Nonlinear magnetic field dependence of the conductance in d-wave 
NIS tunnel junctions

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The ab-plane NIS-tunnelling conductance in d-wave superconductors shows a zero-bias conductance peak which is predicted to split in a magnetic field. In a pure d-wave superconductor the splitting is linear for fields small on the scale of the thermodynamic critical field. The field dependence is shown to be nonlinear, even at low fields, in the vicinity of a surface phase transition into a local time-reversal symmetry breaking state. The field evolution of the conductance is sensitive to temperature, doping, and the symmetry of the sub-dominant pairing channel.

Tunnelling into an unconventional superconductor probes the quasiparticle spectrum associated with a surface superconducting state that is typically strongly deformed, and may have different local symmetry, than the bulk order parameter (OP) \[ \mathcal{O} \]. Indeed, the OP of a pure \( \delta_{x^2-y^2} \) superconductor is suppressed at a [110] surface. The suppression is associated with the formation of zero-energy Andreev states that are bound to the surface (ABS). The ABS is observable as a zero-bias peak (ZBCP) in the tunnelling conductance \[ \mathcal{R} \]. This property makes quasiparticle tunnelling in unconventional superconductors a sensitive probe of broken symmetry. A key signature of a surface ABS is its dependence on an applied magnetic field, or more precisely on screening currents flowing along the surface. For an external magnetic field perpendicular to the conducting plane and parallel to the surface, screening currents produce a Doppler shift \[ \delta \mathcal{R} \] which is observable as a splitting, \( 2 \delta \mathcal{R} \), of the ZBCP with applied field. Some of the predicted field dependence of the splitting has been verified experimentally by Covington et al. \[ \delta \mathcal{R} \], Aprili et al. \[ \delta \mathcal{R} \], and Krupke and Deutscher \[ \delta \mathcal{R} \] for \( \text{YBa}_2\text{Cu}_3\text{O}_{7-p} \) (YBCO) near optimal doping.

It was shown theoretically that a surface phase transition into a state with spontaneously broken time-reversal (T) symmetry should occur for a d-wave superconductor with strong surface pair breaking if there is an attractive subdominant pairing channel \[ \mathcal{Q} \]. A signature of this transition in the tunnelling conductance is a spontaneous splitting of the ZBCP which develops below a surface phase transition temperature, \( T_s \). Such a transition was observed by Covington et al. \[ \mathcal{Q} \] for \( \text{CuI|YBCO} \) junctions, and also by Krupke, et al. \[ \mathcal{Q} \] and Dagan et al. \[ \mathcal{Q} \] for \( \text{InI|YBCO} \) junctions. The latter authors found that the spontaneous splitting of the ZBCP occurred only above a critical doping level, \( p_c \), close to optimal doping. They also showed that the magnitude of the field-induced splitting of the ZBCP is suppressed at low fields for slightly overdoped materials \( p \approx p_c \), while for \( p \approx p_c \), \( \delta \mathcal{R} \) is nonlinear in \( H \) and onsets rapidly. For slightly overdoped YBCO \( (p \gtrsim p_c) \), \( \delta \mathcal{R} \) increases linearly with \( H \) at low field from a non-zero splitting in zero field.

In this Letter we report calculations of the field dependence of the conductance of NIS tunnel junctions in YBCO. We consider a pairing interaction that includes both magnetic and phonon-mediated pairing channels \[ \mathcal{Q} \].

\[
\lambda(q) = \sum_{\delta_{x,y}} \frac{\lambda_{af}}{4} \left( 1 + 4 \xi_{af}^2 \left( \cos^2 \frac{q_{x} - \delta_{x}}{2} + \cos^2 \frac{q_{y} - \delta_{y}}{2} \right) - \lambda_{ep} \right) \tag{1}
\]

The repulsive magnetic contribution to \( \lambda(q) \) results from exchange and short-range spin correlations, and is assumed to dominate a weaker, attractive electron-phonon contribution to the pairing interaction. The interaction depends on the correlation length, \( \xi_{af} \), the incommensurate wave vectors for the spin-excitation spectrum, \( \delta_{x,y} \), and the electron-phonon and magnetic coupling strengths, \( \lambda_{ep} \) and \( \lambda_{af} \). The quasiparticle dispersion relation is modelled by the tight-binding parametrization for YBCO taken from Ref. \[ \delta \mathcal{R} \]. The phonon-mediated interaction is assumed to be attractive in the spin-singlet, s-wave (\( A_{1g} \)) pairing channel. Indirect evidence for an attractive sub-dominant s-wave interaction in the cuprates comes from ab-plane tunnelling measurements on Pr-doped YBCO which show strongly suppressed transitions, \( T_c \lesssim 20 \text{K} \), and no ZBCP indicative of d-wave superconductivity \[ \delta \mathcal{R} \]. For this pairing interaction and band structure we calculated the eigenvalues \( \lambda_{f} \) and eigenfunctions, \( \psi_f(D_{4h}) \), of the linearized gap equation following Refs. \[ \delta \mathcal{R} \]. The eigenfunctions determine the anisotropy of the pairing state in momentum space and form basis functions for the irreducible representations (\( \Gamma \)) of the point group, \( D_{4h} \). The eigenvalues determine the instability temperatures \( T_c^\mathcal{Q} \), for pairing into states with symmetry dictated by the corresponding irreducible representation. The pairing interaction in Eq. (1) allows us to examine the sensitivity of the dominant and sub-dominant pairing channels to the parameters defining the model: \( \xi_{af}, \delta_{x,y} \), and the
coupling parameters, $\lambda_{\text{ep},\text{af}}$, and to consider the doping dependence via these parameters. We consider the one-dimensional, spin-singlet representations, $A_{1g}, A_{2g}, B_{1g}$, and $B_{2g}$. The most attractive eigenvalues calculated for the two-channel interaction are shown in Fig. 1 as a function of $\delta$. Note that all four channels have attractive eigenvalues for incommensurate spin-fluctuations \( \xi_{\text{af}} \) of its eigenfunctions and eigenvalues: $\lambda_{\text{ep}} < 0.1 \lambda_{\text{af}}$.

The eigenfunctions, $\eta_{\text{af}}(p_f)$, also depend on the parameters of the pairing model: $\eta_{A_{1g}}, \eta_{B_{2g}}$, and $\eta_{A_{2g}}$ depend most sensitively on $\xi_{\text{af}}$ and $\delta_{x,y}$, while $\eta_{A_{1g}}$ also depends on $\lambda_{\text{ep}}$. The calculated basis functions are shown in Fig. 1 for $\lambda_{\text{ep}} = 0$; $\eta_{A_{1g}}$ is well described by the simplest $d_{x^2-y^2}$ basis function, $\eta_{\text{af}}(\phi_f) = \sqrt{2}\sin(2\phi_f)$, where $\phi_f$ is the angle $p_f$ makes with respect to the [100] direction of the crystal. For the $B_{2g}$ channel the calculated basis function is not the simplest $d_{xy}$ basis function, $\eta_{\text{af}}(\phi_f) = \sqrt{2}\sin(2\phi_f)$, but a higher harmonic which to a good approximation is $\eta_{B_{2g}}(\phi_f) \approx 2|\sin(2\phi_f)|\sin(6\phi_f)$. The $A_{1g}$ basis function is highly anisotropic for $\lambda_{\text{ep}} < 0.1 \lambda_{\text{af}}$ but nearly isotropic for $\lambda_{\text{ep}} > 0.1 \lambda_{\text{af}}$. The $A_{1g}$ basis function is good approximation given by, $\eta_{A_{1g}}(\phi_f) = (2/\sqrt{1 - 2\alpha + 5\alpha^2})(\alpha - (1 - \alpha)\sin(2\phi_f)\sin(6\phi_f))$, where the parameter $\alpha$ varies between $\alpha = 0$ for $\lambda_{\text{ep}} \ll 0.1 \lambda_{\text{af}}$ and $\alpha = 1$ for $\lambda_{\text{ep}} \gg 0.1 \lambda_{\text{af}}$. In general $\alpha$ varies with doping and provides us with a convenient parametrization of the effect of doping on the pairing eigenfunctions.

The basis functions, $\eta_{\text{af}}(p_f)$, $T_c$, and the relative coupling strengths of the sub-dominant pairing channel are inputs to calculations of the surface phases and tunneling conductance for d-wave models of the cuprates. The surface OP, $\Delta(p_f, R) = \sum_{\text{ep}} \Delta_{\text{ep}}(R)\eta_{\text{af}}(p_f)$, condensate momentum, $p_s$, and excitation spectrum are obtained, selfconsistently, from solutions for the propagator, spectral density and OP describing the superconducting state. The propagator obeys the quasiclassical transport equations [15], and the OP, $\Delta(p_f, R)$, is determined by the anomalous quasiclassical propagator, $\tilde{\Phi}(p_f; R; \epsilon_n)$, through the BCS gap equation,

$$
\Delta(p_f, R) = T \sum_{\epsilon_n} \int d^2p'_f \lambda(p_f - p'_f) \tilde{\Phi}(p'_f; R; \epsilon_n).
$$

The pairing interaction, $\lambda(p_f - p'_f)$, is resolved in terms of its eigenfunctions and eigenvalues: $\lambda(p_f - p'_f) = \sum_{\text{ep}} \lambda_{\text{ep}}\eta_{\text{af}}(p_f)\eta_{\text{af}}(p'_f)$, and we eliminate the interaction parameters, $\lambda_{\text{ep}}$, and cutoff frequency, $\epsilon_n$, in favor of the measurable instability temperatures, $T^2_\text{IN}$. The formulation and application of the quasiclassical transport equations to surface states and tunneling is described in Refs. 2, 15, 14.

The surface superconducting phase is sensitive to magnetic fields that generate surface screening currents. These currents give rise to Doppler shifts of the low-energy surface excitations, $\epsilon_{\text{doppler}} = v_f \cdot p_s(R)$, which modify the relative stability of surface phases described by different local symmetries, and may induce surface phases with broken $T$-symmetry. This type of field-induced transition leads to low-field nonlinearities in the field-dependence of the splitting of the ZBCP, $\delta(H)$. The condensate momentum is given by the phase gradient and gauge-invariant coupling to the vector potential, $p_s(R) = \frac{\hbar}{M}(\nabla \theta - (e/c)A(R))$. For magnetic fields applied along the crystal $\widehat{c}$-axis, $p_s(R)$ is perpendicular both to $\hat{c}$ and to the surface normal $n$, and of order $v_f p_s \sim \Delta(H/H_o)$ where $H_o = (e/c)\Delta/v_f \lambda$ is the pairing field order of a few Tesla in the cuprates. The Fermi velocity, $v_f$ and density of states, $N_f$, determine the zero-temperature penetration depth $1/\lambda^2 = (4\pi e^2/\hbar^2) N_f v_f^2$ in the clean limit, and we take $\lambda/\xi = 100$ for YBCO.

The conductance of a NIS tunnel junction measures an angle-average of the quasiparticle density of states (DOS) at the interface. In the limit of a low-transmission tunnel barrier ($D \ll 1$) the conductance is given to leading order in $D$ by the standard tunnelling result,

$$
dI/dV = \frac{1}{N_f(R_s)} \int d^2p_f D(p_f) N(p_f; R_s; \epsilon) eV
$$

in the limit $T \ll T_c$, where the integral is over trajectories with $p_f n > 0$, $R_s$ is the interface resistance, $N(p_f; R_s; \epsilon)eV = -\frac{3}{4\pi} \text{Im} \Phi_R(p_f, R_s; \epsilon)eV$ is the angle-resolved local DOS of the superconductor evaluated at the surface, $R_s$ and $\Phi_R$ is the diagonal element of the retarded propa-
gator, $\hat{\Theta}^R = \hat{G}(\epsilon_{n} \rightarrow \epsilon + i0^+)$. The angle-resolved local DOS is folded with the trajectory dependent barrier transmission probability, $D(p_f)$. The tunnelling barrier is modelled by a transmission probability that is maximum for quasiparticles with Fermi momenta parallel to the surface normal $(p_f/|n|)$ and decreases with angle as $D = D_0 e^{-\langle\varphi_0 / \varphi_c\rangle^2}$ where $\varphi = \cos^{-1}(p_f \cdot n)$ and $\varphi_c$ is a measure of active tunnelling trajectories. Qualitatively, thick junctions have narrow tunnelling cones, $\varphi_c < \pi/2$, while thinner junctions correspond to a wider range of active tunnelling trajectories.

In Fig. 2 we show results for the tunnelling conductances for the sub-dominant pairing channels with $A_{1g}$ and $B_{2g}$ symmetries. The surface DOS was calculated at fixed temperature just above a surface phase transition with broken $T$ symmetry, $T > T_s$. The conductances were calculated in the clean limit at $T = 0.1 T_c$. Note the nonlinear field evolution shown in Fig. 2b for the $A_{1g}(\alpha = 0.5)$ channel. For the $B_{2g}$ channel the splitting of the ZBCP is suppressed at low fields.

The field induced splitting of the ZBCP, $\delta(H)$, is linear in $H$ for pure d-wave pairing, as shown in Fig. 3. The proximity to a broken $T$-symmetry phase of the form $d +$ enhances the splitting of the ZBCP and generates a field dependence of the shift in the conductance peak that is nonlinear in $H$ for $T > T_c$ (Figs. 2a and 3a). By contrast, the field splitting for the $d_{xy}$ channel is suppressed at low fields; but onsets above a critical field of order $H^c = (T_c^{\text{B2g}}/T_c)H_o$ (Fig. 3). The field dependence of the splitting, $\delta(H)$, and its sensitivity to a sub-dominant order parameter, $\Delta_T$, can be understood by considering the ABS spectrum for an OP that is constant in space, but breaks $T$-symmetry, e.g. $\Delta(p_f) = \Delta_d(p_f) + i\Delta_T(p_f)$. The $d_{x^2-y^2}$ component, $\Delta_d$, changes sign along the scattered trajectory, while the sub-dominant component is unchanged. Thus, $\Delta(p_f)^* = -\Delta(p_f)$ on each trajectory. From the retarded propagator, $\Theta^R(p_f, \epsilon)$, we obtain the ABS pole at an energy shifted away from the Fermi level, $\varepsilon_b(p_f) = -s_f \Delta_T(p_f) - v_f \cdot p_s$, with $s_f = \text{sgn}(\Delta_d(p_f)/\Delta_T(p_f))$.

In the absence of the Doppler shift, a sub-dominant OP shifts the ABS. The magnitude and sign of the shift depend on the magnitude of the sub-dominant OP and the relative phase between $\Delta_d$ and $\Delta_T$, $s_f = \pm$. The bound-state energies for trajectories, $p_f$ and $-p_f$, have opposite signs; this splitting for time-reversed states results in spontaneous surface currents carried by the bound states $A_{1g}$. The two possible directions for the spontaneous current reflect the two-fold degeneracy of the surface state, i.e. $\Delta_d(p_f) \pm i\Delta_T(p_f)$. In a magnetic field screening currents generate a Doppler shift of the surface bound states. For the sub-dominant s-wave OP the Doppler term may generate a shift of the same sign as the spontaneous shift, or the reverse depending on the polarity of the field and the relative phase of the subdominant OP. If the shifts are opposite in sign, the bound state energies move toward the Fermi level with increasing field, until it becomes energetically favorable for the relative phase and bound state current to reverse sign. This reversal occurs at a low field of order $H^c = (T_s/T_c)H_o$ for the sub-dominant s-wave channel as shown in Fig. 3b. Also shown is the field-induced sub-dominant OP that onsets rapidly with field for $T > T_s$, and which is the source of the nonlinearity in $\delta(H)$ shown in Fig. 3a. For $T < T_s$ this splitting is asymmetric about $H = 0$, and hysteretic on a field scale of order $H^c$.

In the doping range where the leading sub-dominant channel is $B_{2g}$, the field evolution is more complex. The angular dependence of the $B_{2g}$ OP, $\Delta_{2g} \sim \sin(2(\phi_p - \pi/2))$, implies that the bound state disperses through the Fermi level as a function of the trajectory angle, $\phi = \cos^{-1}(p_f \cdot n)$. For a [110] surface half of the incident trajectories correspond to ABS above the Fermi level and the other
half have their energies below the Fermi level. When added to their time-reversed partners, these states carry oppositely directed currents. Field-induction of the $d_{x^2-y^2}$ OP for $T > T_s$ produces a different behavior than predicted for $s$-wave sub-dominant pairing; the magnitude of $\Delta_{s\text{xy}}$ remains small, and the corresponding bound state splittings are compensated by the Doppler term, until a threshold field is reached, again of order $H^*$, beyond which the Doppler term cannot be compensated by the shift from the field-induced sub-dominant OP (see Fig. 3 d). For $T < T_s$ the subdominant OP produces splitting of the ZBCP for $H = 0$. The low-field evolution is again different than that of the $s$-wave case; $\delta(H)$ decreases with $H$ until a critical field of order $H^*$ is achieved. This field corresponds to the counter-moving branch of ABS dispersing through the Fermi level. Further increasing the field can drive the sub-dominant OP to very small values, in which case the splitting is given by the Doppler splitting and linear for $H \ll H_0$.

![DIAGRAM](image.png)

**FIG. 4:** (a) Calculated field dependence of the conductance maximum as a function applied field for different values of doping parameter $\alpha$. The model for the transmission probability is $T(\phi) = T_0 \exp[-(\phi/\phi_c)^2]$, with $\phi_c = 12^\circ$. (b) Measured field dependence of the conductance maximum as a function of applied field for different values of doping as reported in Fig. 3 of Ref. [11].

Many of these features appear to be observed in YBCO tunnel junctions. We conclude with a comparison of the theoretical predictions of the surface ABS model for the tunnelling conductance, including the qualitative predictions of the two-channel pairing model, with the tunnelling measurements reported in Ref. [10] for the field dependence of the conductance peaks for YBCO. Calculated splittings of the ZBCP, $\delta(H)$, are shown in Fig. 4a, and are compared with the experimental results shown in Fig. 3b. Experimental observations of the field dependence of the conductance peak in underdoped films are in agreement with theoretical results based on a field-induced $d_{x^2-y^2} + i d_{xy}$ surface state; there is a low-field threshold before a splitting appears, followed by an approximately linear increase in the splitting with $H$. At optimal doping the linear field dependence is recovered with no spontaneous splitting. Further increase in the doping level shows the nonlinear regime for slightly overdoped samples, which is accounted for by an attractive $s$-wave subdominant pairing channel. The evolution with field and doping is systematically reproduced by a $B_{1g} + i A_{1g}(\alpha)$ surface state with anisotropic $A_{1g}$ component closest to optimal doping which evolves as the doping is increased to a nearly isotropic $A_{1g}$ sub-dominant pairing state. The evolution of the ZBCP indicates that the pairing interaction changes with doping; the dominant pairing channels is $B_{1g}$, with a sub-dominant $B_{2g}$ component in the slightly underdoped regime which is overtaken by a sub-dominant $A_{1g}$ component in the overdoped regime. The cross-over occurs close to optimal doping.

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[1] T. Löfwander, V. S. Shumeiko, and G. Wendin, Supercond. Sci. Technol. 14, R53 (2001).
[2] L. Buchholtz, M. Palumbo, D. Rainer, and J. A. Sauls, J. Low Temp. Phys. 101, 1099 (1995). [cond-mat/9511027]
[3] Y. Tanaka and S. Kashiwaya, Phys. Rev. Lett. 74, 3451 (1995).
[4] M. Fogelström, D. Rainer, and J. A. Sauls, Phys. Rev. Lett. 79, 281 (1997).
[5] M. Covington, M. Aprili, E. Paraoanu, L. H. Greene, F. Xu, J. Zhu, and C. A. Mirkin, Phys. Rev. Lett. 79, 277 (1997).
[6] M. Aprili, E. Badica, and L. H. Greene, Phys. Rev. Lett. 83, 4630 (1999).
[7] R. Krupke and G. Deutscher, Phys. Rev. Lett. 83, 4634 (2001).
[8] M. Sigrist, D. Bailey, and R. Laughlin, Phys. Rev. Lett. 74, 3249 (1995).
[9] M. Matsumoto and H. Shiba, J. Phys. Soc. Jpn. 64, 1703 (1995).
[10] Y. Dagan and G. Deutscher, Phys. Rev. Lett. 87, 177004:1 (2001).
[11] R. J. Radtke, S. Ullah, K. Levin, H. Schuttler, and M. Norman, Phys. Rev. B 46, 11975 (1992).
[12] M. Eschrig, J. Ferrer, and M. Fogelström, Phys. Rev. B 63, 220509(R) (2001).
[13] R. J. Radtke and M. Norman, Phys. Rev. B 50, 9554 (1994).
[14] M. Covington and L. H. Greene, Phys. Rev. B 62, 12440 (2000).
[15] L. Buchholtz, M. Palumbo, D. Rainer, and J. A. Sauls, J. Low Temp. Phys. 101, 1079 (1995). [cond-mat/9511027]
[16] M. Eschrig, Phys. Rev. B 61, 9061 (2000).