Short-range impurity in a noncentral cross section of a saddle-point microconstriction

M. I. Lubin
Institute of Microelectronics Technology, Academy of Sciences of Russia, 14232 Moscow District, Chernogolovka, Russia

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The conductance of the saddle-point potential with a short-range impurity in a noncentral cross section of the channel has been calculated for an arbitrary number of transverse modes. A series of downward dips in the conductance versus the Fermi energy has been observed below each threshold. The crossover from resonant dip to a peak near the threshold has also been observed.

Considerable interest has recently been focused on the study of the effect of a single impurity on the conductance of a quantum ballistic microconstriction.[1] Previously we have shown[2] that in the realistic model of a saddle-point potential a short-range impurity located in the central cross section of the waveguide causes a crossover from a resonant dip to a peak near each threshold. We have also investigated the case of a noncentral location of the impurity but only for a pinch-off microconstriction.[3]

Here we develop our model for an arbitrary number of transverse modes, because it is important from both theoretical[4] and experimental[5] points of view.

The main features of our model[2] can be summarized as follows. An impurity changes the conductance of a 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

$$\psi'(r) = -2\pi\psi^0(r_0)\,\frac{G_\epsilon(r, r_0)}{D_\epsilon(r_0)}\,. \tag{1}$$

Here G_ϵ is the Green's function of the confining potential of the microjunction, $\psi^0(r)$ is the incoming field, and $D_\epsilon(r_0)$ is the denominator of the scattering amplitude. The latter one is expressed in terms of the near asymptotic behavior 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, and 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 on 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 its near asymptotic behavior can be calculated.

The waveguide modes in this potential are

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

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

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

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

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

$$T_{n\to n'}=-it(\epsilon'_n)\left[\delta_{nn'}-\frac{\alpha}{D_\epsilon(x_0y_0)}\phi_n(y_0)\phi_{n'}(y_0)\frac{1}{\sqrt{2}}t(\epsilon_{n'})\right.$$
$$\left.\times E(-\epsilon_n,\xi_0)E(-\epsilon_{n'},-\xi_0)\right] \tag{7}$$

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

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

where the complex function H by definition is

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

and $\epsilon\equiv\epsilon_N$. We have used also the convenient representation of the complex Weber's function $E(-\epsilon_n,\pm\xi_0)$ via the real Weber's function[6] $W(-\epsilon_n,\pm\xi_0)$. Then the real part $P(\epsilon,\xi_0)$ and the imaginary part $Q(\epsilon,\xi_0)$ of $H(\epsilon,\xi_0)$ can be easily separated:

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

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

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

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

surprisingly describes the situation with a noncentral 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 $H(\epsilon,\xi_0)$. The bound states are defined[2] as scattering amplitude poles $\bar{\varepsilon}-i\Gamma$, which are roots of the equation

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

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

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

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

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

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

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

These parts 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), and (10b), we decompose the total width $\Gamma=\Gamma_m+\Gamma_t^++\Gamma_t^-$, where the width $\Gamma_m=c^{-1}q_\epsilon$ is due to the decay into the continuous spectra of above-barrier modes $n<N$ (the mixing of modes) and the widths $\Gamma_t^\pm=c^{-1}\cdot 2\pi J_N^\pm$ 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 near the threshold E_N it is possible to expand D_ϵ near $\bar{\varepsilon}$ and, using Eq. (10a) and (12), express Eq. (11) in the form

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

Main result. Let us first analyze the behavior of the conductance below the threshold E_N and above the potential energy $\epsilon_0=-\xi^2/4$ which corresponds to the location of the impurity (i.e., $\epsilon_0<\epsilon<0$). (Note that all bound-state energies are defined with respect to the energy ϵ_0). We see that the function K_ϵ oscillates in this energy interval (the upper part of Fig. 1). This fact leads to the existence of a set of bound states, because

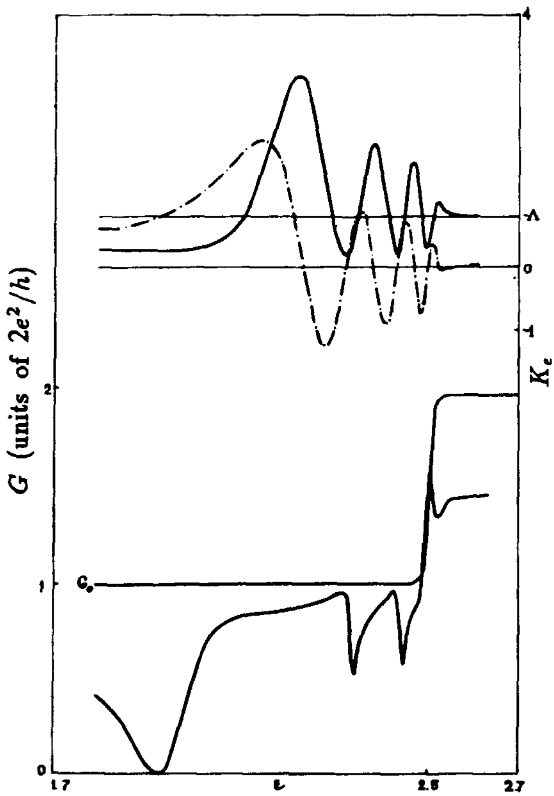

FIG. 1. The dependence of ReK_ϵ (the broken line, upper plot), ImK_ϵ (the solid line, upper plot), and the conductance G (lower plot) on the energy below the threshold 2. The impurity position is determined by the coordinates $y_0=2$ and $\xi_0=6$, $\alpha=5$.

the condition (12) can be satisfied several times. To derive their energies and widths, we introduce a convenient notation $t=|\epsilon|^{-1/3}\cdot(|\epsilon|-\xi^2/4)$ and expand Eqs. (10a) and (10b) into an Airy function[6]

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

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

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

$$\mathrm{Ai}(-t_n)\mathrm{Bi}(-t_n)=\frac{|\Lambda|}{\sqrt{2}\pi\beta}|\epsilon_0|^{1/6}. \tag{18}$$

Here we omitted p_E due to its smallness. Expanding the left side of Eq. (18) in a Taylor series up to the second term and using Wronskian relation[6] $W[\mathrm{Ai}(z), \mathrm{Bi}(z)]=\pi^{-1}$, we obtain the following expression for the energies of the 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. The widths of these bound states can be easily calculated:

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

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

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

These widths are small if we assume that the impurity is strong

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

This means that the impurity is located not far from the bottleneck of the long channel and is in such a place where $\phi_n^2(y_0)$ is large. We 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

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

Assuming $r\approx 1$ in Eq. (16), we obtain narrow downward dips on the conductance curve (the lower part in Fig. 1). Consequently, the "mirror-confined" states[3] become apparent in the case of an arbitrary number of 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 the energy ϵ_0 we obtain additionally one bound state[3] for only the 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 it could be large, as in Fig. 1, due to a slow variation of $\mathrm{Re}K_\epsilon$ in this energy region.

Next, we will investigate the bound state near the threshold E_N. Here we can expand Eqs. (10a) and (10b) in trigonometric functions:[6]

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

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

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

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

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

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

The tunneling of the threshold mode N through the saddle can then be stronger than the decay due to mode mixing. If we assume

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

then Eq. (16) will describe the resonant peak at the threshold (Fig. 1). Substituting Eq. (25) into Eq. (26), we find the condition at which the peak appears:

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

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

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