An explicit model for a quantum channel in 2DEG

VALERI A. FEDIRKO[†], MEI-HSIN CHEN, CHIUNG-CHUAN CHIU, SHI-FONG CHEN,
KAUNG-HSIUNG WU, JENH-YIH JUANG, TZENG-MING UEN, YI-SHUN GOU

Department of Electrophysics, National Chiao Tung University, Hsinchu, Taiwan 30010, Republic of China

A two-parametric model for a channel in a two-dimensional electron gas (2DEG) is proposed which allows for the explicit analytical solution for the problem of quantum electron transport through the constriction. Conductance step smearing appears naturally and a simple criterion for the step occurrence in terms of channel parameters is given.

Key words: quantum electron transport, quantum constriction, conductance quantization, two-dimensional electron gas.

1. Introduction

An interest has persistently been growing in micro- and nano-structures in which an electron can move ballistically through some active region [1]. Quantization of the conductance of a narrow ballistic channel in a two-dimensional electron gas (2DEG) by $G_0 = 2e^2/h$, first discovered by van Wees *et al.* [2] and Wharam *et al.* [3], is, perhaps, one of the most exciting phenomena which can be realized in such structures. Moreover, the differential conductance may also be quantized in such structures as a function of applied bias [4, 5]. Though the principal physical reason for the quantization effects has been clear since the earliest works [2–5], various theoretical approaches have been exploited for treating the problem (see, e.g. [6–23]). Smooth [6–9, 17, 18] and abruptly [10–15] changing channel boundaries were assumed and some channel wall roughness [20, 21] was taken into account. The differential conductance quantization and other effects of non-zero bias [4, 5, 19, 22, 23] were described.

The so-called 'adiabatic' approximation based on the Born–Oppenheimer approach [23] for a hard-wall smooth channel [6–9] is, perhaps, one of the most developed and widely used. Nevertheless no explicit model of a constricting quantum channel has yet been analysed which allows for an exact analytical adiabatic solution for electron quantum transmission. Such a model however, though not a general one in itself, could permit a good physical insight and provide physical criteria for experimental observation of quantization effects in terms of model structure parameters.[1] It is useful for experimental structure evaluation and for experimental data analysis and can be easily generalized. In this paper we propose and analyse a two-parametric model of that kind.

[†]Permanent address: Moscow State University of Technology "Stankin", Moscow 101472, Russia.

[1]Actually, an attempt of that kind was undertaken in [17] but a parabolic potential used there can hardly be brought into correspondence to some real structure and is in fact only an approximation near the bottleneck.
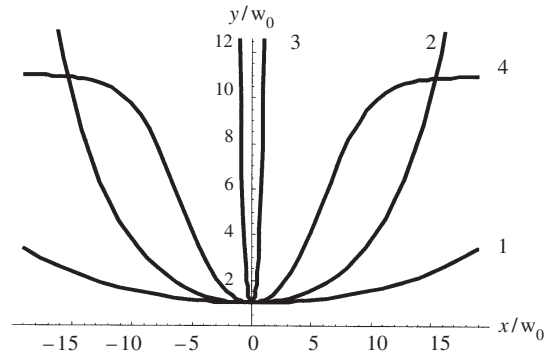
Fig. 1. Schematic picture of model channel boundaries for various values of dimensionless parameter (βw_0): (1) $\beta w_0 = 0.1$; (2) $\beta w_0 = 0.2$; (3) $\beta w_0 = \pi$; (4) boundary defined by ($1'$) for $\beta w_0 = 0.5$, $W/w_0 = 10$.

2. Model

One needs at least two parameters as a minimum set to describe a constricting channel, i.e. the bottleneck width, w_0, and the characteristic channel length, l. Assuming that the 2DEG leads to the channel lies far away from its bottleneck at a distance much longer than l and is much wider than w_0 one can consider a channel, which is broadening smoothly from the bottleneck to infinite 2DEG reservoirs. For a stiff-wall channel model one thus has to find a proper and convenient two-parametric function $y = f(x)$ for an x-dependent channel border, where x is the coordinate along the channel and y is in the perpendicular direction to the plane of the 2DEG sheet. We put $f(x) = 0$ for one border, while for the other we choose $f(x)$ in the form

$$f(x) = w_0 \cdot \cosh(\beta x), \tag{1}$$

which, as one shall see, allows for an exact analytical adiabatic solution for the scattering problem of quantum electron transmission throughout the channel. For such borders the variable width of a channel is:

$$w(x) = w_0 \cdot \cosh(\beta x). \tag{2}$$

Channel boundaries described by eqn (1) are drawn schematically in Fig. 1 for various values of dimensionless parameter βw_0. One can easily see that when $\beta w_0 \ll 1$ we have a *long* channel, while for $\beta w_0 \gg 1$ we have a *short* one. Varying parameters β and w_0 one can adjust such a model channel very close to a number of experimental structures. It is also worth mentioning that the same parameter β^{-1} determines the spatial scale of channel boundary variation so β can be considered as an inverse characteristic length of the channel:

$$\beta \sim l^{-1}.$$

The symmetric channel with boundaries $|y| = f(x)$ can obviously be treated in the same way.

For a particular (usually the lowest) two-dimensional (2D) subband the problem of electron transmission through a stiff-wall channel is that of a solution of a 2D Schrödinger equation for stationary states with zero boundary condition at the channel walls and finite asymptotic at infinity for wavefunction $\Phi(x, y)$

$$\frac{\hbar^2}{2m}\frac{d^2\Phi}{dx^2} + \frac{\hbar^2}{2m}\frac{d^2\Phi}{dy^2} = E\Phi,$$
$$\Phi(x, y = 0) = 0, \qquad \Phi(x, y = f(x)) = 0, \tag{3}$$

where the energy E is measured relative to the edge of the 2D subband. In the adiabatic approximation [6–9, 20] one searches for a stationary solution of (3) as a product

$$\Phi(x, y) = \psi(x)\,\phi(x, y), \tag{4}$$

assuming that $\phi(x, y)$ satisfies the equation

$$\frac{\hbar^2}{2m}\frac{\partial^2\phi}{dx^2} + \frac{\hbar^2}{2m}\frac{\partial^2\phi}{dy^2} + \varepsilon(x)\phi = 0, \tag{5}$$

with the boundary conditions

$$\phi(x, y = 0) = \phi(x, y = f(x)) = 0, \tag{5'}$$

where x is considered as a parameter, but not as a variable.

For that one easily finds a discrete spectrum

$$\varepsilon(x) = \varepsilon_n(x) = \frac{\pi^2 n^2}{w^2(x)}, \tag{6}$$

with

$$\phi(x, y) = \sqrt{\frac{2}{w(x)}}\sin\frac{\pi n}{w(x)}y, \tag{7}$$

and $n = 1, 2, \ldots$ being a transverse mode quantum number.

Substituting (4), (6), (7) into eqn (3) and neglecting slowly ('adiabatically') varying terms [6–9, 20] one finds the one-dimensional (1D) Schrödinger-like equation for a single nth mode wavefunction $\psi_n(x)$ of electron motion along the channel in the effective quasi-potential $\varepsilon_n(x)$:

$$\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} + [E - \varepsilon_n(x)]\psi_n = 0. \tag{8}$$

Transitions between transverse modes are not thus taken into account by the adiabatic approximation.

Intermode scattering breaks the adiabatic approximation when a channel is not smooth enough [6]. However intermode scattering results in a change of a longitudinal momentum of the order of $\pi/w(x)$ for a constant energy, so it is essential only when the spatial scale of channel boundary variation is of the order of $w(x)/\pi$. The latter can be locally characterized by a logarithmic derivative $w'(x)/w(x)$ which for a model under consideration is:

$$w'(x)/w(x) = \beta \cdot \tanh(\beta x).$$

When the dimensionless parameter

$$\lambda^{-1} = \beta w/\pi < 1, \tag{9}$$

intermode scattering is negligible in the region

$$|x| < \beta^{-1}\ln\lambda$$

unless a ballistic regime holds.[1] That is a condition for *local adiabacity* in the vicinity of the bottleneck. However, when λ^{-1} is small (i.e. a *long* channel), one has

$$\beta^{-1}\ln\lambda > 1,$$

so such a channel can be considered as adiabatic at the length longer than its characteristic length, l, i.e. almost '*globally*' adiabatic [8].

Equation (1) may look unsatisfactory because the width of the channel becomes infinite when x tends to infinity. To limit the channel width by some finite value and to formally include into the model the leads of the width $\sim W \gg w_0$ at $x \to \infty$ one can use, for example

$$f(x) = (1 + w_0/W)\frac{w_0\cosh(\beta x)}{1 + (w_0/W)\cosh(\beta x)} \tag{1'}$$

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[1] Adiabatic approximation fails near turning points, however the asymptotic results hold.
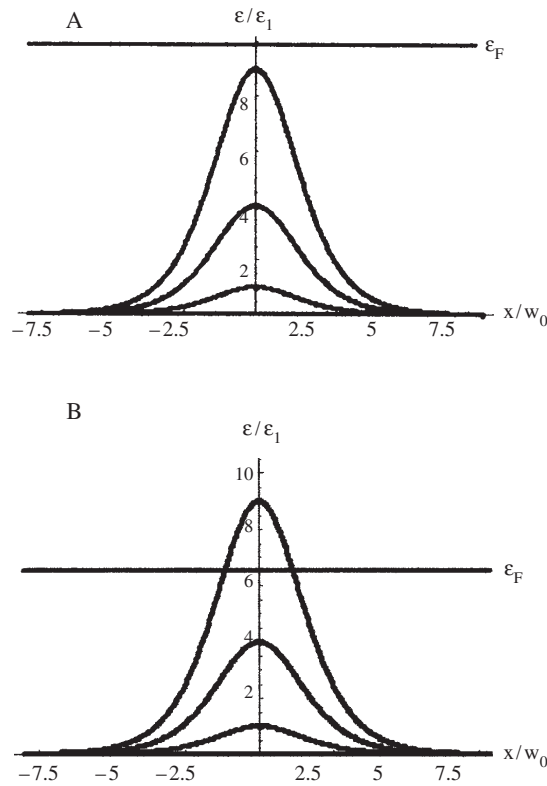
Fig. 2. Effective quasi-potential $\varepsilon_n(x)$ for the first three transversal modes ($n = 1, 2, 3$): A $\lambda = 2\pi$; B $\lambda = 3\pi$; Fermi-energy, ε_F is shown in A and B for the same value of $(k_F/\beta) = 2\pi$.

instead of (1). We show a channel boundary (1′) in Fig. 1 for illustration. The channel length can then be estimated as $L \approx l \ln(W/w_0)$. It, however, has no effect on electron transmission through the channel when $L \gg l$ so eqns (6)–(8) with $w(x)$ in the form of (2) are valid anyway. Yet this may be useful, say, for transversal mode counting.

3. Results and discussion

The problem of electron transmission through a constricted channel is thus reduced to a 1D scattering problem with a potential barrier $\varepsilon_n(x)$. When the channel width $w(x)$ is given by formula (2), eqn (8) leads to the following equation

$$\psi'' + \left(k^2 + \frac{\beta^2\lambda^2 n^2}{\cosh^2 \beta x}\right)\psi = 0, \tag{10}$$

where we put

$$E = \frac{\hbar^2 k^2}{2m} \tag{10′}$$

and λ is defined by (9). Equation (10) is similar to that considered by Pöschel and Teller [24]. The effective quasi-potential $\varepsilon_n(x)$ for the first three modes ($n = 1, 2, 3$) is shown in Fig. 2 for two values of parameter λ: $\lambda = 2\pi$ and $\lambda = 3\pi$.

With the substitution

$$\psi = \cosh^s(\beta x)\, u,$$

where

$$s(s-1) = \lambda^2 n^2, \qquad s = \tfrac{1}{2}\big(1 + i\sqrt{4\lambda^2 n^2 - 1}\big),$$

eqn (10), by introducing the new variable $z = \sinh^2(\beta x)$, is reduced to a hypergeometric equation (see, e.g. [25])

$$z(1-z)u'' + [c - (a+b+1)z]u' - abu = 0, \tag{11}$$

with $a = (s + i\kappa)/2$, $b = (s - i\kappa)/2$, $c = 1/2$, $\kappa = k/\beta$. As follows from (11) the general solution of eqn (10) is of the form

$$\psi = C_1\psi_1 + C_2\psi_2, \tag{12}$$

where

$$\psi_1 = \cosh^s(\beta x) \cdot {}_2F_1(a, b; 1/2; -\sinh^2(\beta x)),$$
$$\psi_2 = \cosh^s(\beta x) \cdot \sinh(\beta x) \cdot {}_2F_1(a + 1/2, b + 1/2; 3/2; -\sinh^2(\beta x)),$$

${}_2F_1$ being the hypergeometric function of corresponding arguments, and C_1 and C_2 are arbitrary constants. So, one can find the exact analytical solution of eqn (10).

To solve the scattering problem one should match the general solution (12) to the boundary conditions at $x = \pm\infty$

$$\psi(x)_{x\to\infty} = e^{ikx} + re^{-ikx}, \quad \psi(x)_{x\to-\infty} = te^{ikx},$$

where r and t are the reflection and transmission amplitude, respectively. That can easily be done using the asymptotic expansion for the hypergeometric function, which leads to the known expression for the transmission coefficient $T = |t|^2$ (see, e.g. [26]) for the nth transversal mode:

$$T_n(k) = \frac{\sinh^2(\pi k/\beta)}{\sinh^2(\pi k/\beta) + \cosh^2\big(\pi\sqrt{4\lambda^2 n^2 - 1/2}\big)}. \tag{13}$$

The reflection coefficient is found immediately as $R = |r|^2 = 1 - T$.

For the above scattering problem we also find the coefficients C_1 and C_2 as

$$C_1 = \frac{\Gamma\big(\tfrac{1}{4} - \tfrac{i}{2}\gamma_-\big)\Gamma\big(\tfrac{1}{4} - \tfrac{i}{2}\gamma_+\big)}{2\Gamma(1/2)\Gamma(-i\kappa)e^{i\kappa \ln 2}}, \qquad C_2 = -\frac{\Gamma\big(\tfrac{3}{4} - \tfrac{i}{2}\gamma_-\big)\Gamma\big(\tfrac{3}{4} - \tfrac{i}{2}\gamma_+\big)}{2\Gamma(3/2)\Gamma(-i\kappa)e^{i\kappa \ln 2}} \tag{14}$$

for any n, where Γ is the gamma function of corresponding argument and we introduce the notations $\gamma_\pm = \kappa \pm \delta$, $\delta = \sqrt{4\lambda^2 n^2 - 1/2}$. Formulae (13) and (14) give full analytical solution of the problem.

For $\kappa, \delta \gg 1$ the transmission coefficient T for any n can be approximated by the simplified expression:

$$T_n = \frac{1}{1 + \cosh^2 \pi\delta/\sinh^2 \pi\kappa} \approx \frac{1}{1 + e^{2\pi(\delta - \kappa)}}. \tag{15}$$

When $\lambda > 1$, $\delta \approx \lambda n$, so

$$\kappa - \delta \approx \left(k - \frac{\pi n}{w_0}\right)\Big/\beta,$$

and eqn (15) shows that T_n are step-like functions of a variable

$$\xi_n = (kw_0/\pi - n)/\beta$$

with a step-smearing width of the order of $\beta w_0/\pi^2 = 1/\pi\lambda$. Steps are thus well-defined for the parameter of eqn (9), $\lambda \geq 1$. Transmission coefficients T_n for some n calculated numerically as a function of ξ at
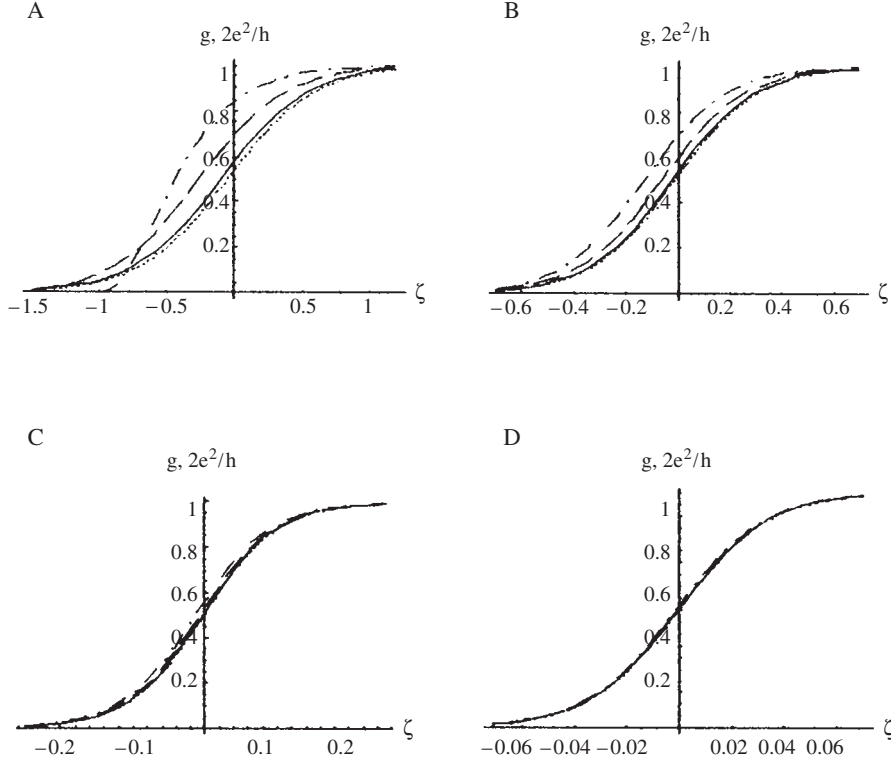
Fig. 3. Dependence of the transmission coefficient T_n on electron energy through the variable $\xi_n = (kw_0/\pi - n)/\beta$ for various values of parameter λ: A $\lambda = 0.5$; B $\lambda = 1$; C $\lambda = \pi$; D $\lambda = 3\pi$; dash-dot line—$n = 1$; dashed line—$n = 2$; solid line—$n = 5$; dotted line—$n = 10$.

various values of parameter λ are plotted in Fig. 3 (due to eqn (10′) this is, in fact, T_n dependence on electron energy). One can see that when $\lambda > 1$ they have a sharp enough stepwise shape, and the step smearing is still less than 1 even for $\lambda = 1$, but it becomes more than 1 when $\lambda = 0.5$. Step smearing is consistent with estimation (15). For $\lambda \leq 1$ the form of a step changes drastically with the mode number, n, but for a few lowest modes only. For $\lambda \geq 1$ the form of a step only slightly depends on a mode number even for low n and this dependence tends to vanish when λ increases.

With the help of eqn (13) one can estimate the ballistic conductance G of a quantum channel in a degenerate 2DEG of geometry (1) at the low temperature limit as

$$G = \frac{e^2}{\pi \hbar} \sum_{n=1}^{\infty} T_n(k_F), \tag{16}$$

where k_F is the Fermi wave-number of 2DEG in the leads (see, e.g. [27]).

In Fig. 4 we present the conductance G, calculated numerically in accordance with (16), as a function of a variable $\xi = (k_F w_0/\pi)$ for a set of values of parameter λ. We sum as many terms $K \gg \xi$ in (16) as necessary to reach the smallest estimated error due to the summation of a finite number of terms for all values of the variable ξ under consideration.

One can see that the step-like dependence of G on ξ survives even when $\lambda = 1$ but only a few (two to three) first steps are apparent enough. However step structure is obviously absent at $\lambda = 0.5$. For $\lambda > \pi$ conductance steps show no marked dependence on the step number up to quite a high number of steps.
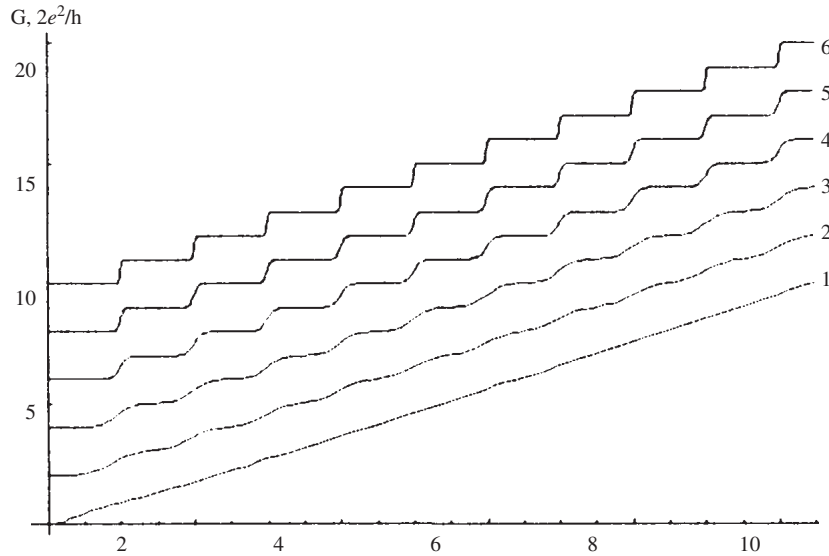
Fig. 4. Conductance, G, of a channel calculated numerically as a function of a variable $\xi = (k_F w_0/\pi)$ for a set of values of parameter λ: (1) $\lambda = 0.5$; (2) $\lambda = 1$; (3) $\lambda = 1.5$; (4) $\lambda = \pi$; (5) $\lambda = 2\pi$; (6) $\lambda = 5\pi$. (Every subsequent curve is shifted up by 1 for clarity).

Actually our calculations show that $N \geq 20$ steps are perfectly apparent, almost without smearing, say, for $\lambda = 2\pi$, i.e. $\beta w_0 = 0.5$. It evidently indicates out that if considerable step smearing, as well as higher order step smearing, is observed in a long smooth channel it likely results from some other reason, probably from scattering by channel wall roughness [20, 21]. The above results, therefore, enable one to evaluate the 'quality' of a channel.

At $\xi < 1$ no free propagating mode exists and the contact behaves as a peculiar tunnelling junction. When $\lambda > 1$ its conductance for the values of ξ not very close to 1 can be estimated in accordance with (15) as:

$$G \approx \frac{e^{2\pi\lambda(\xi-1)}}{1 - e^{-2\pi\lambda}}.$$

It decays exponentially with $k_F w_0$ decreasing as seen in Fig. 5A where some numerical results are presented for a low-mode channel. Low modes dominate the contact conductance if $\lambda \gg 1$ but for smaller λ higher modes contribute significantly due to tunnelling through the quasi-potential barrier. If, e.g. $\lambda = \pi$ one can see at Fig. 5A (2) that $G \approx 0.1$ even when ξ is as small as 0.8.

When $\xi < 2$ a particular case of a single-mode channel is realized. Nevertheless the higher modes may as well contribute significantly to contact conductance by tunnelling through the quasi-potential barrier if λ is not very large. This is well illustrated in Fig. 5A where the first transmission coefficient T_1 is shown in comparison with the whole conductance and with the contribution of higher modes.

In Fig. 5B the conductance of a contact with two propagating modes compared to the contribution of higher modes is shown for various λ which demonstrate typical features for a channel with more propagating modes. Tunnelling modes contribute near the step points $\xi = m$. If $\lambda \approx 2\pi$ their contribution is substantial far enough from the step point, i.e. at $(\xi - m) \sim \pm 1$. For smaller values of λ the contribution of tunnelling modes, with $n > m$, to the channel conductance at $(m - 1) < \xi < m$ is comparable with that of propagating modes, and steps are smeared markedly. When $\lambda > 3\pi$ the conductance for $\xi < m$ is determined mostly by T_n with $n < m$, except for the small vicinity just near the mth step point and step smearing is small, which means that only propagating modes actually contribute to the conductance when parameter λ is large enough.
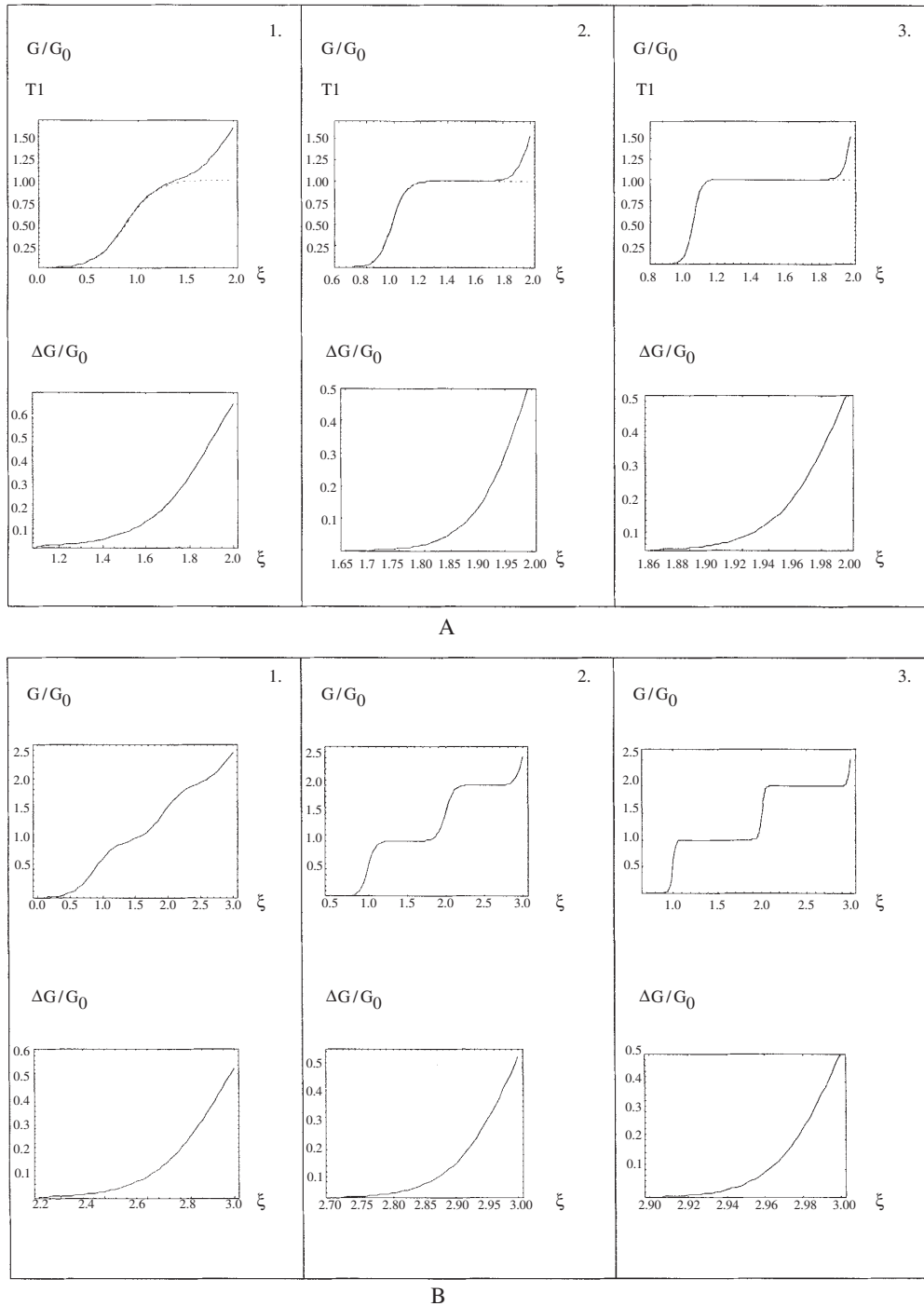
Fig. 5. A Conductance, G, of a contact with none and single propagating mode calculated numerically; also the transmittance T_1 for the lowest mode and the contribution of higher ($n \geq 2$) modes, $\Delta G^{(2)}$ are shown for comparison; G—solid line, T_1—dashed line; B conductance, G, of a contact for the two lowest propagating modes compared to the contribution of higher ($n \geq 3$) modes, $\Delta G^{(3)}$; (1) $\lambda = 1$, (2) $\lambda = \pi$, (3) $\lambda = 3\pi$.

We also draw attention to the fact that at the step points ($\xi = m$) the tunnelling component contribute about $0.5G_0$.

When $\lambda \gg 1$ for $\xi < (m+1)$ far enough from the $(m+1)$th step their contribution can be estimated, using (15), as:

$$\sum_{n=m}^{\infty} T_n(k_F) \approx \frac{e^{2\pi\lambda(\xi-m-1)}}{1 - e^{-2\pi\lambda}}.$$

With the help of (13), (15) one can also estimate the differential conductance of a long channel under some, not very high, bias, V, between the 2DEG reservoirs. There are reasons to believe that in a long narrow channel the electric potential varies monotonously along the x-axis (see also [28]). In that case the approach developed in [4, 21] can be applied using T_n given by eqns (13), (15) instead of the step-like transmission coefficient used in [4, 21]. Assuming that a bias is small enough so one can neglect the change of quasi-potential, we find for the current, I, through a channel

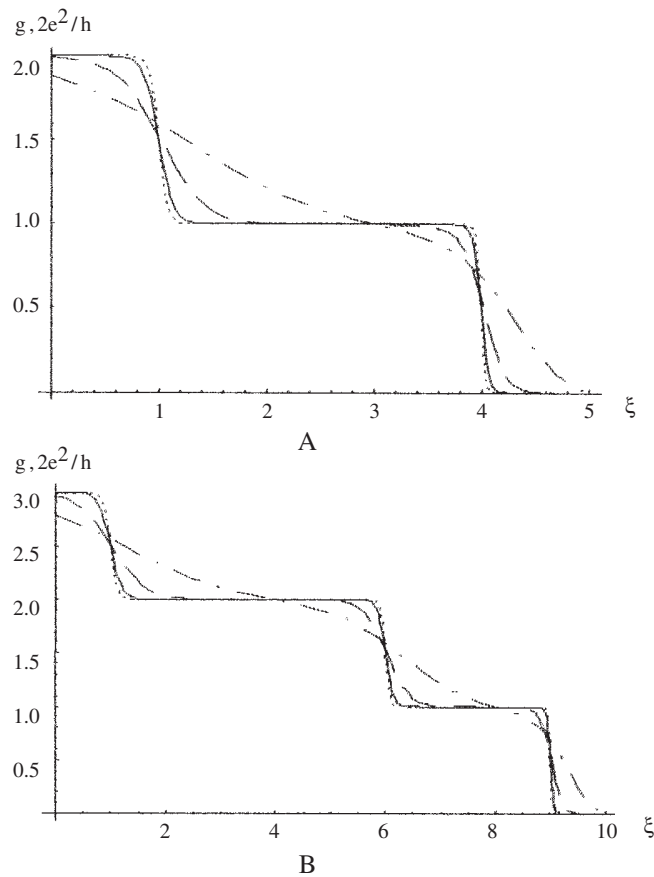$$I = \frac{e}{\pi\hbar} \int_{\varepsilon_F - eV}^{\varepsilon_F} T(E) \, dE, \tag{17}$$

Fig. 6. Low bias voltage dependence of differential conductance, g, of a long narrow channel with m propagating modes: A $m = 2$; B $m = 3$; (1) $\lambda = 1$; (2) $\lambda = \pi$; (3) $\lambda = 3\pi$; (4) $\lambda = 5\pi$.

where:

$$T(E) = \sum_{n=1}^{\infty} T_n(k), \quad E = \frac{\hbar^2 k^2}{2m}.$$

Differential conductance, $g(V) = dI/dV$, then is:

$$g = \frac{e^2}{\pi \hbar} T(\varepsilon_F - eV). \tag{18}$$

Bias dependence of the differential conductance of a narrow channel with only a few, m, propagating modes calculated for various values of λ is shown in Fig. 6. It decreases step-like with increasing bias at [4, 21]

$$V \approx \frac{\varepsilon_F - \varepsilon_n(0)}{e}, \quad n = m, m-1, m-2, \dots, 1 \tag{19}$$

that is a particular feature of 1D flow. The channel reaches its 'saturated' regime when:

$$V > V_m = \frac{\varepsilon_F - \varepsilon_1(0)}{e}. \tag{20}$$

Nevertheless the differential conductance never reaches zero due to higher modes tunnelling. The steps are quite sharp when $\lambda \geq 3\pi$, smear vastly for smaller λ, and disappear when $\lambda \leq 1$.

We should emphasize that the above approach is valid for a *long channel* and for quite *low bias*. It means that the step-wise voltage dependence and saturation of differential conductance can be observed in a long channel with only a few propagating modes, when V_m is *not very high*. For higher bias and for a short channel the potential distribution along the channel should be considered more carefully. We found earlier that space-charge effects at the mouths of a channel became essential at higher bias [21, 22] and results in substantial non-zero differential conductivity at $V > V_m$. So some background is actually always present resulting in non-zero differential conductance at a bias V higher than V_m, and the higher is V_m, the more pronounced are the background effects. Voltage dependence of a conductance for a short channel was estimated in [18, 19, 21, 22] and the results also differ markedly from those given by formulae (18)–(20).

4. Summary

In this paper we consider the problem of electron transport through a constricted quantum channel in a 2DEG. We propose and analyse a convenient two-parametric model for such a channel, which allows for an analytical solution of the scattering problem in the adiabatic approximation. Conditions for observation of channel conductance quantum steps and step-like differential conductance dependence on bias voltage are expressed in terms of model parameters. We found that intrinsic smearing of the quantum steps is not crucial for even quite a short channel—almost up to the limit of adiabatic approximation. The model, by fitting of the parameters, can be used for a good variety of experimental structures, and thus enables one to estimate the quality of a channel and to analyse experimental data.

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