Influence of barrier width on values of spin polarisation measured by point contact Andreev reflection

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A modification of the Blonder-Tinkham-Klapwijk (BTK) model is proposed for the description of the ferromagnet-superconductor (FM/SC) interface. Modelling the contact potential with a rectangular barrier, we investigate the influence of the barrier width at the interface on values of spin-polarisation measured by point contact Andreev reflection. Results suggesting that neglecting the width of the barrier at the interface can lead to overestimation of spin-polarisation using the original BTK model are presented. This effect is particularly strong for low values of polarisation and vanishes for high polarisation. The impact on analysis of the experimental data is also discussed.

Model

The original BTK model [1] is slightly modified. We use a rectangular potential barrier instead of the Dirac's delta potential and we investigate the effect of a finite width of potential barrier on the value of spin polarisation P_{BTK} extracted from the BTK model in the ballistic limit. Modification of the BTK model results from the fact that real FM/SC interfaces are imperfect, i.e. chemical, electronic and structural mismatch between both materials may lead to the conclusion that the rectangular potential barrier is a better approximation for these complex situations. This assumption allows us to include the interference phenomena at the FM/SC interface which are not taken into account in the case of a delta function potential. The potential barrier of the simulated contact is shown in Fig. 1. The height (Z) and width (d) of the potential barrier are free parameters of the model. In the limiting case, when $d \longrightarrow 0$, the model of the contact corresponds to the BTK model.

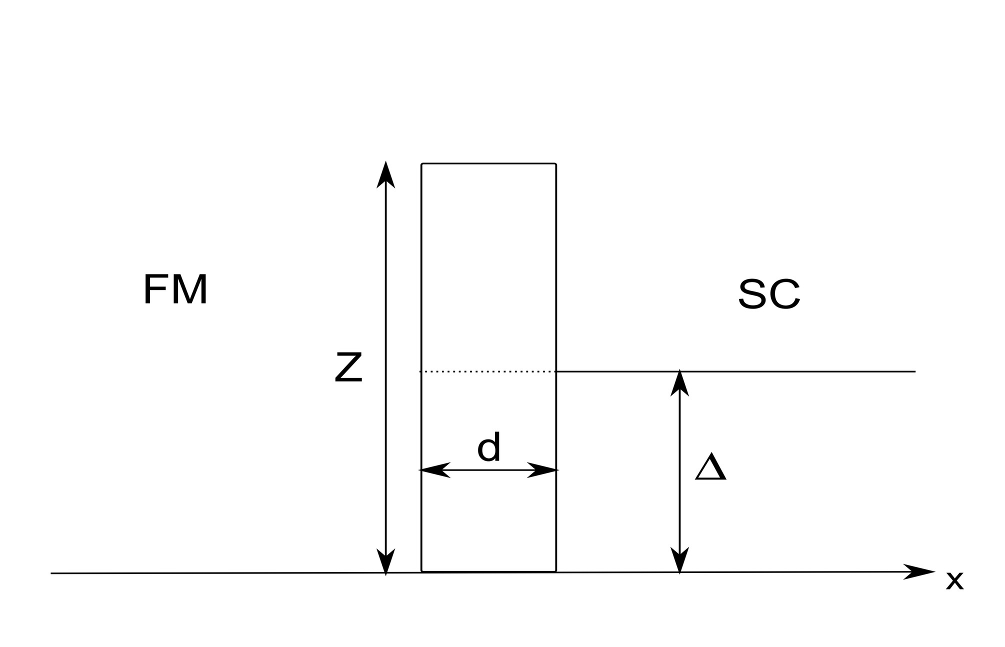

Figure 1. *Scattering potential profile at the interface FM/SC allowing to include quantum interference phenomena. In contrast to BTK theory we assume rectangular potential barrier with height Z and width d.*

Theory

For a small bias voltage, the conductance through the metal–superconductor contact can be evaluated by the formula

$$G_N(V;d,Z) = \frac{e^2}{h}\int_{-\infty}^{+\infty} dE\, \frac{\partial f_{F-D}(E-eV)}{\partial V} \times \left[1 + A_N(E;d,Z) - B_N(E;d,Z)\right], \qquad (1)$$

where V is the bias voltage, $f_{F-D}(E-eV;T)$ is the equilibrium Fermi-Dirac distribution, and $A_N(E;d,Z)$ and $B_N(E;d,Z)$ are the Andreev reflection and normal reflection probabilities, respectively. The probabilities $A_N(E;d,Z)$ and $B_N(E;d,Z)$ can be determined by solving the Bogoliubov-de Gennes equations

$$\begin{bmatrix} H_0(x) & \Delta(x) \\ \Delta^*(x) & -H_0^*(x) \end{bmatrix} \begin{bmatrix} u(x) \\ v(x) \end{bmatrix} = E \begin{bmatrix} u(x) \\ v(x) \end{bmatrix}, \qquad (2)$$

where $\Delta(x)$ is the local energy gap, E is the quasi-particle energy measured from the Fermi level μ_F, and H_0 is the one-particle Hamiltonian in the form

$$H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x) - \mu_F \qquad (3)$$

with the potential energy $U(x) = Z\Theta(x)\Theta(d-x)$, where $\Theta(x)$ is the Heaviside step function.

The BTK model with the Dirac's delta function potential or the rectangular barrier potential can be generalised to include the spin-polarisation P. In this case the total conductance of the contact is given by the formula

$$G(V;d,Z,P) = (1-P)G_N(V;d,Z,P) + PG_H(V;d,Z,P), \qquad (4)$$

where $(1-P)G_N(V;d,Z,P)$ and $PG_H(V;d,Z,P)$ are the fully unpolarised part and the fully polarised part of the total conductance, respectively. The fully polarised part is calculated by putting $A_N(E;d,Z) = 0$ in formula (1). In practice, the equation (4) is used to extract the values of spin-polarisation from the measurements of the total conductance by an appropriate fitting procedure.

Results

Applying the scattering matrix method to solve the Bogoliubov-de Gennes equations we found the probability amplitudes of Andreev and normal reflections as a function of the width of potential barrier for different values of the parameter Z. In particular, Fig. 2 shows the oscillations of the Andreev reflection probability for a few values of parameter Z. These curves are obtained using $Z < \mu_F$, where μ_F corresponds to the Fermi energy in a typical metal. On the other hand, for $Z > \mu_F$ we obtained the exponential decay of the Andreev reflection probability as a function of the potential barrier width.

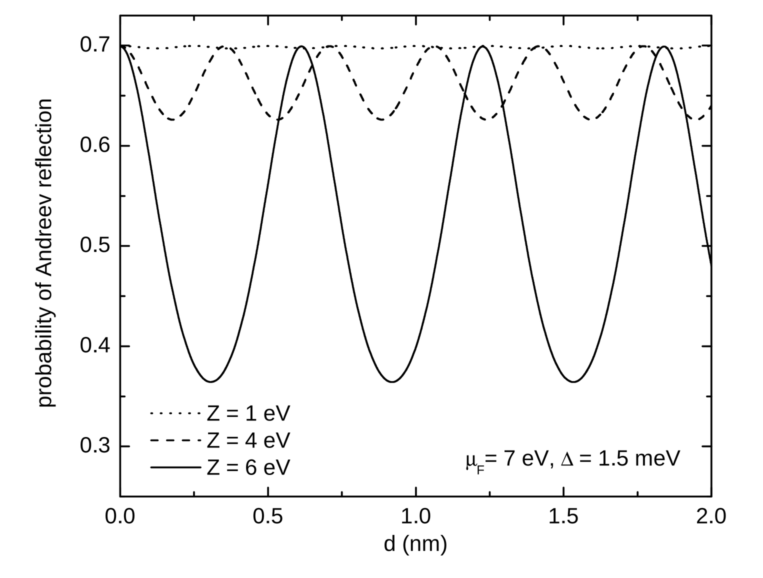

Figure 2. *Calculated Andreev reflection probability as a function of the contact barrier.*

We performed numerical calculations of the total conductance as a function of the bias voltage for the widths of the barrier between 0 and 1 nm assuming four different values of the spin-polarisation, namely 0, 40, 80, and 100 percent. To discuss the situation when the oscillations are strongest the parameter Z was taken equal to 6 eV, see Fig. 2. As a consequence of the periodic nature of the Andreev reflections presented in Fig. 2, we obtain a family of curves describing the conductance as a function of the applied bias voltage. All of the curves are placed between ones corresponding to the minimum and maximum values of the Andreev reflection probability. However, with increasing polarisation the influence of the barrier width becomes less significant. For example if we compare the results for polarisation $P = 0$ with $P = 100\%$ we see a far greater variation in the shape of the conductance curve for the lower value of polarisation.

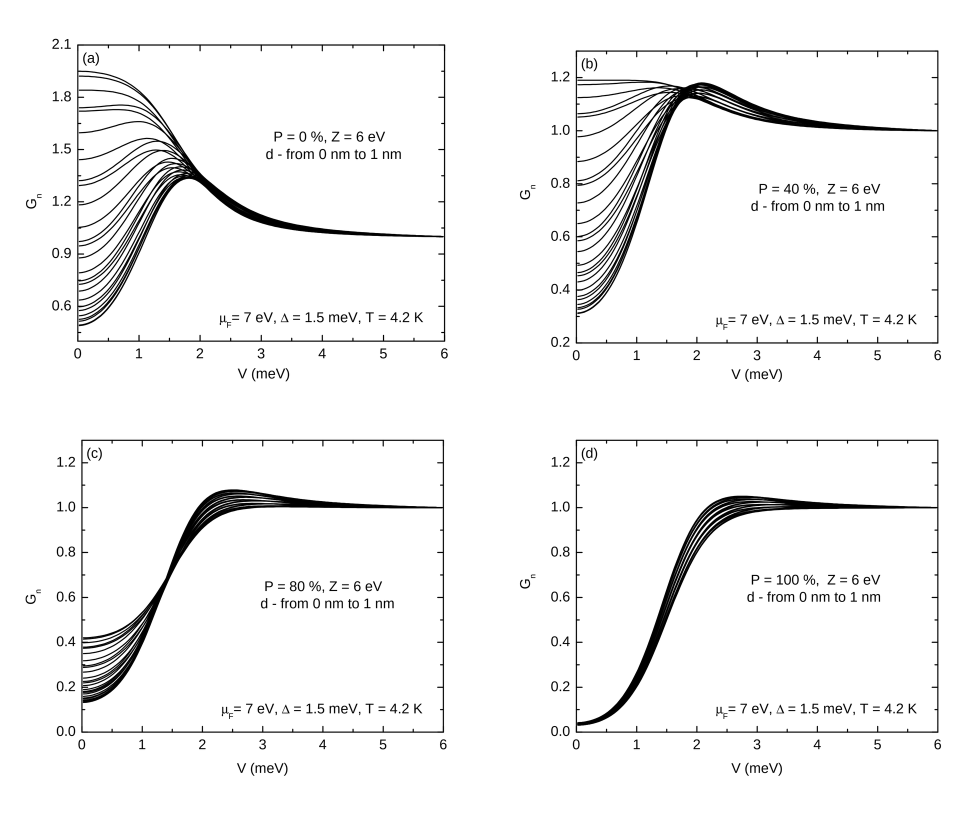

Figure 3. *(Normalized) Conductance calculated for polarisation equal to (a) 0%. (b) 40%, (c) 80% and (d) 100%. Results for the barrier width between 0 and 1 nm.*

In the next step we used BTK theory to fit our theoretical curves for different width of the barrier and fixed value of spin polarisation. The value of polarisation (P_{BTK}) extracted from the BTK model varies significantly from the original value as the barrier width changes. This effect is particularly strong for low values of polarization. For an unpolarised sample the value for P_{BTK} resulting from the BTK fit can vary from 0 to 25% as the barrier width changes (Fig. 4(a)). A similar situation, but on a smaller scale, is observed for $P = 80$ %, with results P_{BTK} between 80% and 85% (Fig. 4(b)). Since we are not able to measure the width of the barrier in experiments we believe that this factor could be responsible for ambiguous results, especially for measuring low spin polarization.

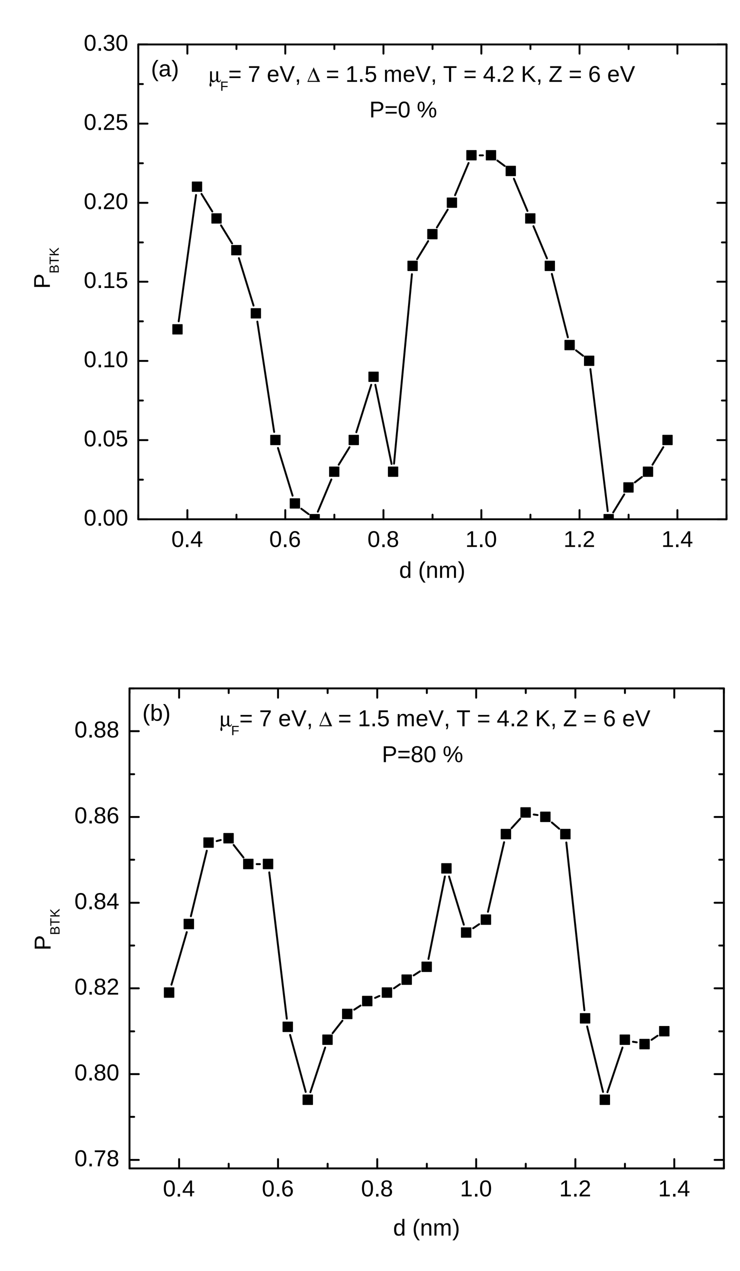

Figure 4. *Polarisation resulting from the BTK model as a function of the barrier width in case of the (a) unpolarised system and (b) polarisation $P = 80\%$.*

Direct evidence of advantage arising from using the rectangular barrier is presented in Fig. 5 showing a comparison between calculated conductance and experimental data obtained for Cu/Nb junction. If the finite-width barrier is assumed (Fig. 5(a)) the fitting procedure gives $P = 0$ as expected, in contrast to results from the original BTK model suggesting $P = 31\%$ (Fig. 5(b)). Additionally, accuracy of the fitting is significantly better in case of the rectangular barrier.

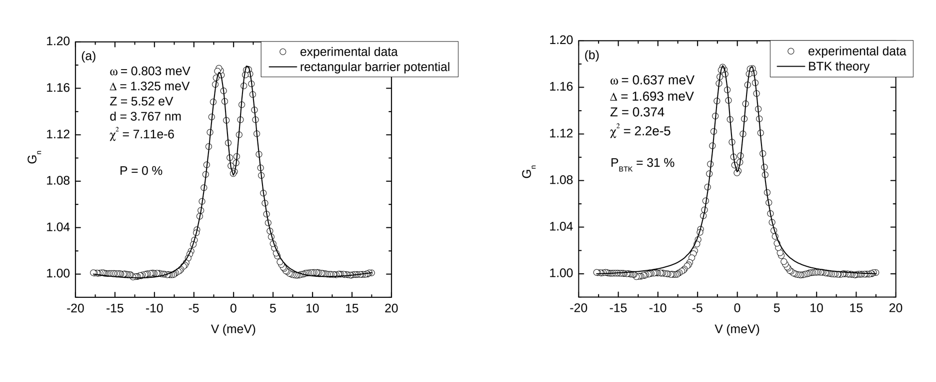

Figure 5. *Measured and calculated conductance for (a) rectangular barrier and (b) BTK model with Dirac's delta.*

Concluding Remarks

In summary, we have investigated the influence of the potential barrier width on values of the spin-polarisation measured by point contact Andreev reflection and we have shown that using a rectangular barrier to model a metal-superconductor interface allows to perform calculations with better accuracy. Neglecting the width of the barrier could lead to an overestimation of the values of spin polarisation extracted from experimental data using the BTK model. The error is larger for lower of spin polarisation.

Acknowledgements

This paper has been supported by the Foundation for Polish Science MPD Programme co-financed by the EU European Regional Development and Physical Sciences Research Council (EPSRC) of the United Kingdom.