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SHORT-RANGE IMPURITY IN A NON-CENTRAL CROSS-SECTION OF A SADDLE-POINT MICROCONSTRICTION

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We calculate the conductance of a saddle - point potential with a short-range impurity in a non-central cross-section of the channel for arbitrary number of the transverse modes. It is found that one observes series of downward dips in the conductance vs Fermy energy below each threshold as well as the crossover from resonant dip to peak around the threshold.

Recently much interest has been raised in study of the effect of a single impurity on the conductance of a quantum ballistic microconstriction [1]. Previosly we have shown [2], that in the realistic model of a saddle point potential, a short-range impurity located in a central cross-section of the waveguide causes the crossover from resonant dip to peak near each threshold. We also investigated a case of a non-central location of the impurity but only for a pinch-off microconstriction [3]. Here, we develope our model for a arbitrary number of the transverse modes, because it is important from both theoretical [4] and experimental [5] point of view.

The main features of our model [2] can be recalled as follows. An impurity changes the conductance of the quantum wire because it scatters the modes which are transmitted through the channel. For a short-range impurity at the point r_0 the scattered field is

$$\psi'(r) = -2\pi\psi^{\circ}(r_0)\frac{G_\epsilon(r,r_0)}{D_\epsilon(r_0)}. \tag{1}$$

Here G_ϵ is the Green's function for confining potential of the microjunction, $\psi^{\circ}(r)$ - the incoming field and $D_\epsilon(r_{\circ})$ - denominator of the scattering amplitude. The latter one is expressed in terms of the near asymptotic behaviour of the Green's function:

$$G_\epsilon(r,r')|_{r,r'\to r_0} = \frac{1}{2\pi}\left[K_\epsilon(r_0) - \ln\frac{|r-r'|}{d}\right] \tag{2}$$

and

$$D_\epsilon(r_0) = \Lambda + K_\epsilon(r_0), \tag{3}$$

where $\Lambda = \ln(d/a)$, a is the scattering length, d is the width of the microjunction.

The saddle-point potential is:

$$V(x,y) = \frac{\hbar^2}{2md^2}\left[-\frac{x^2}{L^2} + \frac{y^2}{d^2}\right]. \tag{4}$$

Here L is the length of the channel, d is of the order of the Fermi wavelength λ_F , and $L \gg d$. The variables can be separated for this potential and thus the Green's function and also it's near asymptotic behaviour may be calculated.

The waveguide modes in this potential are

$$\Psi^{\pm}_{E,n}(x,y) = \Phi_n(y)E(-\varepsilon_n, \pm\xi), \tag{5}$$

where $\Phi_n (n = 0, 1, ...)$ - are the oscillator functions corresponding to energies $E_n = \hbar\Omega(n+\frac{1}{2})$, $\hbar\Omega = \hbar^2/md^2$, $E(-\varepsilon_n, \xi)$ is the complex Weber's functions (according the definition taken from [6]), $\varepsilon_n = (E - E_n)/\hbar\omega$, $\hbar\omega = \hbar^2/mdL$, $\xi = x\,(2/Ld)^{1/2}$. When there is no impurity the conductance of microjunction is (in units of $2e^2/h$) [7]:

$$G_0 = \sum_{n=0}^{\infty} t^2(\varepsilon_n), \tag{6}$$

where $t^2(\varepsilon) = 1 - r^2(\varepsilon) = [1 + \exp(-2\pi\varepsilon)]^{-1}$ is the transmission probability. Therefore for a long channel G_0 versus E have a series of plateau with a width $\hbar\Omega$ and a height $G_0 = N$ (N is the number of transmitted modes), separated by steps of a width $\hbar\omega$.

Using Eq. (1) for ψ', we can take into account the affect of the impurity scattering on the conductance. We also introduced a nondimensional oscillator wave function $\phi_n(y) = (\pi d)^{1/2}\Phi_n(y)$ and the parameter $\alpha = (L/d)^{1/2} = (\hbar\Omega/\hbar\omega)^{1/2}$. Then one can easily obtain the transmission coefficients [2]:

$$T_{n\to n'} = -it(\varepsilon_n)\Big[\delta_{nn'} - \frac{\alpha}{D_\varepsilon(x_0y_0)}\phi_n(y_0)\phi_{n'}(y_0)\frac{1}{\sqrt{2}}t(\varepsilon_{n'})E(-\varepsilon_n,\xi_0)E(-\varepsilon_{n'},-\xi_0)\Big] \tag{7}$$

and compute the conductance according the Landauer formula $G = \sum_{nn'} |T_{n\to n'}|^2$ in the presence of the impurity. In order to simplify this procedure we isolated [2] in D_ε the contribution $\beta H(\varepsilon, \xi_0)$ ($\beta = \alpha\phi_N^2$) from the threshold mode $n = N$ and the contributions p_ε (real part) and q_ε (imaginary part) of other modes $n \neq N$:

$$D_\varepsilon = \Lambda + p_\varepsilon + iq_\varepsilon + \beta H(\varepsilon, \xi_0), \tag{8}$$

where the complex function H by definition is

$$H(\varepsilon,\xi_0) = P(\varepsilon,\xi_0) + iQ(\varepsilon,\xi_0) = \frac{1}{\sqrt{2}}t(\varepsilon)E(-\varepsilon,\xi_0)E(-\varepsilon,-\xi_0) \tag{9}$$

and $\varepsilon \equiv \varepsilon_N$. We use also convenient representation of complex Weber's fuction $E(-\varepsilon_n, \pm\xi_0)$ via the real Weber's function [6] $W(-\varepsilon_n, \pm\xi_0)$. Then the real $P(\varepsilon, \xi_0)$ and imaginary $Q(\varepsilon, \xi_0)$ parts of $H(\varepsilon, \xi_0)$ can be easily separated :

$$P(\varepsilon,\xi_0) = \frac{1}{\sqrt{2}}r(\varepsilon)\cdot 2W(-\varepsilon,\xi_0)W(-\varepsilon,-\xi_0), \tag{10a}$$

$$Q(\varepsilon,\xi_0) = \frac{1}{\sqrt{2}}t(\varepsilon)\Big[W^2(-\varepsilon,\xi_0) + W^2(-\varepsilon,-\xi_0)\Big]. \tag{10b}$$

Substituting Eq.(8)–(10a,b) into (7), one can show after lengthy but direct algebraic manipulations that the expression for the conductance between [2] E_{N-1} and E_{N+1}:

$$G = N + \frac{t^2(\varepsilon)(p_\varepsilon + \Lambda)^2 - r^2(\varepsilon)q_\varepsilon^2}{|D_\varepsilon|^2} \tag{11}$$

suprisingly also describes the situation with a non-central impurity. Now it is obvious that the affect of the position of the impurity along the channel on the conductance is fully described by the function $H(\varepsilon,\xi_0)$. The bound states are defined [2] as scattering amplitude poles $\bar{\varepsilon}-i\Gamma$, which are roots of the equation:

$$\mathrm{Re}D_\varepsilon = \Lambda + \mathrm{Re}K_\varepsilon = \Lambda + p_\varepsilon + \beta P(\varepsilon,\xi_0) = 0. \tag{12}$$

The assumption of the smallness of the width Γ allows us to write it in the form:

$$\Gamma = c^{-1}\cdot \mathrm{Im}K_\varepsilon, \tag{13}$$

where $c = d/d\varepsilon \mathrm{Re}K_\varepsilon|_{\varepsilon=\bar{\varepsilon}}$. On the other hand, $\mathrm{Im}D_\varepsilon(r_0)$ is proportional to the fluxes from δ-function located in r_0 [8]:

$$\mathrm{Im}D_\varepsilon(r_0) = q_\varepsilon + \beta Q(\varepsilon,\xi_0) = 2\pi[J_{n<N}(r_0) + J_N(r_0)]. \tag{14}$$

One can show that the flux $J_N(r_0)$, carried by the threshold mode N, can be devided into two parts:

$$J_N^{\pm} = \frac{1}{2\pi}\beta\frac{1}{\sqrt{2}}t(\varepsilon)W^2(-\varepsilon,\pm\xi_0). \tag{15}$$

They correspond to the fluxes to the right (J_N^+) and to the left (J_N^-) (here we let $\xi_0>0$). Using Eqs. (8), (9), (10b), we decompose the total width $\Gamma=\Gamma_m+\Gamma_t^++\Gamma_t^-$, where the width $\Gamma_m = c^{-1}q_\varepsilon$ is due to the decay into the continuous spectra of above-barrier modes $n<N$ (mixing of modes) and the widthes $\Gamma_t^{\pm} = c^{-1}\cdot 2\pi J_N^{\pm}$ are due to the tunneling of the threshold mode N through the saddle – point potential (Γ_t^-) and the potential of the impurity (Γ_t^+). Below and around the threshold E_N it is possible to expand D_ε near $\bar{\varepsilon}$ and , using Eq.(10a), (12), express Eq.(11) in the form :

$$G = N + \frac{r^2(\varepsilon)(4\Gamma_t^+\Gamma_t^- - \Gamma_m^2)}{(\varepsilon-\bar{\varepsilon})^2+\Gamma^2}. \tag{16}$$

This is a main result of the present work.

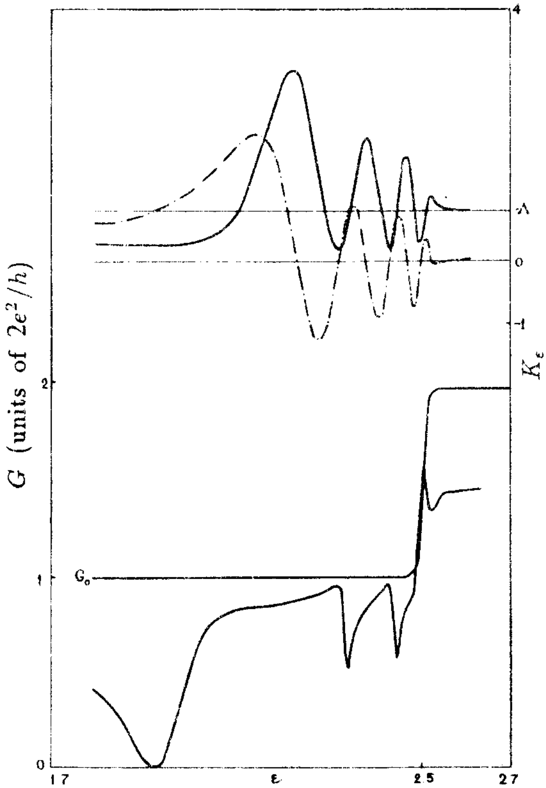
At first, we investigate the behaviour of the conductance below the threshold E_N and above the potential energy $\varepsilon_0=-\xi^2/4$ corresponding to a location of the impurity (i.e. $\varepsilon_0<\varepsilon<0$). (Note, that as following all energies of bound states are defined with respect to the energy ε_0). One can see the oscillations of the function K_ε in this energy interval (the upper part of Fig.1). It is this fact that leads to existance of a set of bound states, because the condition (12) can be fulfilled several times. To derive their energies and widthes we introduce a convenient notation $t=|\varepsilon|^{-1/3}\cdot(|\varepsilon|-\xi^2/4)$ and expand Eq.(10a,b) into Airy function [6]:

$$P(\varepsilon) = \sqrt{2}\pi|\varepsilon|^{-1/6}\mathrm{Ai}(-t)\mathrm{Bi}(-t), \tag{17a}$$

$$Q(\varepsilon) = \sqrt{2}\pi|\varepsilon|^{-1/6}\Big(\frac{1}{4}\exp(-2\pi|\varepsilon|)\mathrm{Bi}^2(-t)+\mathrm{Ai}^2(-t)\Big). \tag{17b}$$

We will search the energies of bound states near zeros t_n of Airy function, determined by equality $Ai(-t_n)=0$. Here $n=1,2..M$ and M is equal to an integer part of $\xi_0^2/4\pi+1$. Then we substitute Eq.(17a) into Eq.(12):

$$\mathrm{Ai}(-t_n)\mathrm{Bi}(-t_n) = \frac{|\Lambda|}{\sqrt{2}\pi\beta}|\varepsilon_0|^{1/6}. \tag{18}$$



The dependence of ReK_ϵ (broken line, upper plot) and ImK_ϵ (solid line, upper plot) and the conductance G (lower plot) on the energy below a threshold 2. The impurity position is determined by coordinates $y_0 = 2$ and $\xi_0 = 6$, $\alpha = 5$

Here we omitted p_E due to its smallness. Expanding left part of Eq.(18) in Taylor series up to the second term and using Wronskian relation [6] $W[\mathrm{Ai}(z), \mathrm{Bi}(z)] = \pi^{-1}$, we have for the energies of bound states:

$$\bar{\varepsilon}_n = -\left(\frac{\xi_0}{2}\right)^{2/3} t_n + \frac{\Lambda}{\beta}\frac{\xi_0}{2}. \tag{19}$$

This type of bound states exists for both signs of the impurity potential. Their widthes can be easily calculated:

$$\Gamma_m = \frac{q_\epsilon}{\sqrt{2}}\frac{1}{\beta}\frac{\xi_0}{2}, \tag{20 a}$$

$$\Gamma_t^- = \frac{1}{4}\pi \mathrm{Bi}^2(-t_n)\left(\frac{\xi_0}{2}\right)^{2/3} \exp(-2\pi|\varepsilon|), \tag{20 b}$$

$$\Gamma_t^+ = \frac{1}{\pi \mathrm{Bi}^2(-t_n)}\left(\frac{\Lambda}{\beta}\right)^2\left(\frac{\xi_0}{2}\right)^{4/3} \tag{20 c}$$

and are small if we assume the impurity is enouth strong

$$|\Lambda| \ll \beta\xi_0^{-1/3}. \tag{21}$$

This means also that the impurity is located not far from the bottleneck of the long channel and in such place where $\phi_n^2(y_0)$ is large . One can see that below the threshold Γ_t^- is due to the tunneling through the wide saddle - point barrier and hence is exponentially small. The condition (21) yields also

$$\Gamma_t^+ \ll \Gamma_m. \tag{22}$$

Assuming $r \approx 1$ in the Eq.(16), we get narrow downward dips on the curve of the conductance (the lower part of Fig.1). In such way the "mirror confined" states [3] become apparent in the case of an arbitrary number of the transverse modes. Indeed, the condition (22) means that the escape through the narrow barrier created by the impurity is small enough and the threshold mode N is "mirror - confined " between the saddle - point potential and the impurity potential at the energies $\bar{\varepsilon}_n$.

Below energy ε_0 we obtain additionally one bound state [3] for only attractive impurities ($\Lambda < 0$) with energy $\bar{\varepsilon}_0 = (\beta/|\Lambda|)^2$. The width of this bound state is

$$\Gamma = \bar{\varepsilon}_0\left[\frac{q_\epsilon}{|\Lambda|} + \exp\left(-\frac{4}{3}\left(\frac{\beta}{|\Lambda|}\right)^3\frac{2}{\xi_0}\right)\right] \tag{23}$$

and maybe large, as in Fig.1, due to slow variation of $\mathrm{Re}K_\epsilon$ in this energy domain.

Next, we investigate the bound state around the threshold E_N. Here we can expand Eq.(10 a,b) into trigonometric functions [6]:

$$P(\varepsilon,\xi_0) = r(\varepsilon)\frac{\sqrt{2}}{\xi_0}\cos\alpha, \tag{24 a}$$

$$Q(\varepsilon,\xi_0) = \frac{\sqrt{2}}{\xi_0}(1 + r(\varepsilon)\sin\alpha), \tag{24 b}$$

where $\alpha = [\xi_0^2/2 + 2\varepsilon\ln\xi_0 + \Phi_2]$ and $\Phi_2 = \arg\Gamma(1/2 - i\varepsilon)$. Assuming that $r(\varepsilon)$ and Φ_2 more slowly varying function than $\cos\alpha$, we obtain following estimates for the widthes about the threshold:

$$\Gamma_m = \frac{1}{r}\frac{q_\epsilon}{\sqrt{2}}\frac{\xi_0}{\beta}\frac{1}{2\ln\xi_0}, \tag{25 a}$$

$$\Gamma_t^- = \frac{1-r}{r}\frac{1}{2\ln\xi_0}, \tag{25 b}$$

$$\Gamma_t^+ = \frac{1}{r^2}\left(\frac{\Lambda\xi_0}{2\beta}\right)^2\frac{1}{(2\ln\xi_0)^3}. \tag{25 c}$$

Then the tunneling of the threshold mode N through the saddle can be stronger than decay due to mode mixing. Indeed, if we assume

$$4\Gamma_t^+\Gamma_t^- - \Gamma_m^2 > 0, \tag{26}$$

than the Eq.(16) describes resonant peak on the threshold (Fig.1). Substituting Eq.(25) into (26) we get the condition when the peak is emerged:

$$r(\varepsilon) < \left[1 + 2\left(\frac{q_\epsilon\ln\xi_0}{\Lambda}\right)^2\right]^{-1}. \tag{27}$$

Note added in proof After completion of this work, I received a copy of work [9] by S.A.Gurvitz and Y.B.Levinson, related to the general analysis of the resonant transmission and reflection due to single impurity in a conducting channel. Their formulae for the conductance is similar to the Eq.(16) of the present work. The essential difference is a reflection coefficient $r(\varepsilon)$ in Eq.(16), because as I mentioned above both tunneling and mixing widthes $\Gamma_t^{\pm}$ and Γ_m have a significance only near the threshold, where $r(\varepsilon) \neq 1$.

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