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LETTER TO THE EDITOR

Symmetry breaking in the tunnelling conductance of a superconducting vortex

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Abstract. Recent STM experiments on *c*-axis tunnelling into a vortex core of YBCO have yielded a sub-gap differential conductance which is not invariant under a reversal of the applied bias. By computing the differential conductance $G(E)$ of a normal–superconducting contact to all orders in the tunnelling strength, we predict that in the absence of open channels in the superconductor, $G(E)$ is necessarily an even function of E and that an asymmetric current–voltage characteristic implies the existence of propagating bound-states within the vortex core.

Symmetries in physical measurements often provide powerful insight into underlying microscopic phenomena. In the tunnelling limit, if the single particle density of states at the Fermi energy is a constant, it is well known that the sub-gap conductance $G(eV)$ of normal–insulating–superconductor (NIS) junctions [1–4] is an even function of the bias voltage V. This symmetry is present in some STM-based experiments on both conventional and high temperature superconductors [5, 6], but in a recent experiment [7] on tunnelling from a normal STM tip into a vortex of YBCO, it is broken.

The aim of this letter is to present an analytic theory of the sub-gap conductance, which highlights the conditions under which asymmetries occur. We present a new result for the conductance between a normal conductor and a superconductor, valid to all orders in the tunnelling strength, which provides a general condition for symmetry breaking. Our key result is that within mean-field BCS theory, the existence of asymmetries implies the presence of propagating quasi-particle states. For the first time, we also present numerical results for the conductance of a vortex, which are valid in the limit that the superconducting coherence length is of order the Fermi wavelength.

When describing transport across the interface between a normal conductor and a superconductor, it is convenient to write the total Hamiltonian H in the form $H = H_{AA} + H_{BB} + H_{AB}$, where H_{AB} has the structure

$$H_{AB} = \begin{pmatrix} 0 & W \\ W^\dagger & 0 \end{pmatrix}$$

and W is a matrix of exchange integrals describing the coupling between the the normal conductor (A) to the superconductor (B). If g_A and g_B are the Green functions of the separate conductors before contact is made, the Green function of the superconductor after making contact is given by [8, 9]

$$G_{BB}^{-1} = g_B^{-1} - \Sigma + \mathrm{i}\Gamma \tag{1}$$

where

$$\Sigma - \mathrm{i}\Gamma = W^\dagger g_A W. \tag{2}$$

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In what follows, we consider the case where the normal conductor is a crystalline, straight wire of constant cross-section, described by a real Hamiltonian and possessing a set of channels $\{|\bar{n}\rangle\}$, of which some are closed, while others are propagating. If the propagating channels are denoted $|n\rangle$, then the Green function of the isolated wire, before contact is made with the superconductor, can be written [8, 9]

$$g_A = \sum_n |n\rangle g_n \langle n| + \sum_{\bar{n}} |\bar{n}\rangle g_{\bar{n}\bar{n}} \langle \bar{n}| = \sum_n |n\rangle g_n \langle n| + \sigma' \tag{3}$$

where the second sum is over states $|\bar{n}\rangle$ orthogonal to open channels and σ' is a Hermitian self-energy matrix. With this notation, one finds $\Sigma - \mathrm{i}\Gamma = \sigma' + \sigma - \mathrm{i}\Gamma$, where

$$\sigma = \sum_n \sigma(n) \qquad \text{and} \qquad \Gamma = \sum_n \Gamma(n) \tag{4}$$

with

$$\Gamma(n) = -W^\dagger |n\rangle [\mathrm{Im}\, g_n] \langle n| W \qquad \text{and} \qquad \sigma(n) = W^\dagger |n\rangle [\mathrm{Re}\, g_n] \langle n| W. \tag{5}$$

In these expressions both $\Gamma(n)$ and $\sigma(n)$ are Hermitian; $\Gamma(n)$ can be viewed as a matrix of inverse lifetimes arising from the presence of channel n and $\sigma(n)$ the corresponding self-energy matrix.

To obtain equilibrium transport properties, we follow references [10, 11], where it is noted that in the absence of inelastic scattering, dc transport is determined by the quantum mechanical scattering matrix $s(E, H)$, which yields scattering properties at energy E, of a phase-coherent structure described by a Hamiltonian H. For a structure possessing open scattering channels labelled by quantum numbers n, the squared modulus of the matrix element $s_{n,n'}(E, H)$ is the outgoing flux of quasi-particles along channel n, arising from a unit incident flux along channel n'. Since channels are associated with quasi-particles labelled by a discrete quantum number α ($\alpha = +1$ for particles, -1 for holes), we write $n = (l, \alpha)$, where l labels all other quantum numbers. With this notation, the scattering matrix elements $s_{n,n'}(E, H) = s_{l,l'}^{\alpha,\beta}(E, H)$ satisfy $s^\dagger(E, H) = s^{-1}(E, H)$ and $s^t(E, H) = s(E, H^*)$. Furthermore if E is measured relative to the condensate chemical potential μ, then the particle–hole symmetry relation $s_{l,l'}^{\alpha,\beta}(E, H) = \alpha\beta[s_{l,l'}^{-\alpha,-\beta}(-E, H)]^*$ is satisfied. For a scatterer formed from contact between a crystalline, normal lead and a superconductor, it is convenient to write $l = (i, a)$, where $i = A$ ($i = B$) for a propagating channel belonging to the normal lead (superconductor). Propagating channels in the superconductor can arise at energies greater than the superconducting energy gap, or under sub-gap conditions in the presence of a vortex. With this notation, and writing $l' = (j, b)$, equilibrium transport properties can be expressed in terms of the quantity

$$P_{i,j}^{\alpha,\beta}(E, H) = \sum_{a,b} |s_{(i,a),(j,b)}^{\alpha,\beta}(E, H)|^2 \tag{6}$$

which is the probability of reflection ($i = j$) or transmission ($i \neq j$) of a quasi-particle of type β in j to a quasi-particle of type α in i. For $\alpha \neq \beta$, $P_{A,A}^{\alpha,\beta}(E, H)$ is referred to as an Andreev reflection probability, while for $\alpha = \beta$, it is a normal reflection probability.

To compute scattering coefficients, we note [9] that the probability of reflecting from channel n of the normal conductor A to channel n' of conductor A can be written

$$|s_{nn'}|^2 = \begin{cases} R_{nn} = |1 - 2\mathrm{i}\,\mathrm{Tr}\{\Gamma(n) G_{BB}\}|^2 & \text{for } n = n' \\ T_{nn'} = 4\,\mathrm{Tr}\{\Gamma(n) G_{BB} \Gamma(n') G_{BB}^\dagger\} & \text{otherwise.} \end{cases} \tag{7}$$

Furthermore at zero temperature [10, 11], the differential conductance at potential difference $v = E/e$ reduces to

$$G(E) = N_A^\alpha(|E|) - P_{A,A}^{\alpha,\alpha}(|E|) + P_{A,A}^{-\alpha,\alpha}(|E|) \tag{8}$$

where $\alpha = \mathrm{sign}(E)$. Writing $n = (A, a, \alpha)$ and $n' = (A, b, \beta)$ and substituting (7) into (6) yields

$$P^{\alpha\beta}_{A,A} = [N - 2\mathrm{i}\,\mathrm{Tr}\{\Gamma(\alpha)(G_{BB} - G^{\dagger}_{BB})\}]\delta_{\alpha\beta} + 4\,\mathrm{Tr}\{\Gamma(\alpha)G_{BB}\Gamma(\beta)G^{\dagger}_{BB}\} \quad (9)$$

where $\Gamma(\alpha) = \sum_a \Gamma(A, a, \alpha)$. From this the conductance (8) becomes

$$G(E) = 2\mathrm{i}\,\mathrm{Tr}\{\Gamma(\alpha)(G_{BB} - G^{\dagger}_{BB})\} - 4\sum_{\beta=\pm 1}\beta\,\mathrm{Tr}\{\Gamma(\beta\alpha)G_{BB}\Gamma(\alpha)G^{\dagger}_{BB}\}. \quad (10)$$

A further simplification is obtained by noting that from equation (1)

$$\begin{aligned}[G_{BB} - G^{\dagger}_{BB}] &= [G_{BB}(G^{\dagger}_{BB})^{-1}G^{\dagger}_{BB} - G_{BB}(G_{BB})^{-1}G^{\dagger}_{BB}] \\ &= [G_{BB}(g^{\dagger}_{B})^{-1}G^{\dagger}_{BB} - G_{BB}(g_{B})^{-1}G^{\dagger}_{BB}] - 2\mathrm{i}G_{BB}\Gamma G^{\dagger}_{BB}\end{aligned}$$

and therefore (10) can be written

$$G(E) = 2\mathrm{i}\,\mathrm{Tr}\{\Gamma(\alpha)[G_{BB}((g^{\dagger}_{B})^{-1} - (g_{B})^{-1})G^{\dagger}_{BB}]\} + 4\sum_{\beta=\pm 1}\mathrm{Tr}\{\Gamma(\beta)G_{BB}\Gamma(-\beta)G^{\dagger}_{BB}\} \quad (11)$$

where $\alpha = \mathrm{sign}(E)$.

Equation (11) is a key result of this letter. It is exact to all orders in the coupling W and immediately highlights the symmetry breaking role of propagating channels in the superconductor. If the superconductor contains no open channels of energy E, then g_B is Hermitian and the first 'single-particle' term on the right-hand-side vanishes. In this case only the second 'two-particle' term survives, which is independent of α and therefore invariant under a reversal of the bias voltage. On the other hand if open channels are present in the superconductor, g_B is no longer Hermitian and the first term survives. Since this term depends explicitly on α, the above symmetry is broken. Hence we conclude that in the absence of inelastic scattering, an asymmetric current–voltage characteristic implies the existence of propagating states in the superconductor.

This symmetry breaking is absent from the theory of reference [4], because it is assumed *a priori* that there are no propagating channels in the superconductor. It is absent from the description of reference [3], because only the density of states averaged over all quasi-particle types is computed. To illustrate this feature, we note that in the tunnelling limit, where G_{BB} is not strongly modified by the presence of the contact, it is useful to expand $G(E)$ to lowest order in Γ and Σ. If g_B is Hermitian the dominant contribution is obtained by replacing G_{BB} by g_B in the second term on the right-hand-side of (11) to yield

$$G(E) \approx 8\,\mathrm{Tr}\{\Gamma(-\alpha)g_B\Gamma(\alpha)g_B\}$$

which is simply $2P^{-\alpha\alpha}_{A,A}$. On the other hand, if g_B is not Hermitian, the dominant contribution is obtained by replacing G_{BB} by g_B in the first term on the right-hand-side of (11) to yield

$$G(E) \approx 2\mathrm{i}\,\mathrm{Tr}\{\Gamma(\alpha)(g_B - g^{\dagger}_{B})\} = -4\,\mathrm{Tr}\{\Gamma(\alpha)[\mathrm{Im}g_B]\}$$

which as noted above, vanishes in the absence of propagating channels in the superconductor. This is a standard result of tunnelling theory and has been used in recent calculations of the tunnelling conductance [12,13]. More generally, in the presence of intimate contact, equation (11) should be used.

Since g_B is a matrix in Nambu space with sub-matrices $g^{\alpha\beta}_{B}$ and $\Gamma(\alpha)$ projects on to α-type quasi-particles, this reduces to $G(E) \approx -4\,\mathrm{Tr}\{\Gamma(\alpha)[\mathrm{Im}g^{\alpha\alpha}_{B}]\}$ and for a point contact at position $\underline{r}$, becomes

$$G(E) \approx 4\pi\Gamma(\alpha, \underline{r})N^{\alpha}_{B}(|E|, \underline{r}) \quad (12)$$

where $N_B^\alpha(|E|, \underline{r})$ is the local density of α-type quasi-particle states and $\Gamma(\alpha, \underline{r})$ characterizes the tunnelling strength. If $\Gamma(\alpha, \underline{r})$ varies only slowly with E on the scale of the superconducting energy gap, this expression demonstrates that in the tunnelling limit, asymmetries occur, whenever the difference $\delta N_B(E) = N_B^+(|E|, \underline{r}) - N_B^-(|E|, \underline{r})$ is non-zero. This situation, which is not described by the theory of [3], arises if the condensate potential μ lies close to a van Hove singularity and therefore the existence of asymmetries in high temperature superconductors should depend sensitively on doping.

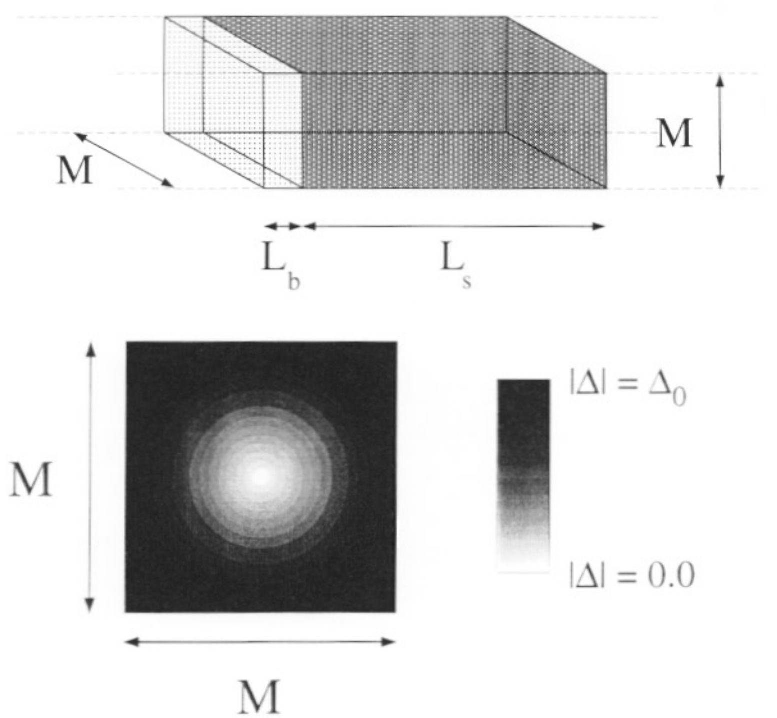

Figure 1. A superconductor of length L_s (shaded) connected to normal wires with the same cross-section as the superconductor. To simulate a NISN structure, a barrier (shown lightly shaded) separates the left-hand normal wire from the superconductor, whereas no such barrier is present at the right-hand N–S interface. (b) The variation of the magnitude of the order parameter within an *a–b* plane of the superconductor.

To verify the above analytic predictions, we now present numerical results for tunnelling into the vortex core of a short-coherence-length superconductor. When ξ is of order the Fermi wavelength, a quasi-classical approach is inappropriate and therefore we analyse a three-dimensional tight-binding system described by a Bogoliubov–de Gennes operator of the form

$$H = \begin{pmatrix} H_0 & \Delta \\ \Delta^* & -H_0^* \end{pmatrix}.$$

In this equation H_0 is a nearest-neighbour Anderson Hamiltonian on a cubic lattice of the form $H_0 = \sum_i |i\rangle\epsilon_i\langle i| - \sum_{ij} |i\rangle\gamma_{ij}\langle j|$ and Δ is a diagonal order parameter matrix. For a system of finite cross-section, once these matrices are specified, the scattering matrix can be computed exactly, as outlined in [10]. In what follows, for a site i belonging to the

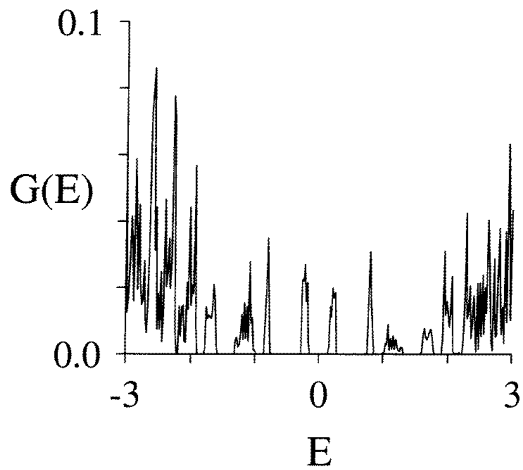

Figure 2. The differential conductance as a function of energy for a system with a uniform barrier of area M^2.

superconductor, Δ has matrix elements $\Delta_{ii} = \Delta(r_i)\exp \mathrm{i}\theta_i$, where the magnitude of the order parameter is chosen to satisfy

$$\Delta(r_i) = \begin{cases} \Delta_0 r_i/\xi & \text{for } r_i \leqslant \xi \\ \Delta_0 & \text{otherwise} \end{cases}$$

and for a vortex lying on the c-axis, $[r_i, \theta_i]$ are the polar coordinates of a site i in the a–b plane. For all other sites, $\Delta_{ii} = 0$.

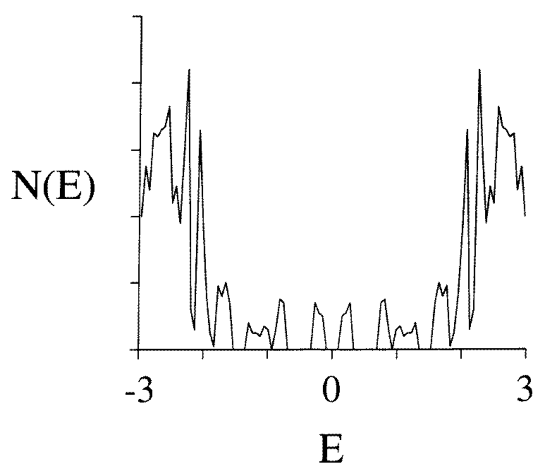

Figure 3. The density of states $N(E)$ corresponding to the conductance of figure 2.

The hopping elements γ_{ij} are non-zero for nearest-neighbour sites only. To simulate an anisotropic Fermi surface and to set the energy scale, if i and j are nearest neighbours belonging to the same a–b plane, or if both belong to a normal wire, then $\gamma_{ij} = 1$, whereas if they are neighbouring sites belonging to adjacent a–b planes and both belong to the superconductor then $\gamma_{ij} = 1/5$.

The simulated structure is the infinitely long parallelopiped shown in figure 1(a), with a–b planes of area M^2 sites and a vortex parallel to the c-axis, passing through the centre of the sample. A superconductor of length L_s sites, is connected to semi-infinite normal wires of cross-sectional area M^2. Between the left wire and the left-hand surface of the superconductor is a tunnel barrier of width L_b sites. For all sites i, except those belonging to the tunnel barrier, the diagonal matrix element $\epsilon_i = \epsilon_0$. If i belongs to the right-hand surface of the superconductor and j to the surface of the right-hand normal lead, then the bulk value $\gamma_{ij} = 1/5$ is assigned. This NISN structure allows for the possibility that sub-gap quasi-particles can propagate through the vortex from the left to the right normal wire. Within the barrier, the diagonal elements of H_0 are set to $\epsilon_0 + 10$ and those of Δ set to zero.

In what follows we shall make use of two models for the barrier. For the results of figures 2 and 3, all hopping elements between barrier sites and the left-hand surface of the superconductor are assigned their bulk value of $\gamma_{ij} = 1/5$ and sites belonging to the barrier are assigned a diagonal element $\epsilon_i = \epsilon_0 + 10$. Figure 2 shows the differential conductance $G(E)$ as a function of E, obtained with the choice $M = 7$, $L_b = 1$ and $L_s = 35$, $\Delta_0 = 2.4$ and $\epsilon_0 = -1$, while figure 3 shows the corresponding quasi-particle density of states. The two sets of results are clearly correlated, but whereas the density of states is an even function of E, the conductance does not possess this symmetry.

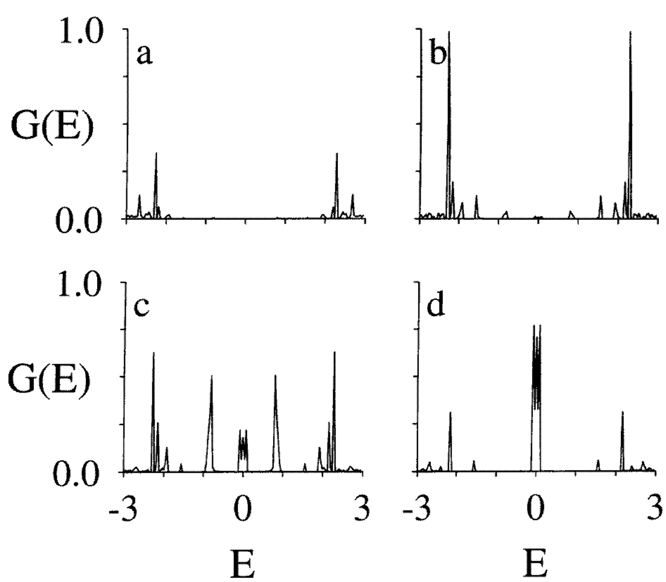

Figure 4. These show the differential conductance as a function of energy when contact is made with four different points along the vortex: (a) corresponds to contact outside the vortex and (d) to contact at the centre of the vortex. For this system $\epsilon_0 = 0$, corresponding to a half-filled band.

The above model describes transport through a barrier of uniform width over the interface between the superconductor and left-hand normal wire. To simulate an STM tip of atomic dimensions, we also analyse a second model, in which diagonal elements of sites belonging to the barrier are assigned a bulk value of $\epsilon_i = \epsilon_0$. However all but

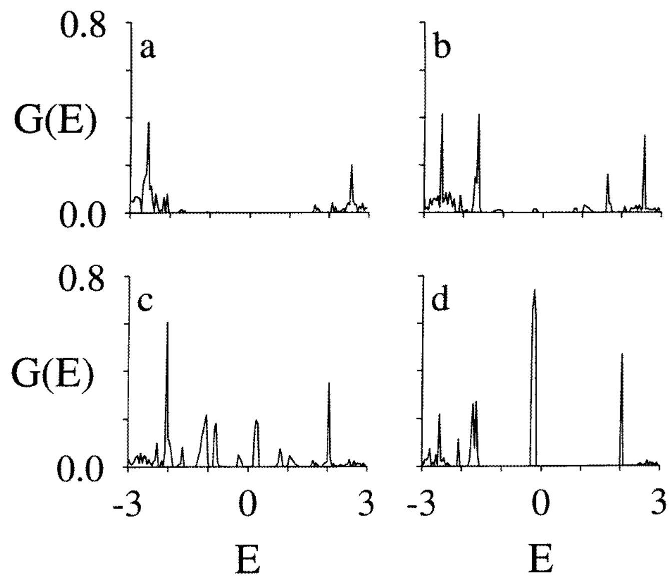

Figure 5. These show the same graphs as figure 4, but with $\epsilon_0 = -1$. Consequently the partial density of states for a single quasi-particle type is no longer an even function of energy.

a single hopping element between barrier sites and those on the left-hand surface of the superconductor are set to zero. To simulate an STM tip, the single non-zero hopping element is assigned a value $\gamma_0 \ll 1$ and the position r_0 of the non-zero element varied to yield different points of contact.

Figure 4 shows four graphs of the differential conductance for contact points starting from $r_0 > \xi$ (part a) and moving towards $r_0 = 0$ at the core (part d). For these results, $M = 9$, $L_s = 35$, $\epsilon_0 = 10^{-6}$ and $\gamma_0 = 1/5$. This choice of ϵ_0 corresponds to half-filling, with $\delta N_B(E) = 0$ and therefore as predicted by equation (12), the conductance is an even function of E. To illustrate the sensitivity to band-filling, figure 5 shows four results obtained with the same parameters as figure 4, except that $\epsilon_0 = -1$. In this case $\delta N_B(E) \neq 0$ and gross asymmetries in the differential conductance are obtained.

In conclusion, we have presented new results for the differential conductance $G(E)$ of a normal–superconducting contact. We predict that whatever the strength of the contact, in the absence of open channels in the superconductor, $G(E)$ is necessarily an even function of E and that an asymmetric current–voltage characteristic implies the existence of propagating states. In the tunnelling limit, symmetry breaking arises from the difference between particle and hole densities of states and if the Fermi energy is close to a van Hove singularity, symmetry breaking will be sensitive to doping.

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