the ZBCP in zero field may persist to higher temperatures. A larger zero-field splitting, which can be provided by, for example, an increase of the tunneling cone, would give better energy resolution and would therefore provide more detailed information on the T_s origin and value.

The FRS theory describes the coupling of the screening currents with the surface bound states in the Meissner limit. In this limit, the superfluid momentum at the surface, and hence the Doppler shift, should increase linearly with applied magnetic field, until the screening currents reach the bulk critical density, $H_C \sim 2.5$ T [11]. SQUID measurements of the bulk magnetization indicate vortex penetration into the YBCO at fields greater than $\sim$0.04 T. Thus, in the range of fields we have investigated, the distribution of the surface currents depends upon the number and distribution of flux quanta. The field dependence of E_m and δ deviates from linearity, as shown in the Fig. 2 inset, and exhibits magnetic hysteresis, as shown in Fig. 3. This hysteresis is consistent with strong vortex pinning at low temperature. No detectable hysteresis is measured at biases above $\sim$25 meV, nor in the magnetic coil without a film. A similar hysteresis observed in thermal conductivity of optimally doped BSCCO remains, to our knowledge, unexplained [21].

The field-induced splitting in the ZBCP and its hysteresis have been observed in junctions fabricated both on (110)- and (103)-oriented films. The tunneling spectra obtained on (103)- and (110)-oriented films is indistinguishable because nanofaceting on the scale of the coherence length ($\xi_{\rm ab} = 20$ Å) allows the ZBCP to be observed in all $(x, y, 0)$-oriented surfaces with comparable spectral weight [11]. In (103)-oriented films this faceting is observed to be 100–200 Å along the (010) direction, as measured by scanning electron microscopy. We point out that for (103)-oriented YBCO/Pb junctions, grain boundaries and junction geometry do not allow precise control of the field orientation with respect to the YBCO c axis. This prevents any quantitative analysis of the field dependence of the ZBCP and also explains why the ZBCP splitting, as opposed to the maximum Doppler shift E_m, is reported in Fig. 3.

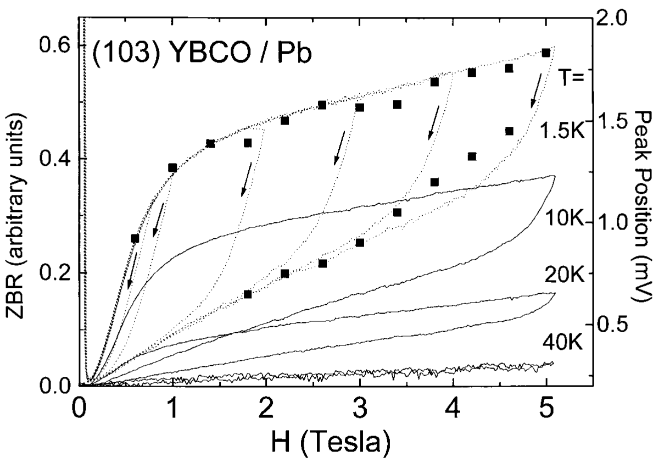

FIG. 3. The hysteresis loops of the ZBCP splitting δ (right axis, squares) and zero-bias resistance, ZBR (left axis, lines), are reported for a (103)-YBCO/Pb junction as a function of magnetic field for several temperatures.

The zero-bias resistance, ZBR, as a function of applied field is plotted along with the points showing the ZBCP splitting in Fig. 3. Note that both exhibit approximately the same field dependence, allowing details of the magnetic behavior of the ZBCP to be studied by measuring the ZBR. We have verified that the ZBR curve is independent of the field rate of change, so dynamical effects do not need to be considered. The ZBR loops, obtained at different temperatures and maximum fields, are also shown in Fig. 3. The loop size decreases in amplitude with increasing temperature and disappears at 40 K, as does the ZBCP [1,8]. The fast decrease of the ZBR at very low field is due to the quenching of the Pb superconducting transition. We measure 0.06 T for the Pb critical field at $T = 4.2$ K. Below $H = 0.5$ T, the field dependence of the ZBR is completely reversible. Hysteretic behavior develops only above $H = 0.75$ T. These hysteresis curves are reproducible, the loops are closed at zero field, and they are symmetric to field inversion. A model of the hysteresis in the ZBCP, which takes into account the ABS coupling with surface supercurrents and includes pinning effects for different vortex densities near the surface for increasing and decreasing field, is under investigation [22].

In summary, the field-dependent DOS is conserved as revealed by the in-plane tunneling conductance of YBCO/Pb tunnel junctions. The magnetic field-induced splitting in the ZBCP shows hysteresis and anisotropy depending on the field orientation. The hysteresis may be related to strong vortex pinning. The anisotropy can be quantitatively accounted for by the FRS theory allowing a k-dependent spectroscopy of the Andreev bound states generated at the surface of an unconventional superconductor [23].

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