Elastic Co–Tunneling in a 1D Quantum Hole Approach

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Abstract

The influence of the phases of tunneling matrix elements on the rate of the elastic co–tunneling at an ultrasmall normal–conducting double–junction is studied in a simple quantum–hole approach at zero temperature. The results are compared with experimental data.

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It is known that besides ordinary tunneling of single charges through ultrasmall double–junctions there is the effect of macroscopic quantum tunneling (q–MQT) via virtual intermediate states \[1, 2\]. Though the current of q–MQT is much smaller than that of ordinary tunneling, it can be observed for voltages below the Coulomb–blockade, where ordinary tunneling is impossible \[3\]. Here we consider only the so–called elastic channel of q–MQT that is qualified by a nonvanishing conductivity at zero voltage as predicted theoretically. Averin and Nazarov \[1, 2\] have presented a theory of elastic q–MQT basing on \[4\] that takes into consideration the phases of tunnel matrix elements yielding the following expression for the conductivity \(G_{el}\) at low voltages \(V\) and temperatures \(T\)

\[
G_{el} = \frac{\hbar G_1 G_2 \Delta}{4\pi e^2} \left( \frac{1}{E_1} + \frac{1}{E_2} \right).
\]

(1)

In this paper we try to give an modified theory of elastic q–MQT where the central electrode is approximated by an 1D quantum hole. This is justified because of its size. We study a simple double–junction, consisting of two ultrasmall tunnel junctions connected in series and possessing capacities \(C_1, C_2\) \((C_\Sigma = C_1 + C_2)\), driven by the voltage \(V\). It is assumed that the external electrodes are metallic bulks. Finally, the result is a formula for the conductivity including the discrete island level spacing \(\Delta_0\) at the Fermi edge. Note, that in the continuous case \(\Delta_0^{-1}\) corresponds to the energy density of states at the Fermi level. \(G_{1,2}\) denote the individual tunnel conductivities of the corresponding junctions. \(E_1\) and \(E_2\) are the electrostatic energy differences connected with tunneling at the respective electrodes and read as

\[
E_{1,2} = \pm \frac{e^2}{C_\Sigma} \left[ n \pm \frac{1}{2} + \frac{C_{2,1} V}{e} \right].
\]

(2)

\(ne\) is the integer–valued charge on the central electrode due to tunneling. In terms of a first order Taylor expansion in the supplied voltage \(V\) the elastic conductivity \(G_{el}\) turns out to be at low temperatures \[1, 2\]

\[
G_{el} = \frac{2\pi e^2}{\hbar} \sum_{k, k'} T_{kk'}^{(1)} T_{kk'}^{(1)*} T_{0k}^{(2)*} T_{0k'}^{(2)} D_0^2 F(\varepsilon_k) F(\varepsilon_{k'}),
\]

(3)

\[
F(\varepsilon) = \frac{1 - f(\varepsilon)}{E_1 + \varepsilon} - \frac{f(\varepsilon)}{E_2 - \varepsilon}.
\]
Here \( f \) denotes the Fermi function and \( D \) the bulk electron density of states. The subscript "0" indicates the Fermi level. In the coordinate representation the tunneling amplitudes \( T \) are expressed by the wave functions \( \psi \) in the following way

\[
T_{km} = \int d^3y d^3z T(y, z) \psi_k^*(y) \psi_m(z).
\] (4)

Note, that the subscripts \( k \) and \( l \) and the coordinates \( y \) belong to the central electrode of the double–junction, whereas the subscripts \( m, n \) and the coordinates \( z \) are used to describe the banks.

Following [1], [2] the conductivities of the single–junctions in Golden–rule type estimation are given by

\[
G_{1,2} = \frac{4\pi e^2}{\hbar} |T(1,2)|^2 \frac{D_0}{\Delta_0},
\] (5)

where \( D_0 \) is the density of states of the banks at Fermi level. In coordinate representation this looks like

\[
G_1 = \frac{4\pi e^2}{\hbar} \int d^3y_1d^3z_1 T^{(1)}(y_1, z_1) T^{(1)*}(y_2, z_2) \psi_0^*(y_1) \psi_0(z_1) \psi_0^*(y_2) \psi_0(z_2) \frac{D_0}{\Delta_0},
\] (6)

and respectively in the case of the other junction.

Owing to the fact that the tunneling matrix elements \( T(y, z) \) drop exponentially outside of the vicinity of the junctions [2], the integrations with respect to \( y \) contribute only for fixed values

\[
y_{1,2} = -\frac{L}{2}, \quad y_{3,4} = \frac{L}{2}.
\] (7)

Then, \( G_{el} \) simplifies to

\[
G_{el} = \frac{\hbar}{8\pi e^2} G_1 G_2 \sum_{k k'} \psi_k^*(-L/2) \psi_k(L/2) \psi_{k'}^*(L/2) \psi_{k'}(-L/2) F(\varepsilon_k) F(\varepsilon_{k'}) \Delta_0^2 / \psi_0^*(-L/2) \psi_0(-L/2) \psi_0^*(L/2) \psi_0(L/2). \] (8)

Using real wave functions according to [2] \( G_{el} \) may be factorized in this approximation with regard to \( k \) and \( k' \), resulting in

\[
G_{el} = \frac{\hbar}{8\pi e^2} G_1 G_2 \left[ \frac{\sum_k \psi_k(-L/2) \psi_k(L/2) F(\varepsilon_k)}{\psi_0(-L/2) \psi_0(L/2) \Delta_0} \right]^2.
\] (9)
Now, the estimation of (9) is done within a quantum hole approximation. This is different to the original approach of Averin and Nazarov. The central electrode is taken as 1D quantum hole with the length \( L \) and the energetic depth \( E \) (counted from the Fermi level, \( E > 0 \)).

Now, the solution of the quantum mechanical problem is done within the variables \[ E = \frac{\hbar^2 k^2}{2 m^*}, \quad \kappa^2 = k^2_E - k^2. \] (10)

In these terms the wave functions are

\[
\begin{align*}
\psi_+(x) &= \begin{cases} 
A_+ \cos k x & 0 \leq |x| \leq L/2 \\
A_+ \cos \frac{k L e^{\kappa(L/2-|x|)}}{2} & |x| > L/2
\end{cases} \\
\psi_+(x) &= \psi_+(x) \\
\frac{1}{A_+^2} &= \frac{1}{k} \left[ \frac{k L}{2} + \sin \frac{k L}{2} \cos \frac{k L}{2} \right] + \frac{1}{\kappa} \cos^2 \frac{k L}{2},
\end{align*}
\[
\begin{align*}
\psi_-(x) &= \begin{cases} 
A_- \sin k x & 0 \leq |x| \leq L/2 \\
A_- \sin \frac{k L e^{\kappa(L/2-|x|)}}{2} & |x| > L/2
\end{cases} \\
\psi_-(x) &= -\psi_-(x) \\
\frac{1}{A_-^2} &= \frac{1}{k} \left[ \frac{k L}{2} - \sin \frac{k L}{2} \cos \frac{k L}{2} \right] + \frac{1}{\kappa} \sin^2 \frac{k L}{2}.
\end{align*}
\]

The finite discrete energy spectrum of the quantum hole results from the solutions of the transcendental equations

\[
\begin{align*}
\tan \frac{k_+ L}{2} &= \frac{\kappa}{k_+}, \\
\tan \frac{k_- L}{2} &= -\frac{k_-}{\kappa},
\end{align*}
\] (11) (12)

for symmetric (+) and antisymmetric (−) wave functions, respectively. Due to the low conductivities of the single junctions the wave function of the island is well approximated by the wave function of the quantum hole.

According to [6], ohmic behaviour of the current can be expected in case of \( eV \ll E \), only. Hence, we simplify the model in terms of \( k \ll \kappa \) which corresponds to \( eV \ll E \) via an uncertainty relation. In this approximation the solutions of Eq. (11) and (12) read as
\[ k_n \approx \frac{\pi n}{L} \left( 1 - \frac{2}{\kappa L} \right), \quad n = 0, 1, 2, \ldots n_E \]  

(13)

with \( \hbar \kappa \approx 2 m^* \sqrt{2 m^*(E - \varepsilon_F)}/\hbar \). \( n_E \) denotes the total number of states in the quantum hole of the energetic depth \( E \). Furthermore, the following Taylor expansion in \( 1/(\kappa L) \) of the required wave function values can be obtained:

\[
\psi_\pm(L/2)\psi_\pm(-L/2) = \pm A_\pm^2 \begin{cases} 
\cos^2(kL/2) \\
\sin^2(kL/2)
\end{cases}
\approx \pm \left( \frac{\pi n}{\kappa L} \right)^2 \left[ 1 - \frac{2}{\kappa L} - \frac{1}{3} \left( \frac{\pi n}{\kappa L} \right)^2 \right] + O \left( \frac{1}{(\kappa L)^0} \right).
\]

(14)

Fig. 1 shows a comparison of different order contributions to \( \psi(L/2)\psi(-L/2) \) at \( \varepsilon(k_n) = \varepsilon_F \).

By means of (14) and the approximation (13) Eq. (9) is given for zero temperature by

\[
G_{el} = \frac{\hbar}{8\pi e^2} G_1 G_2 \left[ \sum_{n=1}^{n_E} (-1)^n \frac{E - \varepsilon_{F}}{E - \varepsilon_{F} - \varepsilon_n} \Delta_0 F(\varepsilon_n) \right]^2
\]

\[
= \frac{\hbar}{8\pi e^2} G_1 G_2 \left[ \sum_{n=1}^{n_F} (-1)^n \frac{E - \varepsilon_{F}}{E - \varepsilon_{F} - \varepsilon_n} \frac{\Delta_0}{\varepsilon_n - \varepsilon_{F} - \varepsilon_n} + \sum_{n=n_F+1}^{n_E} (-1)^n \frac{E - \varepsilon_{F}}{E - \varepsilon_{F} - \varepsilon_n} \frac{\Delta_0}{\varepsilon_n + \varepsilon_{+1}} \right]^2
\]

(15)

Here, \( n_F \) labels the number of states below the Fermi level (\( n_F \leq n_E \)). The contributions of neighboring states possess different signs due to the different symmetry of the respective wave functions. This effect is known from [2]. Formula (13) is our main result. It is much more complicated than expression (1) because the discrete energy spectrum of the central electrode (quantum hole) has been taken into account.

In discussion we are going to compare our results with the experimental data of [3]. For the evaluation numerical values of \( n_F \) and \( \varepsilon_F \) are necessary. According to the experimental setup, the values are chosen as \( n_F = 5.9 \times 10^{22} cm^{-3} \) and \( \varepsilon_F = 5.51 eV \). The quasi–particle mass \( m^* \) is approximated by the free electron mass \( m^* \approx m_0 \approx 9.1 \times 10^{-31} kg \). The parameter \( L \) corresponding to the diameter of the central electrodes is given by the experiment [3]. The second parameter \( E \) describing the barrier height of the quantum hole has to be determined in comparison with the experimental data. Fig. 2 and Fig. 3 show the computed elastic
conductivity $G_{el}$ of sample $A$ and $B$ of [3] in dependence on $E$, respectively. The observed steps arise from the occupation of a new state in the quantum hole. The parameter $E$ is given by the figures where the computed $E$–dependent conductivity $G_{el}$ coincides with the experimental value (independent of $E$). Due to the fluctuations of the numerical curves a least–squares fit was applied to them. This yields the corresponding parameters $E$ of the samples $A$ and $B$; $E_A \approx E_B \approx 2 \ldots 3\, eV$ (cf. Fig. 2 and Fig. 3). This is in good agreement with earlier estimations [8].

The pros of this model are the simple theory behind it. In addition to [2] our result depends on properties of the island characterized by $E$ and $L$. According to the applied model, $\Delta_0 \approx 0.38\, eV$, $1.12\, eV$ is found for sample $A$ and $B$, respectively. These values exceed drastically the data concluded from the experiment [3] in terms of the theory [2] ($\Delta = 0.045\, eV$, $0.126\, eV$). This is not surprising because they are model–dependent parameters.

Our approach is based on the very simple model of an 1D quantum hole, which is far from being general due to the neglect of two dimensions and the idealization of the energetic shape of the barriers. Regarding to the second point it is unlikely within $eV \ll E$ that the shape of the upper end of barriers influences the current dramatically. An influence on the steps observed in Fig. 2 and Fig. 3 could be expected. This approach could be improved by using more sophisticated models of the barrier, as presented for instance by [8], [9]. Additionally, instead of the bulk values for $\varepsilon_F$ and $n_F$ as given above more appropriated values should be taken from the experiment.

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FIGURES

FIG. 1. The evaluation of the different orders of a Taylor expansion of the wave function in a deep quantum hole. – The solid line corresponds to the numerical solution whereas the other curves display the Taylor expansion of given order.

FIG. 2. The comparison of our formulae with the experimental data of sample A. – The figure shows the dependence of the elastic conductivity $G_{el}$ on the barrier height $E$. We compare the numerical solution (solid line) with the fitted value out of the experimental paper (horizontal line). The steps indicate the occupation of a new state within the quantum hole. The straight line corresponds to a $G_{el} = a E^b$ least-square fit of the numerical data. The parameters of the sample are $L = 3 \text{ nm}$, $C_1 = 0.57 \times 10^{-18} F$, $C_2 = 3.4 \times 10^{-18} F$, $G_1 = 1/(3.5 M\Omega)$, and $G_2 = 1/(21 M\Omega)$.

FIG. 3. The corresponding comparison of data like Fig. 1 for sample B. Its parameters are $L = 0.8 \text{ nm}$, $C_1 = 0.095 \times 10^{-18} F$, $C_2 = 0.066 \times 10^{-18} F$, $G_1 = 1/(0.42 M\Omega)$, and $G_2 = 1/(630 M\Omega)$.