Modelling partially coherent transport across an island - multiple Andreev reflection and charging effects

U Schröter and E Scheer
Universität Konstanz, Fachbereich Physik, Universitätsstraße 10, 78464 Konstanz, Germany
E-mail: ursula.schroeter@uni-konstanz.de

Abstract. A Green’s functions technique known to describe transport through a superconducting point contact with multiple Andreev reflection is merged with a rate equation scheme and thus extended to model transport through a series of two junctions enclosing an island between them. In the superconducting state such systems may show an interplay of multiple Andreev reflection and Coulomb blockade. Although not of unique shape calculated current-voltage characteristics exhibit more or less pronounced steps that can be associated to transport processes setting in because of the applied voltage becoming sufficient to overcome certain fractions of the superconductor gap or providing the required charging energy. The speciality of our model, however, lies in regarding all single-charge transfers out of every-order multiple reflection simultaneously instead of adding total rates for processes up to some order. The algorithm can treat series of junctions that are just incoherently coupled via the electrostatic charge on the island as well as transport maintaining coherence across the island. In the latter case we find direct lead-to-lead transport, but interestingly, Coulomb blockade never completely vanishes in our model. In principle, the scheme is also applicable to a mixed situation where interaction between the junctions is partly coherent and partly incoherent.

1. Introduction
Whereas the single-electron-transistor configuration with an island connected by tunnel junctions to the leads of a circuit and capacitively to a gate is well investigated in both normal and superconducting state, in order to model transport properties of a series of two quantum-point contacts of higher transmission, in this work we study the consequences of merging an all-order-interaction Green’s function formalism [1] with rate equations for the island charging. The island is assumed to have sufficiently small capacitance to be sensitive to single-electron charging [2], however, large enough, to act as a bulk reservoir with continuous density of states (DOS). Ensembles of transport channels characterize the junctions. Despite the point contacts having resistances of the order of the quantum resistance $R_k = h/e^2 = 26k\Omega$, we allow for arbitrary transmissions of the channels in all the range between zero and one. Such contacts can, for example, be arranged with break junctions [3], which even provide the possibility to tune their transmission during current-voltage (IV) measurements. It is yet a question under investigation whether in a series of two junctions enclosing an island, multiple Andreev reflection (MAR), see Fig.1b, gets suppressed by Coulomb blockade (CB), see Fig.1a. In orthodox theory valid with low transmission junctions higher-order processes such as Andreev cycles [4, 5], if
allowed from the point of view of their energy outcome, can simply be added as further current paths besides single-particle tunneling. With channels of arbitrary transmission different-order multiple scatterings cannot be regarded as independent of one another any more. This is taken into account by Green’s functions.

2. Method
In both our incoherent [6] and coherent model [7] variant we construct transfer Green’s functions $T$ [8] for each channel in a junction that include the island potential shift with each charging, which is anchored as a phase to the single-hopping amplitudes $\sigma$. With these, renormalized transmission rates $\tilde{G}$ can be expressed for single electrons and holes, be they transferred individually or as a step out of a MAR. Rates from all channels from both junctions (examples here are for single-channel junctions) are added in a way not yet to give a current, but the change of the number of negative excess charges held on the island. Rate equations are then easily solved for the probabilities $P_n$ to encounter the island with a certain charge at any moment of time. We are looking for a stationary state in the sense that the average island charge, or more precisely all the $P_n$, stay constant. With the before obtained transmission rates out of and into any island charge state $n$ and the $P_n$ the net current through the system is determined.

3. Current-voltage characteristics from incoherent model
Fig.s 1c and d show IV-curves from the incoherent model for different ratios of the island charging energy $E_c$ and the superconductor gap $\Delta$ (the same for both leads and the island assumed the same material). Except for a tiny ridge in Fig.1d the onset is at $eV=2\Delta$ and at $eV=2E_c$ in the other case in Fig.1c. The main result of our model is the two-fold voltage threshold for transport processes, where the greater value, of course, becomes decisive. For single-charge tunneling through a junction (for the setup symmetric in capacitances and zero gate voltage) these are $eV \geq 4\Delta$ and $eV \geq 2E_c$. Parameters in Fig.1c and d are such that Andreev reflection (AR) is only important up to first order, and the corresponding thresholds are $eV \geq 2\Delta$ and $eV \geq 2E_c$. Thresholds are here referred to the total applied voltage. For the symmetric case you can just divide by two for one junction. Furthermore the values mentioned here give the requirements to put a charge onto the island through one junction. To get a current through the system, corresponding conditions also have to be fulfilled to take a charge off the island through the other junction. Our threshold is either given by supplying the charging energy or by overcoming the superconductor gap. The outcome of the Green’s functions calculation is such that the initial energy of $2\Delta$ or $\Delta$ per electron to break a Cooper pair in order to create a quasi-particle to be individually transferred or start an AR, does not necessarily seem lost. The above mentioned thresholds are further associated to charging the island from $n=0$ to $n=1$. $6E_c$ in Fig.1c corresponds to going from $n=1$ to $n=2$.

Though no good approximation for the chosen transmissions any more, orthodox-theory calculations - without co-tunneling to compare to our algorithm separately setting up rates for each junction - are also displayed in Fig.s 1c and d. Based on energy balances it needs $2\Delta+E_c$ per junction to create a quasi-particle and charge the island with it. Applying a voltage equivalent of $\Delta + 2E_c$ per junction, sending two (negative) charges through a junction by an AR we get twice this energy, which just suffices to initially break a Cooper pair and provide the charging energy $2^2E_c$. Whereas orthodox theory only considers complete MAR processes, in our model single-charge transfers can take place as if being a step out of a MAR the rest of which may be virtual. In the superconducting state orthodox theory predicts current onsets at clearly higher voltages. Somewhat carefully tuning junction transmissions and the ratio $E_c:\Delta$, IV curves with a step pattern reflecting higher-order AR similar to Fig.1b also for the double junction can be obtained as well. In the normal state our incoherent variant of the Green’s functions model is equivalent to orthodox theory.
4. Coherent variant

The variant of our model with coherent coupling across the island sets a considerably greater mathematical challenge [8, 9] than the incoherent version. Nevertheless, the conception is straightforward. Multiple reflections and MAR extending over both junctions are included in the transfer Green's functions. Then the island charging is again broken down into renormalized single-transfer rates, rate equations are solved for island charge state probabilities, from which then the net current is evaluated. Already in the normal state maintaining coherence between junctions can lead to current onset at lower voltage than for the incoherent case. Onset and step positions are no longer solely determined by the capacitances associated to the junctions and eventually the gate, but also depend on the channel transmissions now. However, as long as $E_c$ remains finite, CB will never completely vanish, even for channels with $t=1$. For an eventual interpretation of measurements a problem may lie in the fact that only being given IV-curves the coherently coupled case will hardly be distinguishable from the incoherent one with asymmetric capacitances.

In the superconducting state the current onset in the coherent model is mostly merely found at slightly lower voltage than in the incoherent variant. The current may exceed that from the incoherent case, but as well fall below it. In the example in Fig.1f the coherent variant, however, clearly loses the step structure in the IV-curve. To find such a linear current contribution dominating rather small $E_c$ is necessary. With $E_c > \Delta$ onset is at $eV=2E_c$ and coherence will not bring it much lower. All these results are due to the following underlying properties: Transport processes coherently leading from lead to lead can pass through any energy level on the island. Single electron tunneling in superconducting state can, for example, set in at $eV=2\Delta$ despite the voltage bridging two junctions. However, all processes involving
only one junction are also still present. Although independent of the island DOS, lead-to-lead transport needs to charge the island up temporarily and can therefore get suppressed by any island-decharging processes which are stronger. Crossed Andreev reflection [10] is suppressed by interferences from backreflection processes. Allowing for spin polarization [11] may, however, render this point to be newly thought about.

5. Channel ensembles and partial coherence
Channel ensembles of single junctions are obtained by diagonalizing some scattering matrix \( \tau^\dagger \tau \). With coherence-maintaining coupling between several modes on the island and in the leads instead of just one per site, the eigenchannel search has to be done for the complete three-site system at once. Resulting channel ensembles will in general differ from those obtained taking each junction as a stand-alone device. However will the diagonalization lead to a system wherein channels are only connected pairwise coherently across the island. This finding will facilitate application of our coherent model variant, which had so far been restricted to one channel per junction, to multichannel junctions.

Modelling partially maintained coherence across the island is possible by splitting island modes into parts coupling to both or only one lead, respectively. Charge change rates are easily mixed from the incoherent and coherent variant at the stage of setting up rate equations.

6. Conclusions and Outlook
A model to simulate transport properties of a single-electron-transistor-like series of junctions, not restricted to the tunnel regime any more, has been presented. An interplay of multiple Andreev reflection and Coulomb blockade can be supposed in such circuits. There is no unique step pattern in calculated current-voltage characteristics. Of two-fold thresholds the superconductor gap or the charging energy may be the decisive one. On the one hand multiple-charge packages on the island are not required to have Andreev reflection going on. On the other hand Coulomb blockade never completely vanishes. The model can assume coherent interaction between both junctions or mere mutual influence via the electrostatic island charge. It has yet to be further developed to also account for Cooper-pair tunneling.

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