Tunneling into Current-Carrying Surface States of High $T_c$ Superconductors

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Theoretical results for the $ab$-plane tunneling conductance in the $d$-wave model for high $T_c$ superconductors are presented. The $d$-wave model predicts surface bound states below the maximum gap. A sub-dominant order parameter, stabilized by the surface, leads to a splitting of the zero-bias conductance peak (ZBCP) in zero external field and to spontaneous surface currents. In a magnetic field screening currents shift the quasiparticle bound state spectrum and lead to a voltage splitting of the ZBCP that is linear in $H$ at low fields, and saturates at a pair-breaking critical field of order $H_c^* \approx 3T$. Comparisons with recent experimental results on Cu/YBCO junctions are presented.

In the $d_{x^2-y^2}$ model for the cuprate superconductors surface states are predicted which should be observable in the sub-gap conductance for $ab$-plane tunneling. Observations of a zero-bias peak (ZBCP) in the in-plane conductance were reported for tunnel junctions on oriented YBCO films by Geerk, et al., Lesueur et al., and Covington et al. The ZBCP splits in a magnetic field of a few Tesla, and recent experiments show that a splitting of a few $meV$ also appears at low temperatures in zero-field. The identification of the ZBCP with surface bound-states associated with $d$-wave pairing is important because the origin of the ZBCP in the $ab$-plane tunneling conductance is the same as that of the $\pi$ phase shift in the Josephson interference experiments. The same sign change that leads to a $\pi$ phase shift in the Josephson current-phase relation is also responsible for a ZBCP in the $ab$-plane quasiparticle tunneling conductance for high impedance junctions. The ZBCP is observed with comparable magnitude for both (110) and (100) orientated surfaces, whereas theoretical calculations predicted no ZBCP for (100) interfaces. We show that a large ZBCP is expected in the $ab$-plane tunneling conductance for all orientations if the interface is microscopically rough.

Several authors have suggested that the surface of $d$-wave superconductors might exhibit spontaneously generated surface currents associated with the presence of a second superconducting order parameter. The surface state of any $d_{x^2-y^2}$ superconductor will exhibit a spontaneously broken time-reversal symmetry phase at sufficiently low temperature. The tunneling spectrum for current-carrying states of d-wave superconductors, externally imposed and spontaneously generated, is the main subject of this letter.

When an excitation reflects elastically off a (110) surface its momentum changes, $p_f \rightarrow -p_f$. Incident and reflected wavepackets propagate through different order parameter fields, $\Delta(p_f, R) \rightarrow \Delta(p_R, R)$, which leads to Andreev scattering, a process of "retro-reflection" in which a particle-like excitation undergoes branch conversion into a hole-like excitation with reversed group velocity. Bound states occur at energies for which the phases of Andreev-reflected particle- and hole-like excitations interfere constructively. This effect is pronounced if the scattering induces a change in sign of the order parameter along the classical trajectory. In this case a zero-energy bound state forms. Surface bound states of this origin were discussed in the context of tunneling into unconventional superconductors by Buchholtz and Zwicknagl, and more recently for the $d_{x^2-y^2}$ pairing model of the cuprates. Reversal of the velocity by Andreev reflection is accompanied by a change in sign of the charge. Consequently Andreev bound states can carry current.

The physics of the surface currents and their influence on the subgap conductance requires a microscopic theory of the surface excitations, the surface order parameter and a transport theory for the coupled surface and bulk excitations and the inhomogeneous pair condensate. We consider low-transmission tunnel junctions between a normal electrode and a cuprate superconductor oriented for tunneling into the $ab$-plane. At $T = 0$ the tunneling conductance measures the excitation spectrum of the superconductor at the surface,

$$dI/dV = \frac{1}{\pi N} \int_{p > 0} d^2 p_f D(p_f) N(p_f, R_e; \epsilon)$$

where $R_e$ is the interface resistance in the normal-state, and $N(p_f, R_e; \epsilon)$ is the superconducting density of states at the interface ($R_e$) for trajectories defined by the Fermi surface position, $p_f$. At finite temperatures the equation for $dI/dV$ must be modified to reflect the thermal occupation of the states contributing to the tunneling current. The tunneling conductance is obtained by folding the angle-resolved density of states at the surface with the barrier transmission probability, $D(p_f)$, for tunneling characteristics labeled by $p_f$. We model the tunneling barrier with a uniform probability distribution, $D = 1/2\phi_c$, within an acceptance cone of angle $2\phi_c$ about the interface normal, and zero outside the cone. A small value of $\phi_c$ represents a thick tunneling barrier, while a large value of $\phi_c$ corresponds to a thin barrier.

The surface excitation spectrum, angle-resolved lo-
cal density of states, \( N(p_f, R; \epsilon) \) and order parameter, \( \Delta(p_f, R) = \sqrt{\Delta(R)(p_{f+}^2 - p_{f-}^2)} \), are obtained by solving Eilenberger’s transport equations. \[13\] For high impedance junctions we can neglect the influence of the tunnel current on the excitation spectrum at the interface. In order to calculate the surface order parameter and density of states we solve the transport equations supplemented by surface boundary conditions. We consider two models: (i) an atomically smooth surface described by continuity of the propagator at the surface for the incident and specularly reflected trajectories and, (ii) a rough or faceted surface modeled as a distribution of microscopic mirror surfaces that are mis-oriented relative to the average interface normal. \[14\]

For specular interfaces the order parameter is strongly suppressed for a (110) surface because the order parameter changes sign along all classical trajectories. Consequently, an Andreev bound state with zero energy is formed for every trajectory. The formation of bound states comes at the expense of the continuum states that form the \( d_{z^2-y^2} \) pair condensate. Conversely, the specular (100) interface is not pairbreaking; the order parameter is constant in magnitude and phase along all incident and specularly reflected trajectories. Figure 1a also shows the effect of surface roughness on the d-wave order parameter for (110) and (100) oriented surfaces. For rough surfaces pair-breaking occurs for all orientations of the surface normal relative to the crystal axes. The key feature to note in Figs. 1c-d is the appearance of a ZBCP with approximately equal spectral weight for both (110) and (100) orientations as a result of surface-induced Andreev scattering by the rough surface. Slight differences in the distribution of spectral weight can be seen as a function of the number of nanofacets.

![Diagram](image)

**FIG. 1.** 1a) The \( d_{z^2-y^2} \) order parameter near (110) and (100) surfaces for specular and rough surfaces. b) The absence of the ZBCP is a special feature of a specular (100) surface. c) The tunneling conductance for nano-faceted (110) and (100) surfaces with three facets (0, ±45°). d) A similar calculation to c) but with seven facets (0, ±22.5°, ±45°, ±67.5°). The acceptance cone is \( \phi_c = 30° \), the width parameter is \( \gamma = 0.05\Delta_0 \), and \( T = 0.3T_c \).

Tunneling experiments performed on oriented YBCO films were carried out in a magnetic field. \[15\] These experiments show a ZBCP which broadens with increasing field and is split by roughly 3 meV at \( H = 1T \). The field evolution of the ZBCP in Pb/YBCO films was initially interpreted in terms of a Zeeman splitting of resonant magnetic impurities in the tunnel barrier. \[16\] The Zeeman shift of the conductance peak in the Appelbaum theory is given by \( \delta = g\mu_B H \), where \( g \) is the g-factor of the paramagnetic centers. Lesueur, et al. \[17\] report a large g-factor to account for the splitting in Pb/YBCO junctions. An alternative way of expressing the Zeeman shift in the Appelbaum model is \( \delta = \Delta_0(H/H_F) \), where \( H_F = \Delta_0/g\mu_B \) is the Pauli field, i.e. the field scale for pair-breaking by the Zeeman energy. The data of Lesueur, et al. \[17\] implies an anomalously low Pauli field \( (H_F \sim 10T \text{ vs. } \Delta_0/2\mu_B = 125T) \) in order to account for the splitting of the conductance peak in a field.

Here we suggest an explanation of the field evolution of the ZBCP that does not invoke paramagnetic tunneling centers, but depends upon the d-wave interpretation of the ZBCP. The surface bound states that give rise to the ZBCP couple to the magnetic field at the interface via the screening current in the superconductor. The electromagnetic coupling that enters the transport equation is \(-\frac{\epsilon}{c}v \cdot A(R)\), where \( A(R) \) is the self-consistently determined vector potential. For a uniform (or slowly varying) supercurrent this coupling leads to a Doppler shift in the continuum excitations given by \( v \cdot p_s \), where \( p_s = \left[ \frac{\epsilon}{c}\nabla \delta - \frac{\epsilon}{c}A(R) \right] \) is the condensate momentum, i.e. excitations co-moving with the superflow are shifted to higher energy while counter-moving excitations are shifted to lower energy. The current also shifts the Andreev bound state spectrum.

Consider the effect of ab-plane screening currents on the tunneling conductance. The screening current is parallel to the surface and proportional to the applied field: \( \mathbf{H} = H\hat{z}, p_s = -(\epsilon/e)A(x)\hat{y} = (\epsilon/e)HA\exp(-x/\lambda)\hat{y} \), where \( \lambda \) is the ab-plane penetration depth. First consider a model for the excitation spectrum of a d-wave superconductor which is not self-consistent, i.e. neglect pair-breaking of the d-wave order parameter at a specular (110) surface. Eilenberger’s equation can then be solved analytically for \( \lambda \gg \xi_0 \); the resulting angle-resolved local density of states is given by

\[
N(p_f, x; \epsilon) = \text{Im} \left\{ \frac{\hat{z} \cdot \hat{R}}{\hat{z} \cdot \hat{R} D^R} \frac{|\Delta(p_f)|^2}{e^{2D^R x/|v_f| \hat{y}}} \right\},
\]

where \( D^R = \sqrt{|\Delta(p_f)|^2 - \epsilon^R(p_f, \epsilon)^2} \) and \( \epsilon^R(p_f, \epsilon) = \epsilon + i\gamma + \frac{\epsilon}{e}v \cdot A(R) \) defines the excitation energy, with impurity broadening approximated by a constant width \( \gamma \). The first term in Eq. 1 is the bulk density of states. The second term gives a bound state contribution near zero energy. At the interface the total (bulk plus surface) continuum contribution to the density of states is given by

\[
N_c = \frac{\sqrt{(|\epsilon - v \cdot p_s|^2 - |\Delta(p)|^2)^2 - |\Delta(p)|^2}}{|\epsilon - v \cdot p_s|^2 - |\Delta(p)|^2}} \Theta((|\epsilon - v \cdot p_s|^2 - |\Delta(p)|^2)^2),
\]
which shows the Doppler shift in the continuum edge. The singularity in the bulk density of states is removed, and spectral weight from the continuum is shifted to the bound state. In the limit $\gamma \to 0$ the bound state contribution becomes $N_0(p_f, x; \epsilon) = \pi|\Delta(p_f)|/\delta(\epsilon - v_f \cdot p_f) \exp(-2|\Delta(p_f)| x/|v_f| x|)$. The spectral weight decays into the bulk as the square of the bound state amplitude. For the trajectory $\hat{x} = \cos \phi_c \hat{x} + \sin \phi_c \hat{y}$ the shift in the bound state is $\epsilon_b = (e/c)^2 H \lambda \sin \phi_c$. A field scale is set by a screening current of order the bulk critical current, $H_0 = (\Delta_c/ev_f\lambda)/\sin \phi_c$, where $\phi_c$ determines the maximum shift observable in tunneling. This field is of order $H_0 \sim (\Delta_c/ev_f\lambda)/\sin \phi_c \sim 1 - 10^T$, and is the field scale observed in the low-field linear region of the splitting of the ZBCP in Pb/YBCO and Cu/YBCO tunnel junctions. The shift in the energy of the bound states calculated from the London screening current and Eq. 4 is strictly valid for $x \gg \xi_0$, where the bound states have little spectral weight. At the interface, where the bound states contribute to the tunneling conductance, a self-consistent calculation of the order parameter and current is required.

![Image](https://via.placeholder.com/150)

**FIG. 2.** a) The current density at different applied fields for a pure $d_{x^2-y^2}$ order parameter and a specular (110) surface. The current density heals to the London screening current, $j \simeq (e/c^2) H/\lambda$, for $x > 5\xi_0$. For $x < 5\xi_0$, the current reverses sign and is carried by the bound states. b) The tunneling conductance vs. $H$ for $T = 0.3T_c$. The splitting of the ZBCP reflects the shift in the surface bound states by the screening current at $x = 0$. The inset shows the linear splitting of the ZBCP at low fields.

Figure 2a shows the self-consistent result for the current density for a specular (110) surface as a function of the applied field $H$ at $T = 0.3T_c$. The current density heals to the London screening current, $j(x) \simeq (e/c^2) H/\lambda$, for $\xi_0 \ll x \ll \lambda$, where it is carried by the continuum states that comprise the condensate. Near the surface, $x \lesssim \xi_0$, the current is carried by Andreev bound states. A similar phenomena is found in the spectral resolution of the current density in vortices. The bound-state current scales linearly with the applied field (in the Meissner region), but is counter-flowing relative to the bulk screening current. As a result the bound-states lead to a small increase in the penetration depth, $\delta \lambda/\lambda_{London} \simeq (\xi_0/\lambda_{London})$. The bound states also lead to a splitting of the ZBCP in a magnetic field. The spectrum is calculated self-consistently with the surface current density. Figure 2b shows the field evolution of the ZBCP for a $d_{x^2-y^2}$ superconductor and a (110) interface. The splitting is symmetric about zero bias, with $\delta \simeq \Delta_0 (H/H_0)$; $H_0 \simeq 6T$ is used in the calculations.

Other current sources will also split the ZBCP. In particular, the spontaneous currents generated at a surface phase transition to a pairing state with mixed symmetry, e.g. $d + is$ surface phase, are due to a shift in the energies of the Andreev bound states in zero field. The relevance of the sub-dominant order parameter depends on the microscopic pairing interaction. Several authors have proposed that superconductivity in the cuprates is mediated by the exchange of anti-ferromagnetic (AFM) spin fluctuations (see Ref. 17 and references therein). This mechanism predicts d-wave pairing with $B_{1g}$ symmetry over a wide range of parameter space of the spin-fluctuation propagator and bandstructure. The AFM mechanism also predicts that the $A_{2g}$ channel $[p_x p_y (p_x^2 - p_y^2)]$ is attractive, but sub-dominant to the $B_{1g}$ channel, i.e. $0 < T_{cA_{2g}} < T_{cB_{1g}}$, and that the pairing interaction in all other channels is repulsive, including anisotropic $A_{1g}$ states that have nodes. Solutions to the linearized gap equation with a tight-binding bandstructure and the spin-fluctuation model of Radtke, et al. [18] lead to sizeable values for the $A_{2g}$ coupling strength, e.g. $T_{cA_{2g}}/T_{cB_{1g}} \simeq 0.3 - 0.4$. Other pairing mechanisms may lead to subdominant pairing with different symmetry, e.g. the electron-phonon interaction may lead to a sub-dominant pairing interaction in the $A_{1g}$ channel. We consider both possibilities.

Surface pair breaking frees up spectral weight at the Fermi surface for the formation of pairs in a sub-dominant pairing channel. For example, a surface order parameter with $A_{1g}$ symmetry will develop near a (110) surface as shown in the inset of Fig. 3a. Figure 3b shows the surface phase diagram as a function of the sub-dominant coupling strength for specular scattering. Below the surface phase transition temperature, $T_s$, a surface order parameter develops which spontaneously breaks $T$-symmetry. The surface phase is doubly degenerate, corresponding to two possible directions for the spontaneous surface current. For $T_{c2} = 0.3T_{c1}$ surface roughness is found to suppress $T_s$ by roughly 30% for the $B_{1g} + iA_{1g}$ transition near a (110) surface. The magnitude of the spontaneous surface current shown in Fig. 3a scales with the amplitude of the subdominant order parameter and can be a sizeable fraction of the critical current density. The spontaneous current is carried by the bound states and is confined to a few coherence lengths of the surface. The ZBCP splits in zero field as $T$ drops below $T_s$ as shown in Fig. 3c for a $B_{1g} \pm iA_{1g}$ surface phase and a sub-dominant coupling constant of $T_{c2} = 0.29T_{c1}$, which gives $T_s = 0.25T_{c1}$, and a zero-field splitting of $\delta_s \simeq 0.15\Delta_0$. The zero-field conductance curves calcu-
lated at points $A$ and $B$ in Fig. 3b are shown in Fig. 3c. The proximity to the surface phase transition, leads to a low-field nonlinear evolution of the splitting of the ZBCP, above and below $T_s$, as shown in the inset of Fig. 3d.

Recent experiments on Cu/YBCO tunnel junctions report a zero-field splitting of $\delta_{\text{exp}} = 1.1 \, \text{meV}$, and a surface phase transition temperature of $T_s \approx 7 \, \text{K}$. These values are in good agreement with the theoretical predictions for a surface phase with $B_{1g} + iA_{1g}$ symmetry and $T_{c2} \approx 0.15 \, T_c$. This provides evidence for a sub-dominant pairing channel and surface-induced broken $T$-symmetry in the high $T_c$ cuprates. The field evolution of the conductance peaks is also accounted for by the shifts of the Andreev bound states. At low temperatures $T \ll T_s$ the low-field nonlinearity is weak, and the shift of the ZBCP is given by, $\delta(H) = \delta_s + v_f \rho_s \sin \phi_s$; at low fields $\rho_s = \frac{2}{c} H \lambda$, and the splitting increases linearly with $H$. However, the screening current is nonlinear at higher fields, and saturates at the pairbreaking critical current. An order of magnitude estimate for the pairbreaking critical field is given by $H_c \approx \frac{\Delta_0}{\rho_s} \sin \phi_s \lambda \approx 1 \, \text{Torr}$ for $\lambda = 1500 \, \text{Å}$ and $\xi_0 = 15 \, \text{Å}$. The nonlinear correction to the screening current is dominated by non-thermal, counter-moving quasiparticles near nodal points of the gap, as described in Ref. [19], and yields the following result for the field evolution of the splitting, $\delta(H) = \delta_s + \Delta_0 (H/H_0) \left[ 1 - \frac{1}{2} (H/H_0^*) \right]$, for $H \leq H_0^*$. This pairbreaking critical field is determined by the excitations in the vicinity of the nodes, and is given by $H_0^* = \frac{\phi_c}{2e N} |\Delta(\vartheta)|/|v_F|$; where $d|\Delta(\vartheta)|/d\vartheta|_{\text{node}}$ is the angular slope of the $d_{x^2-y^2}$ gap at a node, and $v_F$ is the magnitude of the Fermi velocity at node. For the standard $d$-wave model, $|\Delta| \sim |\cos(2\vartheta)|$, and a cylindrical Fermi surface, $H_0^* = 3 \, H_c \approx 3 \, T$. Figure 3d shows a comparison of the data on the splitting of the ZBCP for Cu/YBCO junctions [6] with the theoretical result for $\delta(H)$ (solid line: $H_0^* = 2.5 \, T$, $H_c = 1 \, T$ and $\phi_c \approx 4^\circ$).

The theory of NIS tunneling applied to $d$-wave superconductors accounts for the low-energy features in the $ab$-plane tunneling conductance in terms of Andreev bound states and low-energy continuum excitations near the nodes. The theory accounts for the splitting of the ZBCP in zero-field in terms of a phase transition to a surface state with broken $T$-symmetry, and for the field evolution of the conductance peak in terms of the Doppler shift of the Andreev bound states.

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