Probing Spin Polarization with Andreev Reflection: A Theoretical Basis

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Andreev reflection at the interface between a ferromagnet and a superconductor has become a foundation of a versatile new technique of measuring the spin polarization of magnetic materials. In this paper we will briefly outline a general theory of Andreev reflection for spin-polarized systems and arbitrary Fermi surface in two limiting cases of ballistic and diffusive transport.

Andreev reflection (AR) at the interface between a superconductor and a ferromagnet has been attracting significant interest (e.g., Refs.[1−5]) as the foundation of a new technique[1] to measure the spin polarization in ferromagnets. The technique is based on the idea[6] that the Andreev process is forbidden in half-metals, where only electrons with one spin direction are present at the Fermi level. Correspondingly, in a ferromagnet the Andreev current is partially suppressed, as not all of the conductance channels (CC) are "open" for AR; some channels exist in one spin direction, but not in the other, and thus do not contribute to the Andreev current.

Building a stable and reliable technique for probing spin polarization based on AR is not always straightforward and requires a quantitative theory. Such a theory should take into account the following effects: (1) different number of CC for different spins, (2) finite interface resistance, (3) band structure effects (deviation of the Fermi surface from spherical and the band dispersion from parabolic), (4) effect of an evanescent Andreev hole on quasiparticle current in half-metallic CC, and (5) diffusive transport in the ferromagnet, if needed.

The existing works treat only some of these questions. The first one was taken care of in Ref.[6]. The second one was answered in part in the seminal paper of Blonder, Tinkham and Klapwijk[7], but only for "nonmagnetic" channels (the CC that exist in both spin directions). The third one was dealt with in Ref.[3], but only in the ballistic limit. The fourth one was mentioned in Refs.[2], but not investigated quantitatively. Finally, the last one was briefly touched upon in Ref.[5], but left in the form that could not be directly applied to the experiment. Some aspects of diffusive transport and AR were addressed in Refs.[4].

In this paper, we address all these issues and present a compendium of formulas needed for a quantitative analysis of superconductor-ferromagnet AR. We start with a ballistic contact, whose size is smaller than the mean free path of electrons in the bulk. All electrons with a positive projection of their velocity onto the current direction, x, pass through the contact. Conductance of a ballistic contact is[8,3]

$$G=\frac{e^2}{\hbar}\frac{1}{2}\left\langle N|v_x|\right\rangle A, \tag{1}$$

where A is the contact area, N is the volume density of electronic states at the Fermi level, v is the Fermi velocity, and brackets denote Fermi surface averaging:

$$\frac{1}{2}\left\langle N|v_x|\right\rangle=\frac{1}{(2\pi)^3}\sum_{i\sigma}\int\frac{dS_F}{|v_{\mathbf{k}i\sigma}|}v_{\mathbf{k}i\sigma,x}. \tag{2}$$

Integration and summations are over the states with $v_{\mathbf{k}i\sigma,x}>0$, and Ω is the unit cell volume. $\mathbf{k}$, i, and σ denote the quasimomentum, the band index, and the electron spin, respectively. It is instructive to look at Eq.2 from the "mesoscopic" perspective, using as a starting point the Landauer formula for the conductance of a single electron[9], $G_0=e^2/h$. The total conductance is equal to G_0 times the number of CC, N_{cc}, which is defined as the number of electrons that can pass through the contact. If the translational symmetry in the interface plane is not violated, then the quasimomentum in this plane, $\mathbf{k}_\parallel$, is conserved, and N_{cc} is given by the total area of the contact times the density of the two-dimensional quasimomenta. The latter is $S_x/(2\pi)^2$, where S_x is the area of the projection of the bulk Fermi surface onto the contact plane. Thus $G=\frac{e^2}{h}\frac{S_xA}{(2\pi)^2}\equiv\frac{e^2}{\hbar}\frac{1}{2}\left\langle N|v_x|\right\rangle A$.

This is an important result. To the best of our knowledge, Walter Harrison was the first to spell it out in 1961[10], and there is no lack of the recent paper manifesting proper understanding of this issue (e.g., Ref.[11]). However, till now many otherwise correct and useful paper erroneously identify the number of conductivity channels and the density of states at the Fermi level, that is,

$$\boxed{N_{cc}\propto N(E_F)}=\frac{1}{(2\pi)^3}\sum_{i\sigma}\int\frac{dS_F}{|v_{\mathbf{k}i\sigma}|}. \tag{3}$$

incorrect!

Let us consider now the opposite limit, when the contact size is much *larger* than the mean free path. The conductance is then given by the the bulk conductivity, which is known from the Bloch-Boltzmann theory:

$$\sigma=(e^2/\hbar)\left\langle Nv_x^2\right\rangle\tau, \tag{4}$$

where τ is the relaxation time. The Ohm's law requires that the conductance $G=\sigma A/L$, where L is the length of the disordered region. This can be reproduced within the "mesoscopic" approach[9], taking into account that now each CC, that is, each separate $\mathbf{k}_\parallel$ state, has a finite probability for an electron to get through the disordered region, $0 \leq T \leq 1$, and

$$G = \frac{e^2}{h}\sum_\kappa T_\kappa = \frac{e^2}{h}\int_\lambda^\infty d\zeta P(\zeta)/\cosh^2(L/\zeta), \qquad (5)$$

where $\kappa \equiv \{\mathbf{k}_\parallel, i, \sigma\}$. T_κ is conveniently defined in terms of the probability distribution, $P(\zeta)$, of the localization lengths, ζ. The cutoff λ should be of the order of the mean free path l; in fact, $\lambda = 2l$[9]. (the factor 2 accounts for two possible directions of the electron velocity). Ohm's law requires that $G \propto 1/L$, thus the behavior of $P(\zeta)$ at large ζ must be $const/\zeta^2$. Normalization requires that $const = \lambda N_{cc}$. Substituting that in Eq.5, we get

$$\begin{aligned} G &= \frac{e^2}{h}\int_\lambda^\infty \frac{\lambda N_{cc} d\zeta}{\zeta^2\cosh^2(L/\zeta).} \approx \frac{e^2\lambda N_{cc}}{hL} \\ &= \frac{e^2}{\hbar}\frac{A\lambda}{\Omega L}\sum_{i\sigma}\int\frac{dS_F}{|v_\kappa|}v_{\kappa,x}. \end{aligned} \qquad (6)$$

In the constant τ approximation, used in Eq.4, the average mean free path $l = \sum_{i\sigma}\int \frac{dS_F}{|v_\kappa|}v_{\kappa,x}^2\tau / \sum_{i\sigma}\int\frac{dS_F}{|v_\kappa|}v_{\kappa,x}$, thus $\lambda_\kappa = 2v_{\kappa x}\tau$. Thus

$$\langle G\rangle_L = \frac{e^2}{\hbar}\frac{A}{\Omega L}\sum_{i\sigma}\int\frac{2dS_F}{|v_\kappa|}v_{\kappa,x}^2\tau = \frac{e^2}{\hbar}\left\langle N v_x^2\right\rangle\frac{A}{L} = \sigma\frac{A}{L}.$$

In the diffusive limit the conductance is determined by $\left\langle N v_x^2\right\rangle$, as it should.

The standard theory of AR (BTK)[7], places a specular barrier at the interface, and assumes the ballistic regime and the free electron band structure in the bulk. Let us reproduce the main results of the BTK paper using, instead of their derivation, the "mesoscopic" approach[9]. Probabilities of four processes must be considered: normal reflection, defined as the process where $\mathbf{k}_\parallel$ is conserved, the group velocity in the direction perpendicular to the interface changes sign, AR, when $\mathbf{k}_\parallel$ changes to $-\mathbf{k}_\parallel$, and transmission into the superconductor with or without the branch crossing[7]. The energy is conserved, the electron wave function should be continuous, as well as the current. This gives enough information to find the probabilities, and the total current can be written as

$$\langle G\rangle_{NS} = \frac{e^2}{h}\sum_\kappa T_S(\kappa) = \frac{e^2}{h}\sum_\kappa(1 + A_\kappa - B_\kappa), \qquad (7)$$

where A and B are the probabilities of the normal and Andreev reflection, respectively. Beenakker showed[9] that the "Andreev transparency", the probability of an Andreev process, can be expressed in terms of the normal transparency T_N of the interface. For zero bias :

$$T_S = \frac{2T_N^2(\kappa)(1+\beta^2)}{\beta^2 T_N^2 + [1 + r_N^2]^2} = \frac{2T_N^2(1+\beta^2)}{\beta^2 T_N^2 + [2 - T_N]^2} \qquad (8)$$

where $T_N(\kappa)$ is the normal state transparency, $r_\kappa^2 = 1 - T_N(\kappa)$ is the corresponding normal state reflectance, and $\beta = V/\sqrt{|\Delta^2 - V^2|}$ is the coherence factor. A similar formula can be derived for $V > \Delta$. For a specular barrier, and neglecting the possible Fermi velocity mismatch at the interface, $T_N(\kappa) = 1/[1 + Z^2]$, where Z is the BTK barrier strength parameter[7]. A simple algebra shows that Eq. 8 is equivalent to the BTK formulas.

We will now apply this approach to the diffusive AR. A diffusive Andreev contact can be viewed as a contact between the normal and the superconducting leads, which in addition to the interface, are separated by a diffusive region. The size of the region is larger than the electronic mean free path[5]. In the zero temperature and zero bias limit, Eq.8 reads:

$$\langle G\rangle_{NS} = \frac{e^2}{h}\sum_\kappa T_A = \frac{e^2}{h}\sum_\kappa\frac{2\tilde{T}_\kappa^2}{(2-\tilde{T}_\kappa)^2}, \qquad (9)$$

where now the normal state transmittance for the conductance channel κ is given by the sequential conductor's formula:

$$\tilde{T}^{-1} - 1 = (T_N^{-1} - 1) + (t^{-1} - 1), \qquad (10)$$

where t is the transmittance of the diffusive region, and T_N is the barrier transparency. Using Eq. 5 for the distribution of t's, we find

$$\begin{aligned} \langle G_{NS}\rangle_L &= \frac{e^2}{h}\sum_\kappa\frac{2}{(2/T_N - 2 + 2/t_\kappa - 1)^2} \\ &= \frac{e^2}{h}\frac{\lambda N_{cc}}{L}\int_0^\infty\frac{dy}{[2(1-T_N)/T_N + \cosh y]^2}. \end{aligned} \qquad (11)$$

The last integral can be taken analytically and gives

$$\langle G_{NS}\rangle_L = \frac{e^2}{h}\frac{\lambda N_{cc}}{L}\frac{w\cosh w - \sinh w}{\sinh^3 w}, \qquad (12)$$

where $\cosh w = 2(1-T_N)/T_N$. For the clean (no-barrier) interface, $T_N = 1$, $w = i\pi/2$, and this expression reduces to Eq.6, thus reproducing the known result[12,9] that the diffusive Andreev contact with no interface barrier at zero bias has the same resistance in the superconducting and in the normal states.

Is it possible then to distinguish between the spin-polarization suppression of the Andreev current and possible diffusive transport effect using the experimentally measured conductance? The answer to this crucial question is yes, as we demonstrate in Fig. 1: although it is very difficult to discern the effect of a finite Z in a ballistic contact from the effect of diffusive transport, it is easy to separate both of them from the conductance suppression due to the finite spin polarization.

This brings about a burning question: *Is it possible, by looking at a measured conductance, to tell the spin-polarization suppression of the Andreev current, from the suppression due to a finite barrier resistance and/or to* *possible diffusive transport in the ferromagnet.* The answer is yes, as we will demonstrate below. On the other hand, it is basically impossible to tell the barrier resistance suppression from the diffusive suppression, but fortunately this is of virtually no importance for determining the spin polarization.

We will now derive a full set of formulas for arbitrary bias, temperature, and interface resistance for both ballistic and diffusive regimes, generalizig the BTK formulas[7] in order to be able to use them for the half-metallic CC and in the diffusive limit. These general formulas are summarized in Table I.

We start with extending the BTK approach over the half-metallic CC, which, by definition, correspond to the $\mathbf{k}_\parallel$ allowed in one spin direction, but not in the other. Following BTK, we consider an incoming plane wave and the transmitted plane wave (with and without branch crossing)

$$\psi_{in} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ikx}; \quad \psi_{tr} = c \begin{pmatrix} u \\ v \end{pmatrix} e^{ikx} + d \begin{pmatrix} v \\ u \end{pmatrix} e^{-ikx},$$

assuming, for simplicity, the same wave vector for all the states. Here u and v have the standard BTK meaning, e.g., at $V > \Delta$ $u^2 = 1 - v^2 = (1+\beta)/2\beta$. Unlike BTK, though, now the reflected state is a combination of a plane wave and an evanescent wave:

$$\psi_{refl} = a \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{\kappa x} + b \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ikx}. \tag{13}$$

The total current is $\frac{G_{HS}}{G_0} = \frac{4\beta[1+(K-2Z)^2]}{4(\beta^2-1)Z(K-Z)+[1+(K-2Z)^2][(1+\beta)^2+4Z^2]}$ at $V > \Delta$, where $K = \kappa/k$,) and zero otherwise.

As $V \to \Delta$, $G_{HS}/G_0 \to 0$, and $G_{HS}/G_0 \to G_N/G_0 = 1/(1+Z^2)$ as $V \to \infty$. We will not discuss all the aspects of the non-trivial behavior of G_{HS}/G_0 at intermediate biases. Importantly, G_{HS}/G_0 generally behaves non-monotonically with V, and may have a maximum larger than G_N/G_0 at an intermediate voltage. This maximum is due to the fact that, although the Andreev-reflected hole does not propagate and does not carry any current, the Andreev process itself is allowed at $V > \Delta$ and enhances the transparency of the barrier. This effect does not exist, though, for $Z = 0$, nor for $K \to \infty$. In the formulas given in Table I we used $K \to \infty$, to simplfy the equations, since the actual value of K matters in a relatively narrow region of voltages above the gap. Note that the simple renormalization of the normal current at $V > \Delta$, used in Ref.[1], gives a rather different result: instead of $\frac{4\beta}{(1+\beta)^2+4Z^2}$ it gives $\frac{1+\beta(1+2Z^2)}{(1+\beta)(1+2Z^2)+2Z^4}$, which is discontinuous at $V = \Delta$.

Now we generalize the BTK formulas beyond the ballistic hypothesis. For the nonmagnetic CC the calculation follows Eqs.8 and 10. For zero temperature and a subgap bias voltage $V < \Delta(T)$

$$\langle G \rangle_{NS} = \frac{e^2}{h} \sum_{\mathbf{k}_\parallel, i} \frac{4\tilde{T}_N^2(\kappa)(1+\beta^2)}{\beta^2 \tilde{T}_N^2(\kappa) + [2 - \tilde{T}_N(\kappa)]^2} \tag{14}$$

and

$$\tilde{T}_N^{-1} = T_N^{-1} + t^{-1} - 1 = Z^2 + t^{-1}, \tag{15}$$

with the distribution (5) for t. After some algebra we obtain

$$\langle G_{NS} \rangle_L = \frac{e^2}{h} \frac{\lambda N_{cc}}{L} \int_0^\infty \frac{(1+\beta^2)dy}{\beta^2 + (2Z^2 + \cosh y)^2}. \tag{16}$$

Factor N_{cc} now stands for the number of CC allowed in both spin channels, λ is given by the average mean free path for the channels in question, and thus the total conductance is given by $\langle N v_x^2 \rangle$, averaged over these channels. For $Z = 0$, this gives

$$\langle \sigma_{NS} \rangle = \frac{e^2 \tau}{\Omega} \langle N v^2 \rangle_{\downarrow\uparrow} \frac{\Delta}{V} \log \left| \frac{V+\Delta}{V-\Delta} \right|, \tag{17}$$

which starts from the normal conductivity and logarithmically diverges at $V = \Delta$. For arbitrary Z the conductance still can be cast into an analytical form, namely[14]

$$\langle \sigma_{NS} \rangle = \frac{e^2 \tau}{\Omega} \langle N v^2 \rangle_{\downarrow\uparrow} \frac{1+\beta^2}{2\beta} \mathrm{Im}[F(-i\beta) - F(i\beta)],$$

where

$$F(s) = \cosh^{-1}(2Z^2 + s)/\sqrt{(2Z^2+s)^2 - 1}$$

Similarly, for $V > \Delta$

$$\langle G_{NS} \rangle_L = \frac{e^2}{h} \frac{\lambda N_{cc}}{L} \int_0^\infty \frac{2\beta dy}{\beta + (2Z^2 + \cosh y)} \tag{18}$$

$$\langle \sigma_{NS} \rangle = \frac{e^2 \tau}{\Omega} \langle N v^2 \rangle_{\downarrow\uparrow} \beta F(\beta). \tag{19}$$

At $Z = 0$ this reduces to

$$\langle \sigma_{NS} \rangle = \frac{e^2 \tau}{\Omega} \langle N v^2 \rangle_{\downarrow\uparrow} \frac{V}{\Delta} \log \left| \frac{V+\Delta}{V-\Delta} \right|, \tag{20}$$

an interesting symmetry[13]. At $V \gg \Delta$ we get

$$\langle \sigma_N \rangle = \frac{e^2 \tau}{\Omega} \langle N v^2 \rangle_{\downarrow\uparrow} \frac{\cosh^{-1}(2Z^2+1)}{Z\sqrt{Z^2+1}}, \tag{21}$$

which should be used to normalize the whole conductance curve.

Finally, for for the "half-metallic" CC, there is no conductance at $V < \Delta$. For $V > \Delta$,

$$\langle G_{HS} \rangle_L = \frac{e^2}{h} \frac{\lambda N_{cc}}{L} \int_0^\infty \frac{2\beta dy}{(\beta+1)^2 + 2(2Z^2 - 1 + \cosh y)}$$

$$\langle \sigma_{HS} \rangle = \frac{e^2 \tau}{\Omega} \langle N v^2 \rangle_{\downarrow} \beta F[(\beta+1)^2/2) - 1],$$

where the arrow in the subscript shows that these channels are allowed only in one spin subband.

It is again instructive to see how this expression behaves at $V \gg \Delta$:

$$\langle \sigma_{HS} \rangle = \frac{e^2 \tau}{\Omega} \left\langle N v^2 \right\rangle_{\downarrow} \frac{\cosh^{-1}(2Z^2+1)}{2Z\sqrt{Z^2+1}}, \qquad (22)$$

which is exactly twice less than the corresponding non-magnetic limit.

The formulas derived in this section, and summarized in Table I, finalize our task of generalization of the BTK equations over the finite spin polarization in both ballistic and diffusive limits. The finite temperatures are taken into account straightforwardly in the same way as in the original BTK paper and are not discussed here. We thank E. Demler and I. Zutic for useful suggestions.

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[13] Eqs.17,20 coincide with those obtained in Ref[12] by a different method.

[14] This requires taking non-standard definite integrals of the following form:

$$\int_0^\infty R(\cosh x)dx = \frac{1}{2}\int_{-\infty}^{\infty} R(\cosh x)dx,$$

where R is a rational function. We write this integral as

$$\lim_{\lambda\to 0}\int_{-\infty}^{\infty} R(\cosh x)\exp(i\lambda x)dx.$$

Closing the integration contour in the upper half-plane, we observe that each pole z_j of $R(z)$ generates two rows of simple poles of $R(\cosh x)$ at $x_{jn} = \pm\cosh^{-1}(z_j) + 2\pi i n$. Each simple pole x_{jn} has a residue of $\exp(\pm i\lambda x_{j0})\exp(-2\pi n\lambda)\mathrm{Res}[R(z_j)]/(\pm\sinh x_{j0})$. Summation over n gives

$$\lim_{\lambda\to 0} -2\pi\sum_j \frac{\sin(\lambda x_{j0})\mathrm{Res}[R(z_j)]\exp(\pi\lambda)}{\sinh x_{j0}\sinh(\pi\lambda)} = -2\sum_j \frac{x_{j0}\mathrm{Res}[R(z_j)]}{\sinh x_{j0}}.$$

The same formula holds for the higher order poles, since the difference of the residues of $R(\cosh x)$ and $R(\cosh x)\exp(i\lambda x)$, apart from the factor $\exp(\pm i\lambda x_{j0} - 2\pi n\lambda)$, is of the higher order in λ..

TABLE I. Bias dependence of the total interface current in different regimes: BNM = ballistic non-magnetic[7]; BHM = ballistic half-metallic; DNM = diffusive non-magnetic; DHM = diffusive half-metallic. $F(s)$ is defined in the text

	$E < \Delta$	$E > \Delta$
BNM	$\frac{2(1+\beta^2)}{\beta^2+(1+2Z^2)^2}$	$\frac{2\beta}{1+\beta+2Z^2}$
BHM	0	$\frac{4\beta}{(1+\beta)^2+4Z^2}$
DNM	$\frac{1+\beta^2}{2\beta}\mathrm{Im}\left[F(-i\beta) - F(i\beta)\right]$	$\beta F(\beta)$
DHM	0	$\beta F[(1+\beta)^2/2 - 1]$.

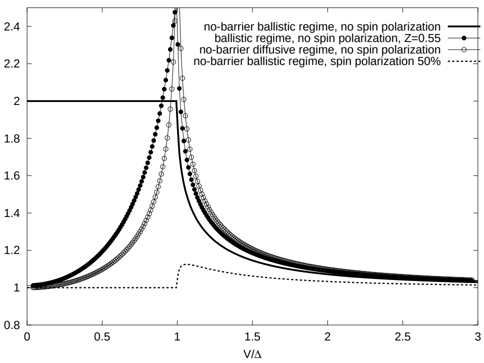

FIG. 1. Andreev conductance in in different regimes.