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1994 J. Phys.: Condens. Matter 6 5957

(http://iopscience.iop.org/0953-8984/6/30/014)

J. Phys.: Condens. Matter 6 (1994) 5957–5964. Printed in the UK

A theoretical study of the tunnelling spectroscopy of an electron waveguide

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Received 27 January 1994, in fianl form 18 March 1994

Abstract. A theoretical study on the tunnelling spectroscopy of an electron waveguide observed by Eugster and del Alamo is presented. A narrow electron waveguide coupled with another much wider one, with a thin barrier between them, is taken as a theoretical model for the leaky electron waveguide used in the experiments of Eugster and del Alamo, and the transport properties of electrons are studied comprehensively through the wavefunction of the system. The results demonstrate that the conductance for the current tunnelling out of the barrier oscillates strongly with the width of the narrow electron waveguide in line with the conductance steps for the current flowing through the narrow waveguide, and the results are in good agreement with that given by experiments. A semiclassical explanation of the electron behaviour in such a leaky electron waveguide is also proposed in the present paper. A comparison between the results from the semiclassical and quantum mechanical views shows that the semiclassical view can reveal some basic physical ideas in such systems. The results also confirm that the oscillations of the tunnelling current can be considered as a spectroscopy of one-dimensional electron density of states (1D DOS) in the electron waveguide as proposed by Eugster and del Alamo.

1. Introduction

Since the experimental observation of the quantized conductance steps $2e^2/h$ of a narrowly confined channel in high-mobility semiconductor heterostructures [1–3], the behaviour of electron waveguides has attracted much attention [4–6]. Electron waveguides with a variety of configurations and structures have been explored to study their transport properties and potential device applications, both theoretically and experimentally [7–17].

Recently, Eugster and del Alamo reported the observation of tunnelling spectroscopy of an electron waveguide, which provides insight into the basic properties of 1D electron systems [18]. By implementing a 'leaky' electron waveguide with a thin tunnelling barrier as one of its confining boundaries, they measured the current flowing through the waveguide as well as the 1D to 2D tunnelling current leaking out of the thin side barrier for various widths of the waveguide. The experiment demonstrated that the tunnelling current showed very strong oscillations lining up with the $2e^2/h$ conductance steps of the waveguide. Interpretation of the oscillations was proposed as a direct spectroscopy of the 1D DOS of the electron waveguide.

In this paper, a theoretical study of such a leaky electron waveguide is carried out. The transport properties of electrons in the waveguide have been studied by solving the single-electron wavefunction of the system. Oscillations of the tunnelling current are demonstrated to be direct evidence of the 1D DOS of the electron waveguide and the results are in good agreement with experiment. First, a semiclassical picture of the system is described, followed by a detailed quantum mechanical calculation.

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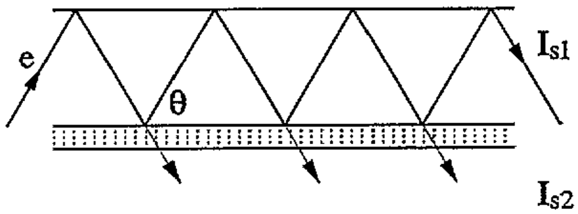

Figure 1. Illustration of the behaviour of electrons in a leaky electron waveguide from a semiclassical point of view. The shaded area represents the barrier. I_{s1} and I_{s2} stand for the currents flowing through the waveguide and tunnelling out of the barrier, respectively.

2. A semiclassical view of the leaky electron waveguide

If the electron is considered as a semiclassical particle, its orbital trajectory in an electron waveguide can be illustrated as shown in figure 1. The incident angle θ_m of electrons in a particular mode m can be expressed by

$$\tan\theta_m = k_{\perp m}/k_{\parallel m} \tag{1}$$

and

$$(\hbar^2/2m^*)(k_{\perp m}^2 + k_{\parallel m}^2) = E_{\mathrm{F}} \tag{2}$$

where $k_{\perp m}$ is the wavevector component normal to the barrier, quantized due to the transverse confinement, $k_{\parallel m}$ is the component parallel to the waveguide, E_{F} is the Fermi energy and m^* is the effective mass of the electron.

Due to their wave nature, electrons may partly tunnel through the barrier and partly reflect back whenever they hit the side wall of the waveguide. An expression for the current tunnelling through the sidewall of the waveguide (I_{s2}) at low temperature can be written as

$$I_{s2} = \frac{e^2\hbar}{m^*}\sum_m k_{\parallel m} N_m T_m g_m^{1\mathrm{D}} \Delta V \tag{3}$$

where contributions from all the excited modes have been taken into account. The bias voltage between the source and drain (ΔV) has been assumed to be small for simplicity. $g_m^{1\mathrm{D}}$ is the 1D DOS of mode m, which is inversely proportional to $k_{\parallel m}$. The transmission coefficient, T_m, can be easily obtained by quantum mechanics and by assuming that the thin side barrier is square. N_m is the number of times an electron meets the barrier during its passage through the waveguide,

$$N_m = Lk_{\perp m}/2Wk_{\parallel m} \tag{4}$$

where L and W are the length and the width of the electron waveguide, respectively.

The tunnelling current and conductance obtained are

$$I_{s2} = \frac{e^2\hbar}{m^*}\sum_m k_{\perp m} T_m g_m^{1\mathrm{D}} \frac{L}{W} \Delta V \tag{5}$$

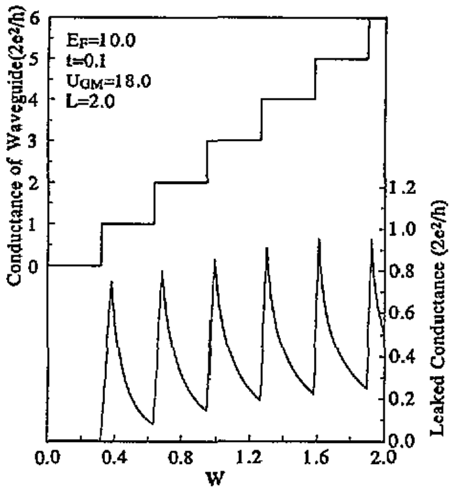

Figure 2. Conductances plotted against W, the width of the electron waveguide, from a semiclassical equation (equation (6)).

and

$$G_{s2} = \frac{e^2\hbar}{m^*} \sum_m k_{\perp m} T_m g_m^{1D} \frac{L}{W}. \tag{6}$$

The formula used is basically the same as equation (2) in [18], except for a multiplier L/W. Both equations show that the tunnelling current is propotional to 1D DOS g^{1D} of the waveguide.

Using the above formulation, G_{s2} against the width of the electron waveguide W has been calculated and the result is shown in figure 2. Conductance steps of the electron waveguide (G_{s1}) are also plotted in figure 2 for reference. In the present paper normalized units are used, i.e. length is in units of W, an arbitrarily chosen length, and correspondingly the wavevector and energy are in units of π/W and $\hbar^2\pi^2/2m^*W^2$, respectively. As observed experimentally, the leaking conductance G_{s2} shows strong oscillations lining up with the rise of steps of G_{s1}.

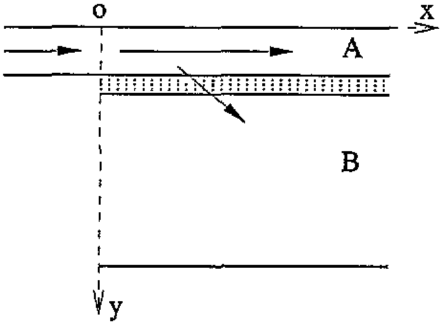

Figure 3. Schematic illustration of the theoretical model applied to simulate a leaky electron waveguide. The shaded area between waveguides A and B represents the tunnelling barrier.

3. Theoretical model

In our theoretical model, an electron waveguide (A) coupled with another much wider one (B) is used to simulate a leaky electron waveguide, as shown in figure 3. Waveguide B is approximately used as a 2D drain for electrons tunnelling out of the electron waveguide A, therefore it should be wide enough for a good simulation. Electrons launching from the left reservoir are confined in waveguide A in the region $x \leqslant 0$, and might tunnel into waveguide B in the region $x > 0$. Assuming that the incoming electrons are in the mth mode of the electron waveguide A, the wavefunction can be expressed as

$$\psi_1^m(x, y) = \phi_1^m(y)\exp(\mathrm{i}k_1^m x) + \sum_n a_{mn}\phi_1^n(y)\exp(-\mathrm{i}k_1^n x) \tag{7}$$

for $x \leqslant 0$, where $\phi_1^n(y)$ is the nth transverse eigenfunction of wave-guide A. For the infinite square-well approximation adopted for the confinement of the waveguide, the eigenfunction is given as

$$\phi_1^n(y) = \left(\frac{2}{W_\mathrm{A}}\right)^{1/2} \sin\frac{n\pi y}{W_\mathrm{A}}. \tag{8}$$

Correspondingly, the nth transverse eigenenergy is

$$E_1^n = \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{W_\mathrm{A}}\right)^2 \tag{9}$$

where k_1^n in equation (7) is the wavevector of the nth mode. The condition for energy conservation gives

$$\hbar^2 k_1^{n2}/2m^* + E_1^n = E_\mathrm{F} \tag{10}$$

where E_F is the Fermi energy of the electron reservoir. The second term of equation (7) represents reflection at the interface of $x = 0$. For $x > 0$, the wavefunction can be written as

$$\psi_2^m(x, y) = \sum_n b_{mn}\phi_2^n(y)\exp(\mathrm{i}k_2^n x) \tag{11}$$

where $\phi_2^n(y)$ satisfies

$$\frac{\hbar^2}{2m^*}\frac{\mathrm{d}^2\phi_2^n(y)}{\mathrm{d}y^2} + U_2(y)\phi_2^n(y) = E_2^n\phi_2^n(y). \tag{12}$$

E_2^n is the nth transverse eigenenergy and $U_2(y)$ is the transverse confinement in region $x > 0$. $U_2(y)$ is defined for various regions by the following relation:

$$U_2(y) = \begin{cases} U_\mathrm{GT} & y \leqslant 0,\ y \geqslant W_\mathrm{A} + t + W_\mathrm{B} \\ U_\mathrm{GM} & W_\mathrm{A} \leqslant y \leqslant W_\mathrm{A} + t \\ 0 & \text{otherwise} \end{cases} \tag{13}$$

where W_A and W_B are the widths of waveguide A and B, U_GT is the potential beyond the waveguides, and t and U_GM are the thickness and height of the barrier, respectively.

$U_{\mathrm{GT}} = -eV_{\mathrm{GT}}$, $U_{\mathrm{GM}} = -eV_{\mathrm{GM}}$, where V_{GT} and V_{GM} are the bias voltages applied on the gates in the experiments [18].

In principle, in equations (7) and (11) n should run over all the modes in two regions, including both the propagating modes whose transverse energies are smaller than E_{F} and evanescent modes whose transverse energies are larger than E_{F}. In our calculation, however, it is found that the required precision can be obtained by taking all the propagating modes and only a few evanescent modes into account.

Continuity of the wavefunction and its first derivative at $x = 0$ gives

$$\phi_1^m(y) + \sum_n a_{mn}\phi_1^n(y) = \sum_s b_{ms}\phi_2^s(y) \tag{14}$$

$$\mathrm{i}k_1^m\phi_1^m(y) - \mathrm{i}\sum_n a_{mn}k_1^n\phi_1^n(y) = \mathrm{i}\sum_s b_{ms}k_2^s\phi_2^s(y). \tag{15}$$

Multiplying equation (14) by $\phi_2^i(y)$ and equation (15) by $\phi_1^j(y)$, respectively, and integrating the resulted equations over y, one obtains a set of algebraic equations for all the coefficients required, where i and j run over all the modes which have been taken into account in the two regions. The solution of this set of equations gives all the coefficients and hence the wavefunctions. The conductance of waveguides A and B with respect to the mth incident mode can be expressed as

$$G_{\mathrm{A}}^m(x) = \int_{\mathrm{A}} e^2\langle\psi_2^m|\hat{j}_x|\psi_2^m\rangle g_m^{\mathrm{1D}}\,\mathrm{d}y \tag{16}$$

$$G_{\mathrm{B}}^m(x) = \int_B e^2\langle\psi_2^m|\hat{j}_x|\psi_2^m\rangle g_m^{\mathrm{1D}}\,\mathrm{d}y \tag{17}$$

where g_m^{1D} is the 1D DOS of the mth mode of waveguide A, and $\hat{j}_x$ is the operator of electron flow. Integrations of equations (16) and (17) are carried out in the regions of waveguides A and B, respectively. The total conductances of waveguides A and B are

$$G_{\mathrm{A}}(x) = \sum_m G_{\mathrm{A}}^m(x) \tag{18}$$

$$G_{\mathrm{B}}(x) = \sum_m G_{\mathrm{B}}^m(x) \tag{19}$$

where m runs over all the excited modes in the input waveguide, G_{A} corresponds to the current flowing through waveguide A, and the leaky conductance G_{B} corresponds to the tunnelling current. Substituting $x = L$, one gets the conductance between source and drain of the waveguides.

In the present model, we have not set a specific boundary condition at $x = L$. However, another model with a boundary at $x = L$ has also been considered and results very similar to those given by the present model have been obtained.

4. Results

The results are shown in figure 4. It can be seen that the results, including both the steps of waveguide conductance G_{A} and the oscillation of leaky conductance G_{B}, are in good agreement with that of the experiment [18]. It is worthwhile noting that in the

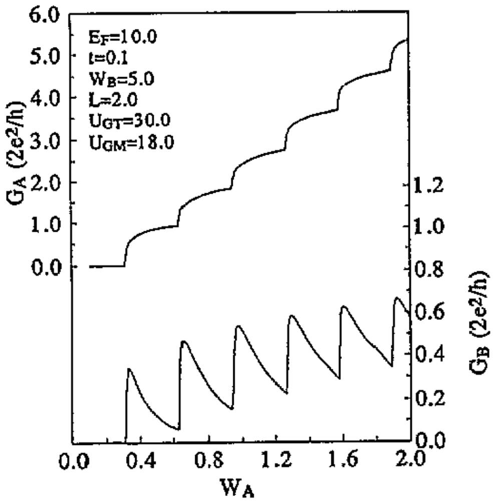

Figure 4. Calculated conductances of the leaky electron waveguide. G_A corresponds to the current flowing through the waveguide and G_B to the current tunnelling out of the barrier.

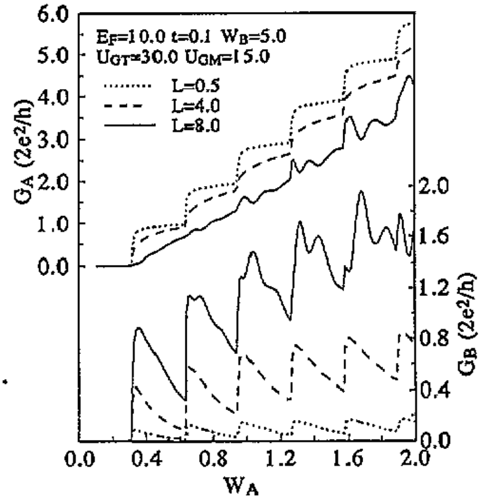

Figure 5. Conductances plotted against W_A for different values of L, the length of the device.

experiment it was the voltage of the upper gate V_{GT} (which is negative) that varied, whereas in our calculation the varying parameter is the width of the electron waveguide A (W_A). Increasing V_{GT} results in a widening of the electron waveguide, however, the relation between U_{GT} and W_A is not linear. This might be one of the factors which cause some detailed differences between the results of the present theoretical calculation and that of the experimental measurements. A comparison between the curves of leaky conductance in figures 2 and 4 shows that the semiclassical model works quite well.

The conductances of our model devices with different length (L) are shown in figure 5. Onsets of steps of G_A and oscillation peaks of G_B are the same for different L as the transverse electronic structure and the Fermi energy remain unchanged. But the value of G_B increases, and G_A decreases correspondingly with increasing L. Meanwhile, the height of the steps of G_A decreases. When L becomes much larger ($L = 8.0$ in figure 5), steps of G_A are not well defined any more and the curve of G_B deviates from the oscillations of small L. This can be expected from our theoretical model, and can be explained as a result of the reflection of the electron wave on the walls of waveguide B. For a device with small length, electrons tunnelling the barrier may flow out of the device without any reflection. On the other hand, the reflection might be significant for a device with large length L. Therefore, the width of waveguide B of our model device must be large enough compared with the length L in order to simulate a long leaky electron waveguide.

The conductances of model devices with different barrier height (U_{GM}) are shown in figure 6. Increasing U_{GM} will result in a decrease in the tunnelling probability, and thus in the tunnelling current. However, the locations of steps of G_A and oscillation peaks of G_B remain unchanged when the carrier density is not modified.

The effect of the variation of the Fermi energy E_F is also studied, and the result is shown in figure 7. When E_F increases, tunnelling current increases with the increase in tunnelling probability, and the onsets of steps of oscillation shift to the left since a greater number of transverse energies pass by the Fermi energy E_F, and the number of steps and oscillations increases since more subbands are occupied.

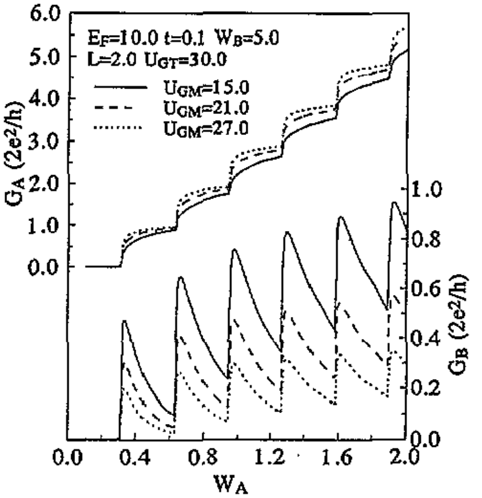

Figure 6. Conductances plotted against W_A for different values of U_{GM}, the height of the barrier.

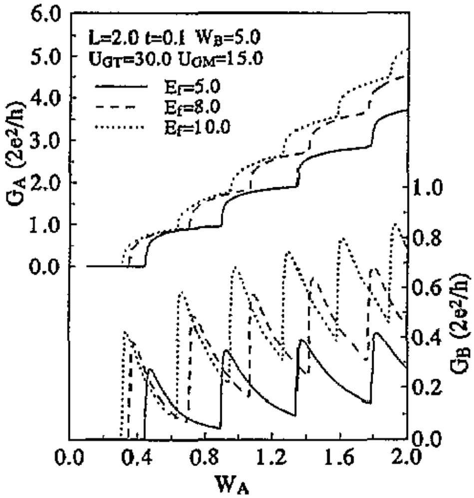

Figure 7. Conductances plotted against W_A for different values of E_F, the Fermi energy of the electron.

In summary, a theoretical study of tunnelling spectroscopy of an electron waveguide has been presented. Oscillations of the conductance of a leaky electron waveguide are theoretically demonstrated. Results of the calculations are in good agreement with experiment. A semiclassical interpretation of tunnelling current oscillations is also proposed and it not only gives the expression of tunnelling current as a linear function of the 1D DOS of the electron waveguide but also shows that some fundamental physical concepts can be revealed. Qualitative agreement between the semiclassical result and quantum mechanical calculation supports the suggestion of Eugster and del Alamo [18] that the tunnelling current oscillation of such a leaky electron waveguide can serve as a spectroscopy for the 1D DOS of the electron waveguide.

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