Chapter 1

Application

The system of interest consists of two dirty superconductors separated by a ferromagnetic barrier. The magnetization of the ferromagnet shall be in the y-direction, parallel to the interfaces with the superconductors. This magnetization introduces two different scattering potentials for incoming electrons, depending on their spin. To formulate the boundary conditions for this system, a scattering matrix approach [1] is employed, where first the interface scattering matrix for an impenetrable interface in the normal state is calculated. In the next step, auxiliary propagators subject to these impenetrable boundary conditions are calculated with the help of the homogeneous solutions to the Usadel transport equation and normalization condition (**??**). Finally, this leads to a matrix current which again goes into the Usadel equation as a boundary condition.

1.1 Interface scattering matrix

First, the scattering matrix of a normal state system consisting of a spin independent potential barrier with height V_2 with different potentials V_1 and V_3 to the left and right will be calculated. The scattering matrix will be of the form

$$\mathbf{S} = \begin{pmatrix} R & \underline{T} \\ T & \underline{R} \end{pmatrix} . \tag{1.1}$$

Here, R and $\underline{R}$ are the reflection coefficients on the left and right side of the interface respectively. T and $\underline{T}$ are the transmission coefficient that characterizes a particle going from left to right of the barrier and vice versa (ADD FIGURE). To calculate R and T, a constant particle current with Fermi energy E_F going from left to right is considered. For an interface parallel to the z-direction, the momentum component parallel to the interface $k_\parallel$ will be conserved and the problem reduces to a one dimensional one. The Hamilton operator for the region $j \in \{1, 2, 3\}$ is then given by

$$\mathcal{H}_j = \left(-\frac{1}{2} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right) + V_j \right) , \tag{1.2}$$

with $\hbar = m = 1$ for simplicity. In the case of a quadratic dispersion relation, the Fermi energy can be expressed as

$$T_j + V_j = E_F \tag{1.3}$$

$$\frac{1}{2} \left(k_j^2 + k_\parallel^2 \right) + V_j = E_F . \tag{1.4}$$

All energies are measured from the chemical potential $\mu = 0$. Therefore, the corresponding wave vectors are defined as

$$k_j = \sqrt{2(E_F - V_j) - k_\parallel^2}\,. \tag{1.5}$$

The incoming particle current can be describes as a plane wave, which leads to the usual ansatz for the wavefunction

$$\psi_E(x) = \begin{cases} \frac{1}{\sqrt{k_1}}\left(e^{ik_1x} + Re^{-ik_1x}\right) & ,x \leq -a \\ \frac{1}{\sqrt{k_2}}\left(A^{ik_2x} + Be^{-ik_2x}\right) & ,-a < x \leq a \\ \frac{1}{\sqrt{k_3}}\left(Te^{ik_3x}\right) & ,a < x \end{cases} \tag{1.6}$$

The factor $1/\sqrt{k}$ ensures normalization of the particle current. The reflected and transmitted portions of the wave are described by Re^{-ik_1x} and Te^{ik_3x} respectively. We now need to match the wave functions through imposing the boundary conditions

$$\begin{aligned} \psi_E(-a_-) &= \psi_E(-a_+) \\ \psi_E(a_-) &= \psi_E(a_+) \\ \frac{d}{dx}\psi_E\Big|_{x=-a_-} &= \frac{d}{dx}\psi_E\Big|_{x=-a_+} \\ \frac{d}{dx}\psi_E\Big|_{x=a_-} &= \frac{d}{dx}\psi_E\Big|_{x=a_+}\,. \end{aligned} \tag{1.7}$$

The index indicates that a limit is taken from the right $(+)$ or the left $(-)$. Plugging in the wave function (1.6) we can solve for the reflection and transmission amplitudes R and T (SEE APPENDIX). Analogously, one can calculate these amplitudes for an incoming wave from the right by making the substitutions $k_{1,3} \to k_{3,1}$ and $x \to -x$. With that, the scattering matrix is

$$\hat{\mathbf{S}}(k_1, k_2, k_3, a) = \begin{pmatrix} R & \underline{T} \\ T & \underline{R} \end{pmatrix} \tag{1.8}$$

$$= \begin{pmatrix} \Gamma\alpha e^{-2ik_1a} & -\Gamma^*\beta e^{i(k_1+k_3)a} \\ \Gamma\beta e^{-i(k_1+k_3)a} & -\Gamma^*\alpha e^{2ik_3a} \end{pmatrix} \tag{1.9}$$

with

$$\alpha = (\kappa_1 - \kappa_3)c + (1 + \kappa_1\kappa_3)s \tag{1.10}$$

$$\beta = 2\sqrt{\kappa_1\kappa_3} \tag{1.11}$$

$$\Gamma = \frac{1}{(\kappa_1 + \kappa_3)c + (1 - \kappa_1\kappa_3)s} \tag{1.12}$$

$$\kappa_{1,3} = \frac{k_{1,3}}{ik_2} \tag{1.13}$$

$$s = \sin(2k_2a) \tag{1.14}$$

$$c = \cos(2k_2a) \tag{1.15}$$

However, for a ferromagnetic barrier, the scattering potential is different depending on the spin of the incoming particle. To account for this, we introduce the wave vectors

$$k_2^{\uparrow,\downarrow} = \sqrt{2\left(E - V_2^{\uparrow,\downarrow}\right) - k_\parallel} \tag{1.16}$$

for spin up or spin down particles respectively. Similarly, each quantity with the superscript $\uparrow$ or $\downarrow$ will depend on $k_2^\uparrow$ or $k_2^\downarrow$ respectively, instead on the k_2 used for the spin independent case. This leads to the full scattering matrix for the system

$$\hat{\mathbf{S}} = \begin{pmatrix} R^\uparrow & 0 & \underline{T}^\uparrow & 0 \\ 0 & R^\downarrow & 0 & \underline{T}^\downarrow \\ T^\uparrow & 0 & \underline{R}^\uparrow & 0 \\ 0 & T^\downarrow & 0 & \underline{R}^\downarrow \end{pmatrix} \tag{1.17}$$

$$= \begin{pmatrix} \Gamma^\uparrow\alpha^\uparrow e^{-2ik_1a} & 0 & -\Gamma^{\uparrow *}\beta^\uparrow e^{i(k_1+k_3)a} & 0 \\ 0 & \Gamma^\downarrow\alpha^\downarrow e^{-2ik_1a} & 0 & -\Gamma^{\downarrow *}\beta^\downarrow e^{i(k_1+k_3)a} \\ \Gamma^\uparrow\beta^\uparrow e^{-i(k_1+k_3)a} & 0 & -\Gamma^{\uparrow *}\alpha^\uparrow e^{2ik_3a} & 0 \\ 0 & \Gamma^\downarrow\beta^\downarrow e^{-i(k_1+k_3)a} & 0 & -\Gamma^{\downarrow *}\alpha^\downarrow e^{2ik_3a} \end{pmatrix} \tag{1.18}$$

$$= \begin{pmatrix} \hat{\mathbf{S}}_{11} & \hat{\mathbf{S}}_{12} \\ \hat{\mathbf{S}}_{21} & \hat{\mathbf{S}}_{22} \end{pmatrix} \tag{1.19}$$

with the elements $\hat{\mathbf{S}}_{ij}$ being 2×2-matrices in spin space. Under the assumption of particle conservation, the reflection- and transmission amplitudes must add up to 1. With the substitution introduced above, this condition reads

$$\left|\Gamma^{\uparrow,\downarrow}\right|^2 \left(\left|\alpha^{\uparrow,\downarrow}\right|^2 + \left(\beta^{\uparrow,\downarrow}\right)^2\right) = 1\,. \tag{1.20}$$

The auxiliary scattering matrix for an impenetrable interface can be obtained by a polar decomposition of $\hat{\mathbf{S}}$ (APPENDIX). We can write the scattering matrix as

$$\hat{\mathbf{S}} = \begin{pmatrix} \sqrt{\hat{1} - CC^\dagger} & C \\ C^\dagger & -\sqrt{\hat{1} - C^\dagger C} \end{pmatrix} \begin{pmatrix} S & 0 \\ 0 & Sul \end{pmatrix}, \tag{1.21}$$

where the matrices S and Sul are unitary matrices in spin space. They contain information about the phase shift for the reflection wave and make up the auxiliary scattering matrix for the impenetrable interface. For this particular system, they evaluate to

$$\begin{pmatrix} S & 0 \\ 0 & Sul \end{pmatrix} = \begin{pmatrix} \frac{\Gamma^\uparrow\alpha^\uparrow}{\left|\Gamma^\uparrow\alpha^\uparrow\right|} e^{-2ik_1a} & 0 & 0 & 0 \\ 0 & \frac{\Gamma^\downarrow\alpha^\downarrow}{\left|\Gamma^\downarrow\alpha^\downarrow\right|} e^{-2ik_1a} & 0 & 0 \\ 0 & 0 & \frac{-\Gamma^{\uparrow *}\alpha^\uparrow}{\left|\Gamma^\uparrow\alpha^\uparrow\right|} e^{2ik_3a} & \\ 0 & 0 & 0 & \frac{-\Gamma^{\downarrow *}\alpha^\downarrow}{\left|\Gamma^\downarrow\alpha^\downarrow\right|} e^{2ik_3a} \end{pmatrix}. \tag{1.22}$$

This matrix structure encodes the reflection and transmission amplitudes for the impenetrable interface. For our purposes, the scattering matrix in particle hole space is needed. With this structure,

1.2 Boundary conditions

1.3 Numerical implementation

Bibliography

[1] Matthias Eschrig et al. “General boundary conditions for quasiclassical theory of superconductivity in the diffusive limit: application to strongly spin-polarized systems”. In: *New Journal of Physics* 17.8 (2015), p. 083037.