IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Theory of electron injection into one-dimensional conductors

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1989 J. Phys.: Condens. Matter 1 305

(http://iopscience.iop.org/0953-8984/1/1/026)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.89
The article was downloaded on 10/05/2010 at 15:54

Please note that terms and conditions apply.

J. Phys. Condens. Matter 1 (1989) 305–309. Printed in the UK

LETTER TO THE EDITOR

Theory of electron injection into one-dimensional conductors

George Kirczenow
Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada, V5A 1S6

Received 10 October 1988

Abstract. A quantum theory of electron injection from a reservoir of higher dimension into a semi-infinite one-dimensional (1D) conductor is presented. Numerical results are given for simple models of narrow quantum channels in semiconductor heterostructures. It is shown that the injection process can strongly influence experimentally measured 1D conductances in ballistic or near-ballistic regimes. It should contribute in a major way to the observed deviations from perfect quantisation of the 1D ballistic conductance. The possibility of resonances in the conductance of finite channels is briefly discussed.

In recent years considerable interest has focused on one-dimensional (1D) electrical conduction in a variety of physical systems (see Landauer 1985, Imry 1986, Stone and Szafer 1988 for reviews). In most cases the transport being considered was controlled by scattering within the 1D system. Because of this the quantum mechanics of electron injection from the physical reservoirs of higher dimensionality into the 1D channel received scant attention, although the fundamental role of this process in 1D transport experiments was not unrecognised. The remarkable, recent experimental studies of ballistic 1D electrical conduction by van Wees *et al* (1988) and by Wharam *et al* (1988), where electrons were *not* scattered within the 1D channel, raise the possibility of studying this injection process in some detail. In this Letter a theory of the injection process is presented which makes it possible to calculate its effects on the conductance of some simple models of ballistic 1D channels. Numerical results are obtained which suggest that the injection and emission processes should be a major source of the experimentally observed deviations from perfect quantisation of the 1D ballistic conductance. No satisfactory explanation of these deviations has previously been proposed.

Perhaps the simplest way to understand the experimentally observed quantisation of the 1D ballistic conductance is in terms of a Landauer-type argument (van Wees *et al* 1988, Wharam *et al* 1988). Its essentials can be summarised briefly as follows. Consider a ballistic channel running from left to right whose electronic structure can be described in terms of a set of 1D sub-bands labelled by an index n and having an energy dispersion ε_{kn}. Assume, for the moment, that the sub-band states in which the electrons are moving to the left are filled up to an energy E and those moving to the right are filled to an energy $E + eV$, where V is the (small) potential difference across the channel. The current through the channel is then given by

$$J = \sum_n e v_{kn} D_n(E) eV \tag{1}$$

0953-8984/89/010305 + 05 \$02.50 © 1989 IOP Publishing Ltd

where the sum is over the occupied sub-bands, the density of states of sub-band n is $D_n(E) = g_s/(2\pi\partial\varepsilon_{kn}/\partial k)|_{\varepsilon_{kn}=E}$, g_s is the spin degeneracy factor, and $\hbar v_{kn} = \partial\varepsilon_{kn}/\partial k$. This yields a conductance

$$G = J/V = \sum_n g_s e^2/h$$

for the channel. For $g_s = 2$, and ν sub-bands containing electrons

$$G = 2\nu e^2/h. \tag{2}$$

This result has been derived in several ways by van Wees *et al* (1988) and Wharam *et al* (1988). Recently Johnston and Schweitzer (1988) obtained it as an exact result in linear response theory at $T = 0$ for a 1D channel of *arbitrary length* arranged in a *closed loop*. If the processes by which electrons are injected into the 1D channel and emitted from it are considered, the closed loop geometry of Johnston and Schweitzer (1988) cannot be used. The above simple argument also fails, because the assumption that the sub-band states in the energy interval $(E, E + eV)$ are completely filled for electrons moving to the right and empty for electrons moving to the left is only approximately correct. The filling of these states is influenced by the processes which occur at the ends of the channel.

To study quantitatively the effects of the injection process *in its simplest form*, consider a semi-infinite 1D channel (C) extending along the x axis for $x > 0$, and a 2D or 3D electron reservoir (an ideal electron gas), filling the left half-space (L) for $x < 0$. An electron incident on the channel opening from the left will be injected or reflected and the probabilities of these events will influence the electric current flowing in the channel. Let us assume that the channel is defined by a potential $U(y)$ which confines the electrons to the vicinity of the x axis, where y stands for the coordinate(s) orthogonal to x. Thus the Hamiltonian for electrons in the channel will be

$$H_C = -\hbar^2(\partial^2/\partial x^2 + \nabla_y^2)/2m^* + U(y) \tag{3}$$

where m^* is the effective mass. In the electron reservoir on the left, the Hamiltonian will be

$$H_L = -\hbar^2(\partial^2/\partial x^2 + \nabla_y^2)/2m^*. \tag{4}$$

Consider an electron incident on the channel from the left with a wavevector $\boldsymbol{k} = (k, K)$ and energy ε_k, where k and K are the components of $\boldsymbol{k}$ parallel and transverse to the channel axis. In the reservoir its wavefunction is

$$\psi_k^L(\boldsymbol{r}) = e^{ikx}\,\varphi_K^L(y) + \sum_{K'} a_{K'}^L\, e^{-ik'x}\,\varphi_{K'}^L(y) \tag{5}$$

where $\varphi_K^L(y) = e^{iKy}$; $k' = (2m^*\varepsilon_k/\hbar^2 - K'^2)^{1/2}$. The sum is over *all* transverse components K', and the convention $(-1)^{1/2} = +i$ is used. This needs to be matched to the wavefunction of the electron in the channel which is of the form

$$\psi_k^C(\boldsymbol{r}) = \sum_n a_n^C\, e^{iq_n x}\,\varphi_n^C(y) \tag{6}$$

where $\varphi_n^C(y)$ is the nth transverse eigenstate of the confining potential $U(y)$ satisfying $H_C\varphi_n^C(y) = \varepsilon_n\varphi_n^C(y)$, $q_n = [2m^*(\varepsilon_k - \varepsilon_n)/\hbar^2]^{1/2}$. The sum is over *all* transverse levels n.

The electric current carried by ψ_k in the channel can be written

$$\langle\psi_k|j_x|\psi_k\rangle = -(\hbar e/m^*)\sum_n^{\mathrm{R}} q_n a_n^{\mathrm{C}*} a_n^{\mathrm{C}} \tag{7}$$

where q_n is as in (6), and the sum is over those 1D sub-bands n for which q_n is real, since evanescent partial waves do not contribute to the current in an infinite channel. To evaluate this current, one can find the coefficients a_n^{C} using the continuity of ψ_k and $\partial\psi_k/\partial x$ at $x = 0$. Equating ψ_k^{L} and ψ_k^{C} at $x = 0$, multiplying by $\varphi_{-Q}^{\mathrm{L}}(y)$ and integrating WRT y yields

$$a_Q^{\mathrm{L}} = -\delta_{QK} + \sum_n M_{-Qn} a_n^{\mathrm{C}} \tag{8}$$

where

$$M_{Qn} = \int_{-\infty}^{\infty} \varphi_Q^{\mathrm{L}}(y)\varphi_n^{\mathrm{C}}(y)\,\mathrm{d}y.$$

Choosing $\varphi_n^{\mathrm{C}}(y)$ to be real, the continuity of $\partial\psi_k/\partial x$ at $x = 0$ yields similarly that

$$q_n a_n^{\mathrm{C}} = kM_{Kn} - \sum_{K'} a_{K'}^{\mathrm{L}} k' M_{K'n} \tag{9}$$

where k, K, q_n, and k' are as defined above. Using (8) to eliminate $a_{K'}^{\mathrm{L}}$ from (9), one finds

$$\sum_n \left(q_n\delta_{mn} + \sum_{K'} k' M_{K'm} M_{-K'n}\right) a_n^{\mathrm{C}} = 2kM_{Km}. \tag{10}$$

Equation (10) is a set of linear equations for the coefficients a_n^{C} which describe the wave function ψ_k in the channel. Notice that in (10) the reflected and evanescent partial waves of ψ_k in the electron reservoir have been eliminated exactly, greatly simplifying the problem.

Expression (1) for the channel current should now be replaced by the current $\langle\psi_k|j_x|\psi_k\rangle$ given by (7), summed over all incident waves ψ_k in an energy interval eV at the Fermi energy E_{F} of the reservoir. For 2D electron reservoirs, as in the experiments of van Wees *et al* (1988) and Wharam *et al* (1988), this yields an expression

$$G = -2\int_{-\alpha}^{\alpha} (m^* e/h^2 k)\langle\psi_k|j_x|\psi_k\rangle\,\mathrm{d}K \tag{11}$$

for the $T = 0$ conductance, replacing equation (2). Here $\alpha = (2m^* E_{\mathrm{F}}/\hbar^2)^{1/2}$, $k = (2m^* E_{\mathrm{F}}/\hbar^2 - K^2)^{1/2}$.

In order to see how the simple result (2) is modified by the effects of electron injection, it is necessary to solve the system of equations (10) and evaluate the conductance (11) numerically. This has been carried out for two models of the confining potential $U(y)$ which are frequently used in modelling channels in semiconductor heterostructures, namely, the parabolic potential $U(y) = cy^2 + U_0$, and the square-well potential $U(y) = U_0$ for $|y| < W/2$, $U(y) = \infty$ for $|y| > W/2$. Here y is the coordinate orthogonal to x in the plane of the heterostructure; very strong out-of-plane confinement is assumed. According to the work of Laux *et al* (1988) the parabolic potential should be a good approximation for the narrowest channels, while square well may be more appropriate for wider ones. A numerical solution requires that the infinite system of equations (10)

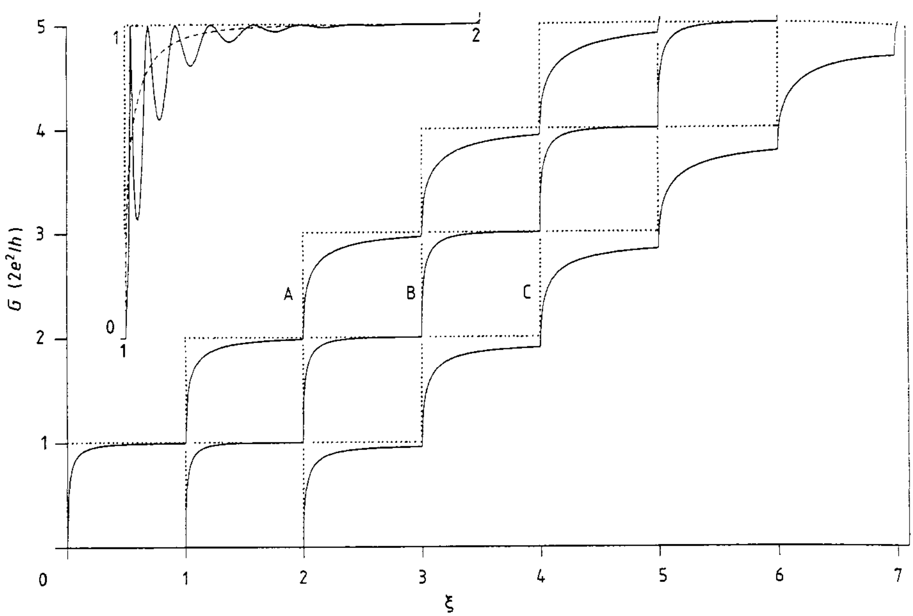

Figure 1. Conductance G versus ξ for semi-infinite ballistic channels. Curve A: parabolic confinement with $\hat{U}=0$. Curves B, C: square-well confinement with $\hat{U}=0$, $\hat{U}=\hat{E}_F/2$ respectively. Full curves: present theory. Dotted curves: ideal result (2) which does not include electron injection effects. Horizontal scale is for curve B; curve A (C) is offset by 0.5 (1.0) to the left (right). Inset: see text. Ideal result (2) (dotted), semi-infinite channel as for curve B (broken curves), finite channel of length $5W$ (full curves).

be truncated. However, the convergence of G with increasing cutoff was very good and the numerical errors in the results presented here are negligible.

The $T=0$ conductance G for these potentials depends on two variables chosen here as the normalised 2DEG Fermi energy $\hat{E}_F$, and the normalised height of the potential step encountered by the electron on entering the constriction $\hat{U}$. For the square-well case let us define $\hat{E}_F = E_F/\Delta$ and $\hat{U} = U_0/\Delta$, where $\Delta = h^2/8m^*W^2$ so that $\varepsilon_n = n^2\Delta + U_0$. For parabolic confinement define $\hat{E}_F = E_F/\hbar\omega$ and $\hat{U} = U_0/\hbar\omega$, with $\omega = (2c/m^*)^{1/2}$ and $\varepsilon_n = (n+\frac{1}{2})\hbar\omega + U_0$. It is convenient to plot the conductance as a function of a dimensionless energy variable ξ which is chosen as $\xi = (\hat{E}_F - \hat{U})^{1/2}$ for the square well and $\xi = \hat{E}_F - \hat{U}$ for parabolic confinement.

Some representative results are shown in figure 1. Curve A is for parabolic confinement with $\hat{U}=0$. Curves B and C are for square-well confinement with $\hat{U}=0$ and $\hat{U}=\hat{E}_F/2$ respectively. The full curves are the present results for a semi-infinite channel, while the dotted curves show the ideal result (2) which does not include electron injection effects. The horizontal scale is for curve B; curve A (C) is offset by 0.5 (1.0) to the left (right) for clarity. It is clear that the quantisation of the conductance is not exact although it can be quite accurate in the plateau regions. The accuracy of the quantisation is lower for the higher plateaus, and it is also reduced for non-zero U_0. It should be noted that $\hat{U}$ is likely to decrease and the confining potential to become more square-well-like with increasing ξ (Laux *et al* 1988), moderating this trend somewhat in the experimental systems.

Qualitatively the present results, including the lower accuracy of quantisation for the higher plateaus, are in agreement with the experiments of van Wees *et al* (1988) and Wharam *et al* (1988), however some potentially important effects have not been included here. Firstly, any residual scattering in the ballistic channel, including that caused by irregularities in the channel walls, will further reduce the accuracy of the quantisation and tend to smooth the 'corners' of the curves shown in figure 1. Secondly, for a *finite* ballistic channel, the quantum mechanics of electron emission from the channel also needs to be considered. This problem can be solved using similar techniques to those described above and will be addressed in detail elsewhere. Here only the main result will be indicated: the inset in figure 1 shows the lowest plateau of curve B magnified by a factor of 3. The dotted curve is again the ideal conductance given by (2), the conductance of the semi-infinite channel is shown as a broken curve, and the full curve is the conductance calculated for a finite channel of length $5W$. The conductance of the finite channel oscillates about that for the semi-infinite channel caused by interference effects caused by multiple internal reflections of the electrons at the ends of the channel. An equivalent interpretation is that the peaks in the conductance occur when the Fermi energy of the 2D electron reservoirs matches the energies of longitudinal resonant electron states in the channel.

In summary: the first quantitative theory of electron injection into a 1D quantum channel has been presented. The theory can explain the experimentally observed deviations from perfect quantisation of the 1D ballistic conductance, and suggests that finite ballistic quantum channels may exhibit resonant conduction.

I would like to thank E Castano and W M Que for helpful discussions. This work was supported by the Natural Sciences and Engineering Research Council of Canada.

References

Imry Y 1986 *Directions in Condensed Matter Physics* ed. G Grinstein and G Mazenko (Singapore: World Scientific) p 101

Johnston R and Schweitzer L 1988 *J. Phys. C: Solid State Phys.* **21** L861

Landauer R 1985 *Localization Interactions and Transport Phenomena* ed. B Kramer, G Bergmann and Y Bruynserade (Heidelberg: Springer) p 38

Laux S E, Frank D J and Stern F 1988 *Surf. Sci.* **196** 101

Stone A D and Szafer A 1988 *IBM J. Res. Dev.* **32** 384

van Wees B J, van Houten H, Beenakker C W J, Williamson J G, Kouwenhoven L P, van der Marel D and Foxon C R 1988 *Phys. Rev. Lett.* **60** 848

Wharam D A, Thornton T J, Newbury R, Pepper M, Ahmed H, Frost J E F, Hasko D G, Peacock D C, Ritchie D A and Jones G A C 1988 *J. Phys. C: Solid State Phys.* **21** L209