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Theory of the sign of multi-probe conductances for normal and superconducting materials

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Abstract. We examine equivalent forms of the current–voltage relationship applicable to mesoscopic superconductors and use one of these to derive general conditions for the sign of the conductance in a four-probe measurement. For disordered systems, with well separated voltage probes, where the normal-state conductance is positive, we predict that the sign of the longitudinal four-probe conductance of superconducting wires can be reversed by varying an applied magnetic field, and that at certain critical values of the field, the conductance passes through a singularity.

1. Introduction

During the past few years, descriptions of charge transport in mesoscopic superconductors have focused mainly on either normal–superconducting (N–S) boundary conductances, two-probe conductances of N–S–N structures or the Josephson effect in S–N–S systems [1–17]. There currently exist no detailed theoretical results for multi-probe measurements, even though the multi-probe conductance formulae to be evaluated have been known for some time [2, 4]. It is well known that in phase-coherent, normal structures both positive and negative four-probe electrical conductances can occur, whereas the corresponding two-probe conductances are necessarily positive [18, 19]. More recently it was shown that the longitudinal conductance of a normal disordered wire can have arbitrary sign only if the disorder is sufficiently weak, whereas in superconductors negative conductances can arise whatever the degree of disorder [20], suggesting that superconductivity itself can induce sign changes. In this paper we present a detailed analysis of the sign of the four-probe conductance of phase-coherent structures.

A key complication which arises when deriving formulae for transport properties in interacting mesoscopic systems is the need to impose detailed balance in the steady state. Perhaps the simplest example of this arises within mean-field BCS theory, when describing the effect of superconductivity on transport properties, where it is known [2] that the condensate chemical potential μ must be chosen self-consistently to ensure charge conservation. For non-interacting systems [19] this complication does not arise, and for simple N–S interfaces can be avoided by choosing the superconductor as one of the external voltage probes [1]. However, for multi-probe measurements in which the current-carrying leads are normal [2–4], this minimal level of self-consistency is crucial.

One consequence of the absence of automatic quasi-particle charge conservation is the explicit appearance of μ in current–voltage relations applicable to mesoscopic

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superconductors. For a system connected by perfect normal leads to N external reservoirs at potentials v_i, $i = 1, 2, \ldots, N$, these take the form [2, 4]

$$I_i = \sum_{j=1}^{N} a_{ij}(v_j - v) \tag{1}$$

where $v = \mu/e$, I_i is the current carried by lead i and a_{ij} is a matrix element formed from linear combinations of quasi-particle reflection and transmission coefficients [2].

The appearance of $\mu = ev$ on the right-hand side of equation (1) is a manifestation of two key features; first, there exists a superconducting condensate possessing a well-defined chemical potential; and second, the condensate acts as a source and sink of charge. Equation (1) is extremely general and contains all known results for phase-coherent superconducting and non-interacting normal systems as special cases. It should be noted that except in a trivial adiabatic limit, it does not describe measurements in which superconductors with different condensate potentials are present, since in such structures order parameter phase differences varying at the Josephson frequency are present and therefore a theory based on time-independent scattering theory cannot be applied.

One can recast equation (1) in many equivalent forms, some of which are particularly useful when dealing with specific problems. In the following section, we highlight two such forms, one of which is used in section 3 to address the question of negative four-probe conductances in normal and superconducting structures. The analysis of section 3 suggests that the behaviour of longitudinal four-probe conductances in the presence of magnetic fields in the localized regime, should be markedly different for normal and superconducting systems, and in section 4 we show the results of a numerical simulation in two dimensions, which illustrate these differences.

2. Equivalent forms of the current–voltage relation

Our motivation for rewriting equation (1) stems from the fact that in the presence of Andreev scattering, the sum of elements of each row and column of the matrix $\{a_{ij}\}$ are non-zero. In [4], the quantities

$$x_i = \sum_{j}^{N} a_{ij} \tag{2}$$

and

$$y_j = \sum_{i}^{N} a_{ij} \tag{3}$$

were therefore identified as natural variables, which characterize the effect of Andreev scattering on transport properties. In another context, Büttiker has further noted that an approximate description of finite-frequency transport [24] yields an equation of the same form as (1), with non-zero parameters x_i, y_j. In the latter context these quantities were referred to as *emissivities* and *injectivities* respectively.

Starting from equation (1), one can write down two admittance matrices, with elements $\{a'_{ij}\}$ and $\{a''_{ij}\}$, satisfying

$$I_i = \sum_{j=1}^{N+1} a''_{ij} v_j \qquad i = 1, 2, \ldots, N+1 \tag{4}$$

$$I_i = \sum_{j=1}^{N} a'_{ij} v_j \qquad i = 1, 2, \ldots, N \tag{5}$$

where in equation (4) we have written $v_{N+1} = v$ and

$$I_{N+1} = -\sum_{i=1}^{N} I_i$$

with I_{N+1} the total current flowing out of the superconductor. For $i, j \leqslant N$ one finds $a''_{ij} = a_{ij}$, $a''_{i,N+1} = -x_i$, $a''_{N+1,j} = -y_j$ and $a''_{N+1,N+1} = s$, where

$$s = \sum_{j=1}^{N} y_j = \sum_{i=1}^{N} x_i .$$

Clearly equation (4) treats the superconductor on the same footing as other reservoirs and is particularly relevant when μ is determined by external means, as in a typical boundary resistance measurement.

Equation (5) on the other hand is more relevant when the net current into the superconductor is zero, in which case μ can be eliminated through the condition

$$\sum_{i=1}^{N} I_i = 0$$

to yield

$$a'_{ij} = a_{ij} - x_i y_j / s . \tag{6}$$

Since

$$\sum_{i=1}^{N} a'_{ij} = \sum_{j=1}^{N} a'_{ij} = 0$$

the formal structure of multi-probe conductance formulae based on matrix elements $\{a'_{ij}\}$ is identical for normal and superconducting structures. It is interesting to note that for situations in which there is no quasi-particle transmission between different reservoirs, the matrix $\{a_{ij}\}$ is diagonal and therefore at first sight equation (1) suggests that charge does not flow between different reservoirs. Such a conclusion would be incorrect, because reservoirs are coupled through the steady-state condition

$$\sum_{i=1}^{N} I_i = -I_{N+1}$$

where I_{N+1} is the current leaving the superconductor. Indeed for the case of a superconductor connected to two normal probes, for which $N = 2$ and $I_3 = 0$, one finds $I_1 = -I_2$ and therefore a non-zero current, mediated by the superconductor, flows from probe 1 to probe 2. Equations (4) and (5) yield the same result, but since $\{a'_{ij}\}$ and $\{a''_{ij}\}$ are not diagonal, the coupling of reservoirs in the absence of quasi-particle transmission is more transparent.

3. Analysis of the sign of four-probe conductances

In the presence of $N = 4$ probes, writing $I_i = -I_j = I_{ij}$ and for $k, l \neq i, j$, choosing $I_k = I_l = 0$, one defines the four-probe conductance $G_{ij,kl}$ through the relation $G_{ij,kl} = I_{ij}/(V_k - V_l)$. Starting from equation (2), or equivalently equations (4) or (5), this expression can be evaluated once the matrix elements $\{a_{ij}\}$ are known. In units of $2e^2/h$, these are given by [4] $a_{i,j\neq i} = T_{ij}^{\mathrm{A}} - T_{ij}^{\mathrm{O}}$, $a_{ii} = M_i + R_i^{\mathrm{A}} - R_i^{\mathrm{O}}$, where T_{ij}^{O} and R_j^{O} are normal transmission and reflection coefficients for quasiparticles incident at probe j, and T_{ij}^{A} and R_j^{A} are the corresponding Andreev coefficients [2, 4]. At zero temperature these quantities are the scattering probabilities of zero-energy quasi-particles, whereas at finite temperature they are thermal averages of such probabilities. At zero temperature M_l is the number of channels in probe i and at finite temperature it is the corresponding thermally averaged number of channels. Since

$$R_i^{\mathrm{O}} + R_i^{\mathrm{A}} + \sum_{j\neq i}(T_{ij}^{\mathrm{O}} + T_{ij}^{\mathrm{A}}) = R_i^{\mathrm{O}} + R_i^{\mathrm{A}} + \sum_{j\neq i}(T_{ji}^{\mathrm{O}} + T_{ji}^{\mathrm{A}}) = M_i$$

the matrix $\mathbf{A}$ has the property that any diagonal element is necessarily greater than or equal to the sum of any subset of the other elements on the same row and similarly for any subset of elements in the same column. The emissivities and injectivities are given by

$$x_i = \sum_j a_{ij} = 2\left(R_i^{\mathrm{A}} + \sum_{j\neq i} T_{ij}^{\mathrm{A}}\right) \qquad y_j = \sum_i a_{ij} = 2\left(R_j^{\mathrm{A}} + \sum_{i\neq j} T_{ij}^{\mathrm{A}}\right).$$

Examples of $\mathbf{A}'$ for a device connected to two, three and four probes are shown in table 1. The formulae in the table illustrate that the diagonal elements a'_{ii} are always positive; a result which is proved in the appendix. As a consequence, raising the potential of a reservoir causes more net current to be drawn from that reservoir. In contrast, the examples in table 1 show that the off-diagonal elements may be of either sign, and therefore raising the potential of one reservoir may result in an *increase* or *decrease* in the net current supplied to each of the others. This is unlike the situation for normal materials, where the off-diagonal elements of $\mathbf{a}'$ are always negative, so raising the potential of one reservoir necessarily results in an increase in the net current supplied to each of the others. The requirement that the rows and columns of $\mathbf{A}'$ sum to zero also implies that for two probes, the off-diagonal elements are necessarily negative, whereas no such restriction arises for $N \geqslant 3$. As a consequence superconductors connected to three or more probes may exhibit new phenomena which are absent from simpler two-probe structures. To illustrate this feature, it is convenient to rewrite the multi-channel conductance formulae derived in [2, 4], in terms of elements a'_{ij} rather than a_{ij}. Since the N equations of (5) are linearly dependent we eliminate the Nth equation and write

$$\begin{pmatrix} I_1 \\ \vdots \\ I_{N-1} \end{pmatrix} = a'_N \begin{pmatrix} V_1 - V_N \\ \vdots \\ V_{N-1} - V_N \end{pmatrix} \tag{7}$$

where $\mathbf{a}'_N$ is the minor of $\{\mathbf{a}'\}$ obtained by deleting row and column N. The inverse of equation (7) is

$$\begin{pmatrix} V_1 - V_N \\ \vdots \\ V_{N-1} - V_N \end{pmatrix} = \frac{1}{d}\begin{pmatrix} b'_{11} & \cdots & b'_{N-1,1} \\ \vdots & & \vdots \\ b'_{1,N-1} & \cdots & b'_{N-1,N-1} \end{pmatrix} \begin{pmatrix} I_1 \\ \vdots \\ I_{N-1} \end{pmatrix} \tag{8}$$

where $d = \det \mathbf{a}'_N$, b_{ij} is the ijth element of the cofactor matrix of $\mathbf{a}'_N$ and if $N = 2$ we define $b'_{11} = 1$. It is shown in the appendix that the value of d is independent of which row and column are deleted from equation (5), even though the cofactor matrix is not. For simplicity we compute $G_{ij,kl}$ by taking $k = N-1$ and $l = N$. This choice simplifies the working but has no physical significance as we may label the probes in any order. From equation (8), writing $I_i = -I_j$, $I_k = 0$ for $k \neq i, j$, and defining $b_{i,N} = b_{N,i} = 0$, yields

$$G_{ij,N-1,N} = d/(b'_{i,N-1} - b'_{j,N-1}). \tag{9}$$

The determinant d can most easily be computed using the relation

$$d = \det \mathbf{A}'_N = \det \mathbf{A}_N - \frac{1}{S}\sum_{i=1}^{N-1}\sum_{j=1}^{N-1} x_i y_j b'_{ij} \tag{10}$$

where $\mathbf{A}_N$ is the minor obtained by deleting row and column N from $\mathbf{A}$. This relation is also proved in the appendix.

Table 1. Expressions for $\mathbf{A}'$ for simple systems. Top row: a single superconducting wire. Middle row: a device connected to three probes, with the dominant scattering processes Andreev reflection of particles incident from reservoir 3 and Andreev transmission between probes 1 and 2. This device illustrates the fact that off-diagonal coefficients of $\mathbf{A}'$ may be positive. Bottom row: a superconducting wire in the localized limit with two probes at each end of wire.

SYSTEM	A	A'
Single superconductor connected to 2 probes	$A = \begin{pmatrix} M - T_{11} & -T_{12} \\ -T_{21} & M - T^{O}_{22} \end{pmatrix}$ where $T_{ij} = T^{A}_{ij} - T^{O}_{ij}$	$A' = \begin{pmatrix} a'_{11} & -a'_{11} \\ -a'_{11} & a'_{11} \end{pmatrix}$ where $a'_{11} = T^{O}_{12} + T^{A}_{12} + 2(R^{A}_1 R^{A}_2 - T^{A}_{12}T^{A}_{21})/(R^{A}_1 + R^{A}_2 + T^{A}_{12} + T^{A}_{21})$
3-probe device	$A = M\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	$A' = M\begin{pmatrix} 1/3 & 1/3 & -2/3 \\ 1/3 & 1/3 & -2/3 \\ -2/3 & -2/3 & 4/3 \end{pmatrix}$
Long wire with negligible quasi-particle transmission along the wire.	$A = \begin{pmatrix} M - T_{11} & -T_{12} & 0 & 0 \\ -T_{21} & M - T^{O}_{22} + T_{22} & 0 & 0 \\ 0 & 0 & M - T_{33} & -T_{34} \\ 0 & 0 & -T_{43} & M - T_{44} \end{pmatrix}$ where $T_{ij} = T^{A}_{ij} - T^{O}_{ij}$	$a'_{11} = T^{O}_{12} + T^{A}_{12} + 2R^{A}_1 S_{BR}/S + (R^{A}_1 R^{A}_2 - T^{A}_{12}T^{A}_{21})/S$ $a'_{12} = -T^{O}_{12} + T^{A}_{12} S_{BR}/S - (R^{A}_1 R^{A}_2 - T^{A}_{12}T^{A}_{21})/S$ $a'_{13} = -(T^{A}_{12} + R^{A}_1)(T^{A}_{43} + R^{A}_3)/S$ $a'_{14} = -(T^{A}_{12} + R^{A}_1)(T^{A}_{34} + R^{A}_4)/S$ other a'_{ij} can be deduced by symmetry

Writing equation (9) in terms of a'_{ij} yields for a device connected to two probes

$$G_{12,12} = a'_{11} \tag{11}$$

in agreement with [2, 4]. For a device connected to three reservoirs equation (9) becomes

$$G_{ij,ik} = -d/a'_{jk}. \tag{12}$$

Finally for a device connected to four probes we find

$$G_{ij,kl} = d/(a'_{ki}a'_{lj} - a'_{kj}a'_{li}) \tag{13}$$

provided $i \neq j \neq k \neq l$.

Equations (11)–(13) show that G is always of the form $d/(\text{terms in } a'_{ij})$, so the sign of G is determined by the relative signs of d and the denominator. In the case where the system has two, three or four probes a key result is that d is always positive or zero, and provided some of the probes are not completely decoupled from the device d is always positive. We have proved this by using equation (10) to simplify d, substituting

$$a'_{ii} = 2R^{\mathrm{A}}_i + \sum_{j\neq i}(T^{\mathrm{O}}_{ij} + T^{\mathrm{A}}_{ij}) \qquad a'_{i,j\neq i} = T^{\mathrm{A}}_{ij} - T^{\mathrm{O}}_{ij}$$

and using a computer algebra package to evaluate the sign of d for three and four probes. In both cases the result was a sum of positive products of transmission probabilities. For two probes, $d = a'_{11}$ and remains positive. For more than four probes, the analysis was not possible, because the number of terms in the resulting expression for d exceeded the memory of our available computers.

We are now in a position to make firm statements about the sign of G for different arrangements. Result (11), along with the appendix, shows that a two-probe conductance is always positive. For the three-probe case, the sign of $G_{ij,il}$ tells us the sign of the effective transmission between the current-only probe and the voltage-only probe. For a normal material the three-probe conductance is always positive, but for a superconductor, if Andreev scattering dominates, it may be negative. The sign of the four-probe conductance in normal systems has been the subject of much experimental and theoretical work [21, 22]. For a normal system, equation (13) reduces to $G_{ij,kl} = d/(T_{ki}T_{lj} - T_{kj}T_{li})$, which was interpreted by Avishai and Band [22] as showing that if the current from probe i has a high probability of being transmitted to voltage probe k, while T_{kj} is small, then reservoir k will need to supply a large current to ensure that $I_k = 0$, so $V_k \approx V_i$. A similar argument shows that if $T_{lj} \gg T_{kj}$ then $V_l \approx V_j$, so $V_k > V_l$ and $G_{ij,kl}$ is positive. This situation can be understood by reference to the long wire shown in figure 1(a), connected to reservoirs labelled 1, 2, 3, 4. If we choose $i = 1$, $j = 2$, $k = 3$ and $l = 4$ then $G_{ij,kl}$ measures the longitudinal conductance along the wire which would be expected to be positive if the transmission along the wire is weak.

In the presence of Andreev scattering, the sign of $G_{ij,kl}$ has a similar interpretation, which allows one to understand the physical reason for a recent prediction [20] that the longitudinal conductance of a superconducting wire in the localized regime can be negative, whereas the corresponding normal-state conductance is positive. As indicated by the expressions in the third row of table 1, whereas for strongly disordered normal materials a'_{31} and a'_{42} vanish, in the presence of Andreev scattering they are both negative and can have larger magnitudes than a'_{32} and a'_{41}. Hence negative conductances occur because the effective coupling between probes at opposite ends of the wire is greater than that across the wire.

4. Magnetoconductance of a wire

While the above analysis demonstrates that sign changes due to the onset of superconductivity are possible, it does not identify systems for which such changes are probable. In this section we examine in more detail the longitudinal conductances $G_{12,34}$ and $G_{14,32}$ of long normal and superconducting wires of the kind shown in figure 1(a) and show that the sign of these conductances may be reversed by the application of a magnetic field. In [20], it was shown that in the limit of vanishing quasi-particle transmission along the wire, $G_{12,34}$ is given by

$$G_{12,34} = -\left(\frac{T^{\mathrm{A}}_{31} - T^{\mathrm{O}}_{31}}{d_{\mathrm{TL}}} + \frac{T^{\mathrm{A}}_{42} - T^{\mathrm{O}}_{42}}{d_{\mathrm{BR}}}\right)^{-1} \tag{14}$$

with a similar expression for $G_{14,32}$. In this expression, d_{TL} and d_{BR} are positive quantities, so the crucial factor determining the sign of G is the relative strengths of the normal and Andreev scattering probabilities across the wire. If the wire is thin, these coefficients will be appreciable. Numerical work [23, 25] has suggested that in this limit, for homogeneously disordered samples with no applied magnetic field, normal transmission will dominate. Therefore in order to observe a sign change the geometry must be chosen to enhance T^{A}.

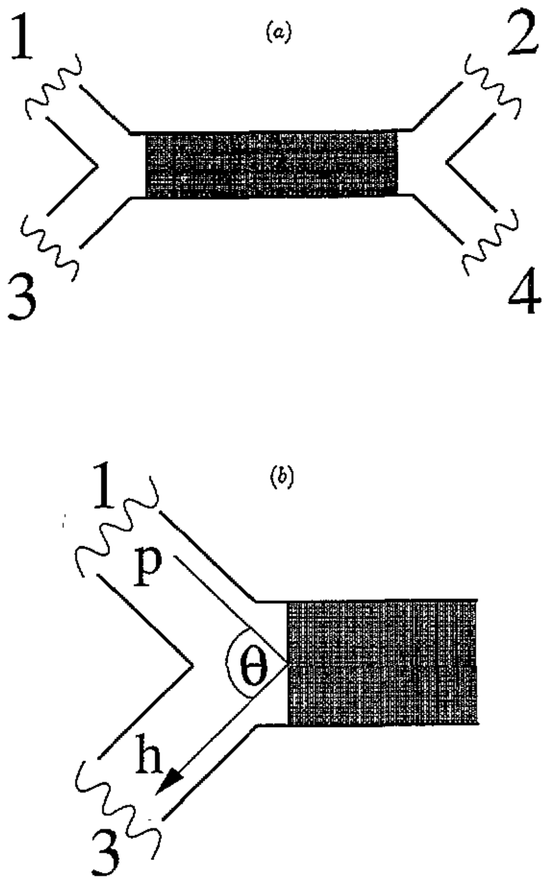

Figure 1. (*a*) A wire connected to four external probes. (*b*) A possible trajectory of an Andreev-reflected quasi-particle incident from probe 1, which has a high probability of being transmitted into probe 3.

Such a geometry is shown in figure 1(*a*), for which the probes at each end are situated opposite each other, but a potential barrier prevents direct transmission across the sample. In the presence of a magnetic field it becomes possible for a particle incident from probe 1 to evolve into a hole emitted into probe 2, via Andreev *reflection* at the superconducting interface, as illustrated by figure 1(*b*). Since the angle θ in the figure increases with applied magnetic field, one expects the conductance to reverse sign over certain ranges of B, such that θ is sufficient to redirect a high proportion of Andreev reflected particles from probe 1 into 2.

Simulations were performed using the tight-binding model and with the transfer matrix based algorithm described in [4]. Because this algorithm imposes a current flow at the external connections perpendicular to the slices, the precise geometry simulated is shown in figure 2. The dimensions (labelled in the figure) used were $i = 5$ sites, $j = 5$ sites, $k = 30$ sites, and the potential barriers at the ends of the wires were one site wide $\times$ five sites long. Quasi-particles were prevented from entering the potential barriers by large on-site potentials in the barrier region. In the shaded region the site potentials were chosen at random from a uniform distribution between limits $-\delta U$ and δU, and when required a constant superconducting order parameter $\Delta = 0.2$ was assumed.

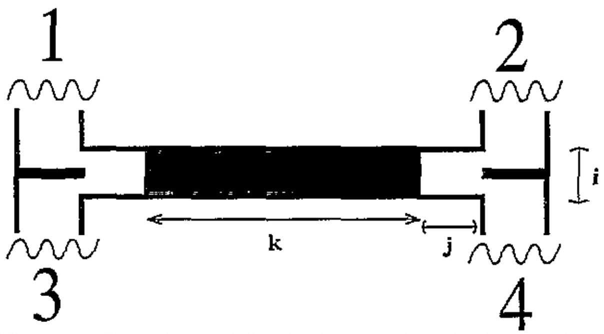

Figure 2. The wire modelled in the numerical simulations. The black areas are potential barriers which quasi-particles are unable to penetrate; the shaded area is the region in which normal potential disorder and a constant order parameter exist.

Typical plots of conductance against magnetic field are shown in figures 3 and 4 for $G_{12,34}$ and figures 4 and 5 for $G_{14,32}$. Figures 3 and 5 show the case of small disorder, $\delta U = 0.5$, where as figures 4 and 6 show that for a large disorder, $\delta U = 1.0$. Plots for four different realizations of disorder are shown in each figure, one realization in each column. The upper plots are for superconducting systems. the lower plots are for the equivalent normal structures in which Δ is set to zero everywhere, but all other potentials are unchanged. In figures 3 and 5 the large conductances for the normal devices show that the transmission probabilities along the wire are high, so all the terms in the denominator of (13) are of comparable magnitude. Consequently the conductance changes sign whether or not there is a superconducting order parameter. In contrast, for the strongly disordered case shown in figures 4 and 6, where the small normal-state conductances imply negligible longitudinal transmission along the wires, the normal conductances remain positive, consistently with [20]. However, when the superconducting order parameter is switched on, sign changes reappear in the magnetoconductance. An interesting feature of figures 3 to 6 is that the sign changes always occur via a singularity in G, so the conductance never passes smoothly through zero. This is a consequence of the positivity of d in expression (13), which implies that a sign change can only occur when the *denominator* passes through zero. In practice, we expect the conductance to be bounded by the fact that when the current flow becomes large, we are no longer in the linear response regime. Nevertheless, our results suggest that close to a sign reversal, the four-probe magnetoconductance of superconducting wires in the ballistic and localized regimes will show sharp features. Since the effect does not depend on the degree of localization, such features should be measurable in both conventional and high-T_c superconductors.

5. Summary

We have shown how the fundamental current–voltage relations introduced in [2, 4] can be recast in a form which resembles those of a normal structure and which makes no explicit reference to the condensate potential. Since the condensate can be regarded as a source and sink of charge, this is formally equivalent to a technique pointed out by Büttiker [19] which recursively eliminates those reservoirs that are not actively used in the conductance measurement. This procedure allows equations for multi-probe conductances to be written in the same form for both normal and superconducting samples, at the expense of relaxing certain restrictions on the signs of admittance matrix elements a'_{ij}. Starting from

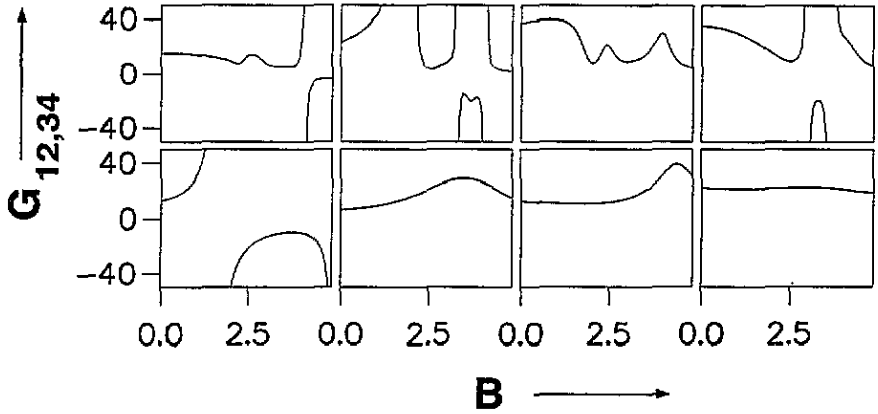

Figure 3. Plots of $G_{12,34}$ against applied magnetic field for the device shown in figure 1, with $\delta U = 0.5$. Each column shows a different realization of disorder. The top plots show the case for a superconductor, the lower plots the equivalent devices with no superconducting order parameter but with all other potentials unchanged.

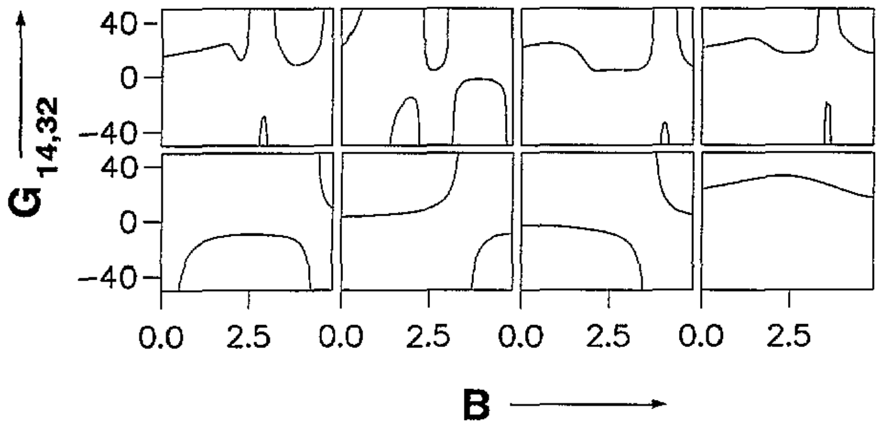

Figure 4. As figure 3, but showing a plot of $G_{14,32}$.

these equations, we have derived conditions for the sign of the multi-probe conductance of samples connected to up to four reservoirs. The numerical results of figures 3 to 6 show that for superconducting materials in the localized and diffusive regimes, applying a magnetic field may change the sign of the longitudinal conductance.

Acknowledgments

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Appendix

In this Appendix we prove some properties of the transport matrix $\mathbf{A}'$ and its minors.

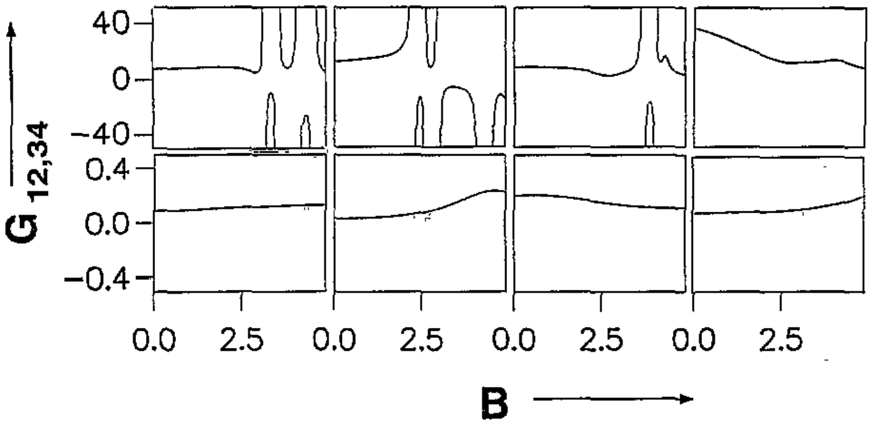

Figure 5. As figure 3, but with $\delta U = 1.0$.

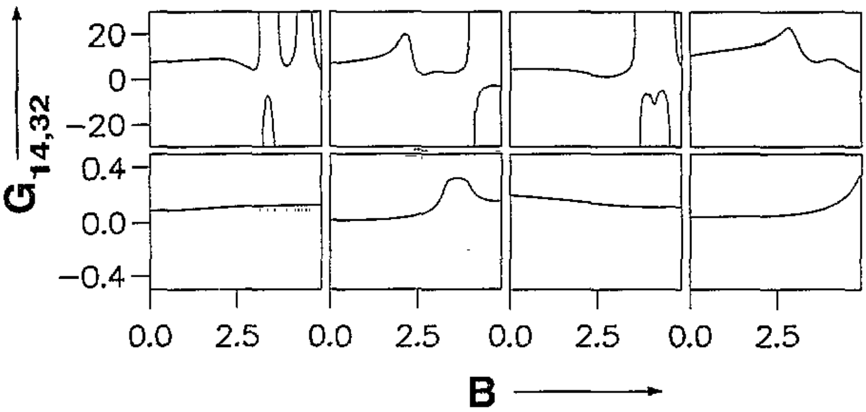

Figure 6. As figure 4, but with $\delta U = 1.0$.

A1. Proof that the diagonal elements of A′ are positive

This follows by writing

$$a_{ii} = 2R_i^{\mathrm{A}} + (1/2)\sum_{j\neq i}(T_{ij}^{\mathrm{A}} + T_{ij}^{N} + T_{ji}^{\mathrm{A}} + T_{ji}^{N})$$

where all sums are taken over the range 1 to N unless otherwise indicated. Hence

$$\begin{aligned} Sa'_{ii} = {} & \left(4R_i^{\mathrm{A}} + \sum_{j\neq i}(T_{ij}^{\mathrm{A}} + T_{ij}^{N} + T_{ji}^{\mathrm{A}} + T_{ji}^{N})\right)\left(\sum_j (R_j^{\mathrm{A}} + \sum_{k\neq j} T_{kj}^{\mathrm{A}})\right) \\ & -4\left(R_i^{\mathrm{A}} + \sum_{j\neq i} T_{ij}^{\mathrm{A}})(R_i^{\mathrm{A}} + \sum_{j\neq i} T_{ji}^{\mathrm{A}}\right) \\ = {} & \left(\sum_{j\neq i}(T_{ij}^{\mathrm{O}} + T_{ji}^{\mathrm{O}})\right)\left(\sum_j (R_j^{\mathrm{A}} + \sum_{k\neq j} T_{kj}^{\mathrm{A}})\right) \\ & + \left(R_i^{\mathrm{A}} + \sum_{j\neq i}(T_{ij}^{\mathrm{A}} + T_{ji}^{\mathrm{A}})\right)\left(\sum_{j\neq i} R_j^{\mathrm{A}} + \sum_{k\neq i,j} T_{jk}^{\mathrm{A}}\right) + \sum_{j\neq i}(T_{ij}^{\mathrm{A}} - T_{ji}^{\mathrm{A}})^2. \end{aligned} \qquad (1)$$

Since all the terms are positive it follows that $a'_{ii} > 0$.

A2. Proof of expression (10)

The proof follows by defining $N \times N$ matrices $\mathbf{C}^{(n)}$, $\mathbf{Q}^{(n)}$ and $\mathbf{R}^{(n)}$ with $n \leqslant N$ as follows:

$$c_{ij}^{(n)} = \begin{cases} c_{ij} & \text{for } i < n \\ c_{ij} - x_i y_j / S & \text{for } i \geqslant n \end{cases} \tag{2}$$

$$q_{ij}^{(n)} = \begin{cases} c_{ij} & \text{for } i < n \\ -x_i y_j / S & \text{for } i = n \\ c_{ij}^{(n)} & \text{for } i > n \end{cases} \tag{3}$$

$$r_{ij}^{(n)} = \begin{cases} c_{ij} & \text{for } i < n \\ -x_i y_j / S & \text{for } i = n \\ c_{ij} & \text{for } i > n. \end{cases} \tag{4}$$

Since $\mathbf{Q}^{(n)}$ may be obtained from $\mathbf{R}^{(n)}$ by subtracting row n of $\mathbf{R}^{(n)}$ from each of the rows $(n+1), \ldots, N$ we have that

$$\det \mathbf{Q}^{(n)} = \det \mathbf{R}^{(n)}. \tag{5}$$

Also, by expanding along row n of $\mathbf{C}^{(n)}$ we find

$$\det \mathbf{C}^{(n)} = \det \mathbf{C}^{(n+1)} + \det \mathbf{Q}^{(n)} \tag{6}$$

and

$$\det \mathbf{C}^{(n)} = \det \mathbf{C}^{(n+1)} + \det \mathbf{R}^{(n)}. \tag{7}$$

Hence

$$\det \mathbf{C}^{(1)} = \det \mathbf{C}^{(N)} + \sum_{j=1}^{N} \det \mathbf{R}^{(j)}. \tag{8}$$

Expression (10) now follows by expanding $\det \mathbf{R}^{(j)}$.

A3. Proof that $\det \mathbf{A}'_j$ is independent of j

We consider the jjth and NNth minors $\mathbf{A}'_j$ and $\mathbf{A}'_N$ of $\mathbf{A}'$, and construct a new matrix $\mathbf{B}$ by adding all rows (except row j) to row j in $\mathbf{A}'_N$, then adding all columns (except column j) to column j, and finally exchanging row j with row $N-1$ and column j with column $N-1$. Since adding the rows and columns leaves the determinant unchanged, while each exchange reverses its sign, we have that $\det \mathbf{B} = \det \mathbf{A}'_N$. However, as the sum of any column of $\mathbf{A}$ is zero, it follows that the sum of column i of $\mathbf{A}'_N$ is a'_{Ni}. Similarly the sum of row k of $\mathbf{A}'_N$ is a'_{kN}. Hence $\mathbf{B} = \mathbf{A}'_j$, and $\det \mathbf{A}'_j = \det \mathbf{A}'_N$.

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