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Electron scattering in an arbitrarily bent planar quantum channel

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Abstract. The bend region of a two-dimensional quantum channel of constant width is shown to generate a well-type effective potential in the problem of electron wave scattering. For narrow channels the longitudinal modes of electron propagation should be considered as approximately independent. In the one-mode approximation the coefficient of electron reflection is calculated and its non-monotonic dependence on the incident electron momentum and the channel bend angle is determined. The local maxima in the reflection coefficient decrease exponentially with increasing electron momentum and increase with increasing channel bend.

It is known that the electron mobility in the plane of contact of the heterostructures, such as GaAs–$Al_{1-x}Ga_xAs$, exceeds greatly that in the transverse direction [1]. An additional restriction to the geometry of electron motion could be caused by applying a negative potential of definite configuration in the plane of the heterojunction [2] or by making narrow channels and other elementary devices [3] on the basis of lithographic technologies [4–6]. A small value (10–100 nm) of at least one of the inherent sizes of these quasi-two-dimensional structures together with a small effective mass $m = 0.07m_e$ of the charge carriers results in essentially quantum effects even in a relatively easily available temperature interval (2–200 K). Moreover, in high-quality structures, where the free path of the charge carriers is larger than the inherent longitudinal size of the device (channel), the so-called ballistic regime of electron transfer [1] is realized. Recently this regime has been studied intensively in the framework of the standard two-dimensional Schrödinger equation with such or another fixed boundary conditions [7–9].

In the present work on the ballistic electron transport in an arbitrarily bent quantum channel we started with a quite natural desire to choose a coordinate system that would simplify the boundary conditions and later make it possible to convert our two-dimensional problem into a one-dimensional problem. In this approach the coordinate system should be adequate for the channel geometry. This can be realized easily at least for channels of constant width (in contrast with the channel used in the paper by Lent [8]) and continuous bend with a constant sign of curvature.

Consider an infinitely long two-dimensional quantum channel of constant width d for which the internal boundary in a Cartesian system of coordinates x, y coincides with the curve $y = f(x)$, $f''(x) > 0$. The concrete form of the function $f(x)$ is not, in principle, necessary for further development of the theory but for illustration we often refer to the curve

$$y = f_b(x) \equiv L \tan\beta\{\sinh^{-1}[\cot\!an\,\beta \cosh(x/L)] - \ln(\cot\!an\,\beta)\} \qquad (1)$$

which models well the internal boundary of the channel such as symmetric bend with the asymptotic $y = \pm x \tan\beta$ at $x/L \to \pm\infty$. The function $f_b(x)$ has the following advantages: the possibility of regulating the angle $\pi - 2\beta$ between two straight parts of the channel and the smoothness of the junction by means of parameters β and L respectively ($0 < \beta < \frac{1}{2}\pi$, $L > 0$).

The parametric relations

$$\begin{aligned} x &= \tau + \rho f'(\tau)/\sqrt{1 + f'^2(\tau)} \\ y &= f(\tau) - \rho/\sqrt{1 + f'^2(\tau)} \\ s &= \int_0^\tau \mathrm{d}\xi\, \sqrt{1 + f'^2(\xi)} \end{aligned} \tag{2}$$

give the system of orthogonal $\nabla\rho \cdot \nabla s = 0$ curvilinear coordinates $\rho = \rho(x, y)$, $s = s(x, y)$ (figure 1). The coordinate $\rho \geqslant 0$ varies across the channel so that $\rho = 0$ at the internal channel boundary and $\rho = d$ at the external boundary. The coordinate $-\infty < s < \infty$ changes along the channel so that $s \to -\infty$ for the channel input and $s \to \infty$ for the channel output. The metric tensor components [10], necessary to record the Laplace operator, in these coordinates are written as

$$\begin{aligned} g_{\rho\rho} &\equiv (\partial x/\partial\rho)^2 + (\partial y/\partial\rho)^2 = 1 \\ g_{ss} &\equiv (\partial x/\partial s)^2 + (\partial y/\partial s)^2 = [1 + \rho f''(\tau)/s'^3(\tau)]^2 \equiv [1 + a(s/L)\rho/L]^2. \end{aligned} \tag{3}$$

For a symmetrically bent channel (1) for example, the function $a(s/L)$ (the function of channel bend) is as follows:

$$a_b\left(\frac{s}{L}\right) = \frac{\sin\beta\cos^2\beta}{\sinh^2[(s/L)\cos\beta] + \cos^2\beta}. \tag{4}$$

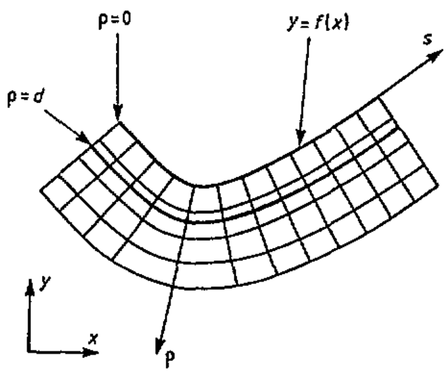

Figure 1. The orthogonal curvilinear coordinates ρ, s and their fastening to the internal wall of the channel $y = f(x)$.

Now we can find the stationary Schrödinger equation

$$-[1+\varepsilon ra(\varepsilon\sigma)]^{-1}\frac{\partial}{\partial\sigma}\left([1+\varepsilon ra(\varepsilon\sigma)]^{-1}\frac{\partial\psi}{\partial\sigma}\right)-[1+\varepsilon ra(\varepsilon\sigma)]^{-1}\frac{\partial}{\partial r}\left([1+\varepsilon ra(\varepsilon\sigma)]\frac{\partial\psi}{\partial r}\right)$$
$$+U(r)\psi=\mathcal{E}\psi \qquad \left(\varepsilon\equiv\frac{d}{L}\right). \tag{5}$$

On the basis of this we shall consider the electron scattering problem in the above-mentioned two-dimensional arbitrarily bent quantum channel. Here the coordinates ρ and s have been made dimensionless by the channel width d, i.e.

$$\rho=rd \qquad s=\sigma d \tag{6}$$

and the electron energy E by the typical energy $\hbar^2/2md^2$ of transverse quantization, i.e.

$$E=\hbar^2\mathcal{E}/2md^2. \tag{7}$$

The potential $U(r)$ models channel walls which will be assumed to be impenetrable to electrons:

$$U(r)=\begin{cases}0 & 0<r<1\\ \infty & r\leqslant 0,1\leqslant r.\end{cases} \tag{8}$$

It is easily seen that, for the channel input $\sigma\to-\infty$ and for its output $\sigma\to\infty$, where $a(\varepsilon\sigma)\to 0$, our equation (5) does not differ from the Schrödinger equation for a straight channel.

The difference between straight and bent channels is the largest in the region where $|\sigma|\lesssim L/d$, and this is the reason for electron reflection. The situation is close to that known in the gauge field theory when the system with broken symmetry (in the given case with bent geometry) is completely equivalent to that with restored symmetry but in the presence of an additional field [11]. Since we are interested in longitudinal electron motion, then we first eliminate terms with a first derivative in σ in the Laplacian by the substitution

$$\psi=\sqrt{1+\varepsilon ra(\varepsilon\sigma)}\Phi \tag{9}$$

and then we decompose Φ in the eigenfunctions

$$P_n(r)\equiv\sqrt{2}\sin(\pi nr) \qquad n=1,2,3,\ldots,\infty \tag{10}$$

of the Laplacian transverse part for a straight channel:

$$\Phi=\sum_{m=1}^{\infty}F_m(\sigma)P_m(r). \tag{11}$$

As a result we obtain a one-dimensional but infinite system of coupled equations for the functions $F_n(\sigma)$:

$$\frac{-\mathrm{d}^2F_n(\sigma)}{\mathrm{d}\sigma^2}+L_{nn}(\sigma)F_n(\sigma)+\sum_{m=1}^{\infty}(1-\delta_{nm})M_{nm}(\sigma)F_m(\sigma)=0 \qquad n=1,2,3,\ldots,\infty. \tag{12}$$

It should be noted that the conditions for which the function Φ satisfies at the input and output of a channel must coincide with those for the function ψ since $\lim_{\sigma\to\pm\infty}[a(\varepsilon\sigma)] = 0$.

The above-proposed approach can be fully applied obviously to channels of arbitrary width ($\varepsilon \equiv d/L$ is arbitrary).

Further we shall consider narrow channels when $\varepsilon \ll 1$. Then, on the one hand, in the expressions for $L_{nn}(\sigma)$ and $M_{nm}(\sigma)$ one can be confined by terms not larger than those of the first order in ε, i.e.

$$
\begin{aligned}
L_{nn}(\sigma) &\simeq \int_0^1 \mathrm{d}r\,[1 + 2\varepsilon r a(\varepsilon\sigma)] \left[\left(\frac{\mathrm{d}P_n(r)}{\mathrm{d}r} \right)^2 - \mathcal{E} P_n^2(r) \right] \\
M_{nm}(\sigma) &\simeq \int_0^1 \mathrm{d}r\, 2\varepsilon r a(\varepsilon\sigma) \left(\frac{\mathrm{d}P_n(r)}{\mathrm{d}r} \frac{\mathrm{d}P_m(r)}{\mathrm{d}r} - \mathcal{E} P_n(r) P_m(r) \right)
\end{aligned}
\tag{13}
$$

and, on the other hand, owing to smoothness of the function $a(\varepsilon\sigma)$ the solutions of the set of equations (12) can be found by semi-classical (WKB) methods [12]:

$$
F_n = A_n \exp\left(\frac{\mathrm{i}}{\varepsilon} Q(u) \right) \qquad u \equiv \varepsilon\sigma. \tag{14}
$$

Combining the relations (12)–(14), with accuracy to ε inclusively, we find an aggregate of normal longitudinal modes that corresponds to the energy $\mathcal{E}$:

$$
\mathrm{d}Q_n^{\pm}/\mathrm{d}u \simeq \pm q_n[1 + \tfrac{1}{2}\varepsilon a(u)] \qquad n = 1, 2, 3, \ldots, \infty \tag{15}
$$

where

$$
q_n \equiv \sqrt{\mathcal{E} - (\pi n)^2}. \tag{16}
$$

Modes with $q_n^2 > 0$ are able to propagate along the channel while those with $q_n^2 < 0$ are not. It should be noted that the result (15) and (16) obtained with the adopted precision does not depend on the availability of the crossed terms in equation (12). In other words, in this approximation each equation

$$
\varepsilon^2 \mathrm{d}^2 F_n/\mathrm{d}u^2 + q_n^2[1 + \varepsilon a(u)]F_n = 0 \tag{17}
$$

describes completely one of the normal longitudinal modes of the bent channel. From here the function $a(u)$ of the channel bend is seen to affect electron wave propagation similar to a potential well, but the depth of such a well is determined by the longitudinal part of the incident electron energy.

Since the longitudinal modes are separated, we shall consider the propagation of an arbitrary mode (but such that $q_n^2 > 0$). The approximate basic solutions of equation (17) obviously (from (14) and (15)) have the form

$$
F_n^{\pm}(0 \mid u) \simeq \exp\left(\pm\mathrm{i}\frac{q_n}{\varepsilon} \int_0^u \mathrm{d}\xi\,[1 + \tfrac{1}{2}\varepsilon a(\xi)] \right) \qquad q_n^2 > 0. \tag{18}
$$

By certain superpositions of these two solutions any precise solution both for the channel input and for the channel output can be approached with asymptotic precision. The scattering problem under consideration consists indeed in establishing the correspondence between asymptotics such as the incident $F_n^+(0 \mid u)$ and the reflected $F_n^-(0 \mid u)$ waves for the input and asymptotics such as the outgoing $F_n^+(0 \mid u)$ wave for the output. Unlike precise solutions where input and output asymptotics are correlated automatically, such correlation is a specific problem for semi-classical solutions [12–14] because in the complex plane near roots of the equation

$$1 + \tfrac{1}{2}\varepsilon a(z) = 0 \tag{19}$$

the basic solutions (18) become invalid. The problem is complicated by the proximity of the roots of equation (19) to those of the equation

$$1/a(z) = 0 \tag{20}$$

(i.e. to the poles of the function $a(z)$); thus using the standard Zwaan approach [12, 13] appears to be impossible. In this case the most suitable approach is that of Pokrovskiy and Khalatnikov [14] dealing with the agreement of the input and output asymptotics in the complex plane on the anti-Stokes line

$$\mathrm{Im}\left(\int_{z_0}^{z} \mathrm{d}\zeta[1 + \tfrac{1}{2}\varepsilon a(\zeta)]\right) = 0. \tag{21}$$

Here z_0 is the root of equation (19) nearest to the real axis (further let $\mathrm{Im}\, z_0 > 0$). The essence of the above concordance consists in joining the input and output asymptotics with suitable (exact at the point Z_0) solutions of the one-mode equation (17).

Let us consider the case, which is most important from the physical point of view, when the pairing roots z_0 and z_p of equations (19) and (20) nearest to the real axis are far from the other pairing roots. Then, near the points z_0 and z_p,

$$1 + \tfrac{1}{2}\varepsilon a(z) \simeq k\frac{z - z_0}{z - z_p} \qquad (\mathrm{Im}\, z_0 > \mathrm{Im}\, z_p). \tag{22}$$

Therefore, after the replacement

$$\zeta = -2\mathrm{i}k(q_n/\varepsilon)(z - z_p) \qquad \lambda = -\mathrm{i}(q_n/\varepsilon)(z_0 - z_p) \tag{23}$$

the one-mode equation (17) is reduced to the standard Whittaker equation [15]

$$\mathrm{d}^2 F_n/\mathrm{d}\zeta^2 + (-\tfrac{1}{4} + \lambda/\zeta)F_n = 0. \tag{24}$$

The constant k is close to unity and, for example in the case of a symmetrically bent channel (4), has the form

$$k = 1 - \tfrac{1}{4}\varepsilon \operatorname{cotan} \beta \qquad \varepsilon < \beta < \tfrac{1}{2}\pi - \varepsilon. \tag{25}$$

For unambiguous interpretation of the fundamental solutions $W_{\lambda 1/2}(\zeta)$ and $W_{-\lambda 1/2}(\zeta \exp(\pm \mathrm{i}\pi))$ of the equation obtained (equation (24)) we make a vertical cut in the complex plane upwards from the point z_p so that $\arg \zeta = 0$ on the right-hand bank and $\arg \zeta = -2\pi$ on the left-hand bank. Then with the aid of the asymptotics [15]

$$W_{\mu\nu}(z) \simeq \exp(-\tfrac{1}{2}z + \mu \ln z) \qquad |z| \gg 1, |\arg z| < \pi \tag{26}$$

we find that to the right of z_0 on the anti-Stokes line the solution $W_{\lambda 1/2}(\zeta)$ transforms into the outgoing wave

$$W_{\lambda 1/2}(\zeta) \to F_n^+(z_0 \mid z) \exp(\lambda \ln(2\lambda/e)). \tag{27}$$

Applying additionally the property [15]

$$W_{\lambda 1/2}(\zeta) = \exp(-2\mathrm{i}\pi\lambda) W_{\lambda 1/2}(\zeta \exp(2\mathrm{i}\pi)) - \frac{2\mathrm{i}\pi \exp(-\mathrm{i}\pi\lambda)}{\Gamma(1-\lambda)\Gamma(-\lambda)} W_{-\lambda 1/2}(\zeta \exp(\mathrm{i}\pi)) \tag{28}$$

side by side with the asymptotics (26) we see that to the left of z_0 on the anti-Stokes line the solution $W_{\lambda 1/2}(\zeta)$ changes into the desired superposition of the incident and reflected waves

$$\begin{aligned} W_{\lambda 1/2}(\zeta) \to F_n^+(-\infty \mid z) F_n^+(z_0 \mid -\infty) \exp\left[\lambda \ln\left(\frac{2\lambda}{e}\right)\right] - F_n^-(-\infty \mid z) F_n^-(z_0 \mid -\infty) \\ \times \exp\left[-\lambda \ln\left(\frac{2\lambda}{e}\right)\right] \frac{2\mathrm{i}\pi \exp(-2\mathrm{i}\pi\lambda)}{\Gamma(1-\lambda)\Gamma(-\lambda)}. \end{aligned} \tag{29}$$

The solutions for the input and output of the channel are correlated in such a way that asymptotics typical of the scattering problem are obtained. Hence, the modulus square of the ratio of the coefficient of the reflected wave to that of the incident wave gives the reflection coefficient

$$\begin{aligned} R_n = \left(\frac{2}{\pi}\right)^2 \Gamma^4(\lambda+1) \frac{\sin^4(\pi\lambda)}{\lambda^2} \exp\left[-4\lambda \ln\left(\frac{2\lambda}{e}\right)\right] \\ \times \exp\left[-4\frac{q_n}{\varepsilon} \operatorname{Im}\left(\int_{-\infty}^{z_0} \mathrm{d}\xi \, [1 + \tfrac{1}{2}\varepsilon a(\xi)]\right)\right] \qquad q_n^2 > 0. \end{aligned} \tag{30}$$

It should be emphasized that here (contrary to the case of the potential barrier [14]) $\operatorname{Re}\lambda > 0$, and therefore the reflection coefficient R_n is the oscillatory function of λ. This situation is typical for potential wells with varying depth and/or a width when the reflection coefficient can repeatedly go to zero [16]. Analogy with the non-reflecting potential can easily be seen in the case of a channel such as a symmetric bend because then

$$\lambda \equiv -\mathrm{i}(q_n/\varepsilon)(z_0 - z_p) \simeq q_n/4\cos\beta \tag{31}$$

and the longitudinal momentum q_n, as it is known, regulates the depth of the effective potential well. In general, non-monotonic dependence of the reflection coefficient on the momentum is also known in the problem of one-dimensional scattering by the square well potential [16] but there it has a distinct nature. Using the general formula (30) for the channel such as the symmetric bend (4) with a precision that keeps the basic qualitative effects gives

$$R_n \simeq \left(\frac{q_n + 4\cos\beta}{q_n}\right)^2 \sin^4\left(\frac{\pi q_n}{4\cos\beta}\right) \exp\left(-4\frac{q_n}{\varepsilon}\frac{\frac{1}{2}\pi - \beta}{\sin(\frac{1}{2}\pi - \beta)}\right). \tag{32}$$

This relation is true for channels bent within the angles $\varepsilon < \beta < \frac{1}{2}\pi - \varepsilon$ when the roots $z_0 \approx \mathrm{i}(\frac{1}{2}\pi - \beta + \frac{1}{4}\varepsilon)/\cos\beta$ and $z_p = \mathrm{i}(\frac{1}{2}\pi - \beta)/\cos\beta$ are far from other roots of equations (19) and (20). These moderately bent channels, unlike the very straight $\beta < \varepsilon$ and the very bent $\frac{1}{2}\pi - \varepsilon < \beta < \frac{1}{2}\pi$ channels, are the most applicable for practical use.

Considering R_n as a function of incident electron momentum q_n, one can see that with increasing q_n together with the periodicity of the reflection coefficient an exponential decrease in its local maxima also takes place. It should be noted that, at the right-angle bend $\beta = \frac{1}{4}\pi$, one of the minima of the reflection coefficient (namely $q_{n\,\mathrm{min}} = 4\sqrt{2}$) coincides with one of the minima in the paper by Lent [8], although this comparison is not quite justified because of the essential difference in the situations under consideration (in our case $\varepsilon \ll 1$ and in Lent's paper $\varepsilon \gtrsim 1$).

Generally, the dependence of R_n on the angle β of channel bending is also oscillatory but with increasing β the local maxima of reflection coefficient also increase.

It should be mentioned that the classical analogue of the scattering problem considered above leads to channel non-reflectability independently of the ratio d/L as well as the bending angle 2β. This can be understood in the framework of a simple geometrical billiards-like treatment of a point particle in a channel with rigid walls. However, we would prefer here an analytical explanation based on the Lagrangian

$$\mathcal{L} = \tfrac{1}{2}m(\dot{\rho}^2 + g_{ss}\dot{s}^2) - V(\rho) \qquad V(\rho) \equiv \frac{\hbar^2}{2md^2}U\left(\frac{\rho}{d}\right) \tag{33}$$

of the classical particle under study. The corresponding Lagrange equations in terms of the longitudinal velocity component $\mathrm{v}_s = \sqrt{g_{ss}}\dot{s}$ and the transverse velocity components $\mathrm{v}_\rho = \dot{\rho}$ are as follows:

$$\begin{aligned} &\dot{\mathrm{v}}_s + \frac{\mathrm{v}_s \mathrm{v}_\rho}{L(s,\rho)} = 0 \\ &\dot{\mathrm{v}}_\rho + \frac{1}{m}\frac{\partial V(\rho)}{\partial \rho} - \frac{\mathrm{v}_s^2}{L(s,\rho)} = 0 \end{aligned} \tag{34}$$

where

$$L(s,\rho) \equiv \rho + L/a(s/L). \tag{35}$$

Rewriting the first of these equations in the form

$$\mathrm{v}_s(t) = \mathrm{v}_s(t_0)\exp\left(-\int_{t_0}^{t}\frac{\mathrm{d}\xi\,\mathrm{v}_\rho(\xi)}{L(s(\xi),\rho(\xi))}\right) \tag{36}$$

we come to the straightforward conclusion that the s-independent potential $V(\rho)$ of walls is incapable of changing the sign of the particle's longitudinal velocity. As a result the reflection coefficient of a collection of classical point particles should be equal to zero.

Returning to the quantum scattering problem it is appropriate to point out that the coefficients of electron reflection may be explicitly connected with the conductance G, which is the experimentally observable quantity. For example, if we choose the external 'wire' to be a perfect conductor, a two-terminal conductance at vanishing bias and temperature is evaluated using the linear conductance formula [17–19]

$$G = \frac{e^2}{\pi\hbar}\sum_{nm} T_{nm}\left(\frac{2md^2E_{\mathrm{F}}}{\hbar^2}\right) \tag{37}$$

where E_F is the Fermi energy and the sum runs over the propagating modes, since evanescent modes do not contribute to the current in an infinite channel. The transition coefficients $T_{nm}(\mathcal{E})$ in our case are as follows:

$$T_{nm}(\mathcal{E}) = (1 - R_n)\theta(q_n^2)\delta_{nm} \tag{38}$$

so that the quantities R_n are responsible for the deflection of the conductance $2md^2E_F/\hbar^2$-dependence from a perfect staircase-like shape. For channels with a large d/L-ratio this effect should undoubtedly be more clearly observable. As the bending angle 2β tends to zero, the above-mentioned deflection becomes negligible.

Another kind of imperfection in the conductance staircase-like $2md^2E_F/\hbar^2$-dependence may, for example, be caused by the finiteness of the channel [20].

In conclusion we recall that the basic formula for the reflection coefficient (30) is obtained under a sufficiently general assumption about the form of the quantum channel bend. The specific character of the concrete channel is determined by the form of function of its bend $a(u)$ and the roots of equations (19) and (20) associated with this function.

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