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A theoretical investigation of the effects of a single scatterer on a leaky electron waveguide

Aiguo Fei†, Lin Jiang†, Guangzhao Xu†, Ping Jiang‡† and Xide Xie†

† State Key Laboratory of Surface Physics, Fudan University, Shanghai 200433, People's Republic of China§

‡ CCAST (World Laboratory), PO Box 8730, Beijing 100080, People's Republic of China

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Abstract. Effects of a single scatterer on the transport properties of a leaky electron waveguide are investigated theoretically. The δ-function is used to simulate the scattering potential. The results show that the presence of even a single scatterer located in the waveguide will lead to obvious distortion of the shape of conductance steps, and will greatly influence the oscillations of the tunnelling current observed in clean waveguides. However, the effects of the scatterer being located outside the tunnelling barrier on either the conductance steps or the oscillations of the tunnelling current are negligible.

In recent years, transport properties of electron waveguides have been widely studied experimentally and theoretically [1–12]. Electron waveguides are thought to be an important kind of quantum electronic device. From a practical point of view it is necessary to understand the effect of undesirable impurities which may exist occasionally in such quantum devices. Some experimental and theoretical studies have been reported [10, 13–20], which demonstrated the degradation and destruction of conductance quantization by the presence of impurities. In this paper, a theoretical investigation of the effect of a single impurity (scatterer) in a special electron waveguide, a 'leaky' electron waveguide, is presented.

A leaky electron waveguide was first implemented by Eugster and del Alamo by using a thin tunnelling barrier as one of its confining boundaries [9]. Their experiment showed that the tunnelling current oscillated strongly in line with the $2e^2/h$ conductance steps of the waveguide, which could be considered as a spectroscopy of 1D DOS (one-dimensional density of states) in the electron waveguide. They also reported experimentally the effect of a local scatterer on the transport properties of a dual-electron waveguide and on the tunnelling characteristics of a leaky electron waveguide [10]. Using a model coupled dual-electron waveguide, the present authors have theoretically demonstrated the transport and tunnelling properties of the leaky electron waveguide [12]. In the present paper, a δ-function is used to simulate the scattering potential, and the transport and tunnelling characteristics of a leaky electron waveguide, with one single scatterer located within the waveguide or outside the tunnelling barrier, are calculated. The results give some insight into the problem concerned, i.e. the effects of existence of impurities.

As in our previous work [12], an electron waveguide (A) coupled with another much wider one (B), as shown in figure 1, is used to simulate a leaky electron waveguide. The δ-

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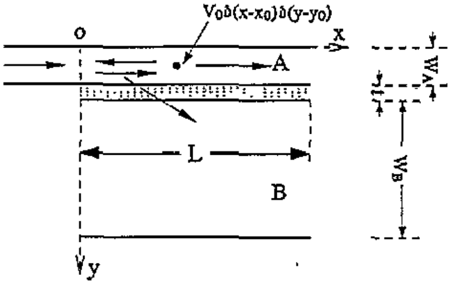

Figure 1. Schematic illustration of the theoretical model used to simulate a leaky electron waveguide. The shaded area between waveguide A and B represents the tunnelling barrier. The small solid circle in waveguide A stands represents the impurity (the scatterer).

function approximation is used to simulate the scatterer. The scattering potential is assumed to be

$$V(x, y) = V_0\delta(x - x_0)\delta(y - y_0) \tag{1}$$

where (x_0, y_0) is the location of the scatterer, which can be either in waveguide A or in waveguide B. V_0 can be either negative or positive to simulate either an attractive or repulsive scatterer correspondingly. Electrons launched from the left reservoir, which is not shown in figure 1, are confined in input waveguide A in the region $x \leqslant 0$, and might tunnel into waveguide B in the region $x > 0$ where the scattering is assumed to happen.

By assuming that the incoming electrons are in the mth mode of electron waveguide A, the wavefunction can be expressed as

$$\psi_1^m(x, y) = \phi_1^m(y)e^{ik_1^m x} + \sum_n a_{mn}\phi_1^n(y)e^{-ik_1^n x} \tag{2}$$

for the region $x \leqslant 0$, where $\phi_1^n(y)$ is the nth transverse eigenfunction of waveguide A. For the infinite square-well approximation adopted in the present work for the confinement in this region,

$$\phi_1^n(y) = \sqrt{\frac{2}{W_A}}\sin\frac{n\pi y}{W_A} \tag{3}$$

where W_A is the width of waveguide A. Energy conservation gives

$$\frac{\hbar^2}{2m^*}\left(\frac{n\pi}{W_A}\right)^2 + \frac{\hbar^2 k_1^{n2}}{2m^*} = E_F \tag{4}$$

where k_1^n is the wavevector of the nth mode and E_F is the Fermi energy of the electrons. The second term of equation (2) stands for the electron waves reflected at the interface $x = 0$.

For the region $0 < x \leqslant x_0$, the wavefunction can be written as

$$\psi_2^m(x, y) = \left(\sum_n a_{mn}^+ e^{ik_2^n x} + \sum_n a_{mn}^- e^{-ik_2^n(x-x_0)}\right)\phi_2^n(y). \tag{5}$$

Here the second term stands for electron waves reflected from the scatterer. For $x > x_0$

$$\psi_2^m(x, y) = \sum_n b_{mn}\phi_2^n(y)e^{ik_2^n(x-x_0)}. \tag{6}$$

In equations (5) and (6), $\phi_2^n(y)$ satisfies

$$-\frac{\hbar^2}{2m^*}\frac{d^2\phi_2^n(y)}{dy^2} + U_2(y)\phi_2^n(y) = E_2^n\phi_2^n(y) \tag{7}$$

while

$$E_2^n + \frac{\hbar^2 k_2^{n2}}{2m^*} = E_F \tag{8}$$

where E_2^n is the nth transverse eigenenergy in the region $x > 0$. $U_2(y)$ is defined as

$$U_2(y) = \begin{cases} U_{GT} & y \leqslant 0, y \geqslant W_A + t + W_B \\ U_{GM} & W_A \leqslant y \leqslant W_A + t \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

where W_B is the width of waveguide B, U_{GT} is the transverse confinement adopted for the waveguides in the region $x \geqslant 0$, t and U_{GM} are the thickness and height of the tunnelling barrier, respectively. $\phi_2(y)$ can be solved by the transfer matrix method as we did before [8]. Meanwhile, $\psi_2^m(x, y)$ should satisfy

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2 + U_2(y) + V(x, y)\right]\psi_2^m(x, y) = E_F\psi_2^m(x, y) \tag{10}$$

where $V(x, y)$ is the scattering potential shown in equation (1).

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

$$\phi_1^m(y) + \sum_n a_{mn}\phi_1^n(y) = \left(\sum_s a_{ms}^+ + \sum_s a_{ms}^- e^{ik_2^s x_0}\right)\phi_2^s(y) \tag{11}$$

$$ik_1^m\phi_1^m(y) - \sum_n ik_1^n a_{mn}\phi_1^n(y) = \sum_s ik_2^s\left(a_{ms}^+ - a_{ms}^- e^{ik_2^s x_0}\right)\phi_2^s(y). \tag{12}$$

Continuity of the wavefunction at $x = x_0$ gives

$$\sum_s (a_{mn}^+ e^{ik_2^n x_0} + a_{mn}^-)\phi_2^n(y) = \sum_l b_{ml}\phi_2^l(y). \tag{13}$$

Orthonormality of ϕ_2^n yields

$$a_{mn}^+ e^{ik_2^n x_0} + a_{mn}^- = b_{mn} \tag{14}$$

where n runs over all the modes that are taken into account. Integrating equation (10) from $x_0 - \varepsilon$ to $x_0 + \varepsilon$ gives

$$\frac{\hbar^2}{2m^*}\left(\frac{\partial\psi_{2\text{right}}^m}{\partial x} - \frac{\partial\psi_{2\text{left}}^m}{\partial x}\right)\bigg|_{x_0} = V_0\delta(y - y_0)\psi_2^m(x_0, y) \tag{15}$$

if $\varepsilon \to 0$. Multiplying equation (11) by $\phi_2^i(y)$ and equation (12) by $\phi_1^j(y)$ respectively, where i or j runs over all the modes which are taken into account, and integrating the resulting equations over y yields a set of algebraic equations. Multiplying equation (15) by $\phi_2^j(y)$, where j also runs over all the modes taken into account, and integrating the resulting equation over y yields another set of algebraic equations. Solution of the two sets of equations combined with equation (14) gives all the coefficients and hence the wavefunctions.

The conductances of waveguides A and B with respect to the mth input mode can be expressed as

$$G_A^m = \int_A e^2\langle\psi_2^m|\hat{j}_x|\psi_2^m\rangle g_m^{1D}\,dy\big|_{x=L} \tag{16}$$

$$G_B^m = \int_B e^2\langle\psi_2^m|\hat{j}_x|\psi_2^m\rangle g_m^{1D}\,dy\big|_{x=L} \tag{17}$$

where L is the length of the tunnelling region and g_m^{1D} is the 1D DOS of the mth mode of the input waveguide at E_F, and $\hat{j}_x$ is the operator of electron flow. Integrations of equations (16) and (17) are carried out for waveguide A and waveguide B, respectively. The total conductances of waveguide A and waveguide B are

$$G_A = \sum_m G_A^m \tag{18}$$

$$G_B = \sum_m G_B^m \tag{19}$$

where m runs over all the excited modes in the input waveguide ($x < 0$). G_A corresponds to the current flowing through the waveguide A, while the leaky conductance G_B corresponds to the tunnelling current.

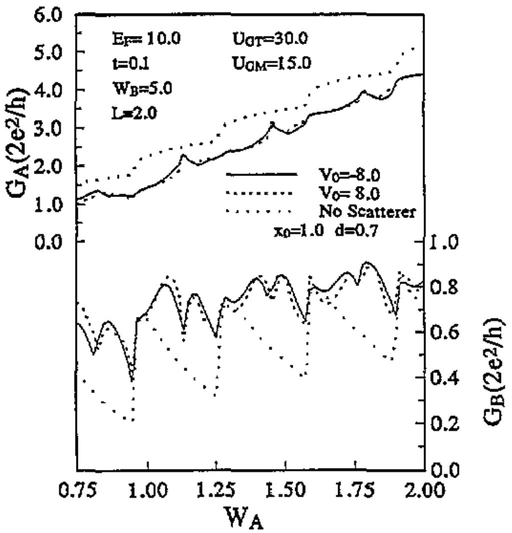

Figure 2. Calculated conductances of the leaky waveguide with an attractive or a repulsive impurity in waveguide A in comparison with that of a clean waveguide. G_A corresponds to the current flowing through the waveguide and G_B to the tunnelling current.

In principle, in equations (2) and (5), n should run over all the modes in the corresponding regions, including both the propagating modes and evanescent modes. However, it has been found that the required precision could be obtained by taking all the propagating modes and only a few lowest evanescent modes into account.

In the present paper we use normalized units, i.e., length is in units of W, an arbitrarily chosen length, correspondingly the wavevector and energy are in units of π/W and $\hbar^2\pi^2/2m^*W^2$ respectively.

It should be noticed that in the 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 widening the electron waveguide though the relation between V_{GT} and W_A is not linear [12]. Besides, to locate the position of the scatterer, a parameter d, which is the distance from the scatterer to the tunnelling barrier, is used in our calculation. For a scatterer in waveguide A, $y_0 = W_A - d$; for scatterer in waveguide B, $y_0 = W_A + t + d$. While W_A is varied in our calculation, d is kept constant, which agrees with the experiments. In the experiments [9, 10], the middle-gate bias voltage was kept constant while the side-gate voltage was varied which means that the local scatterer had a constant distance from the middle gate (the tunnelling barrier).

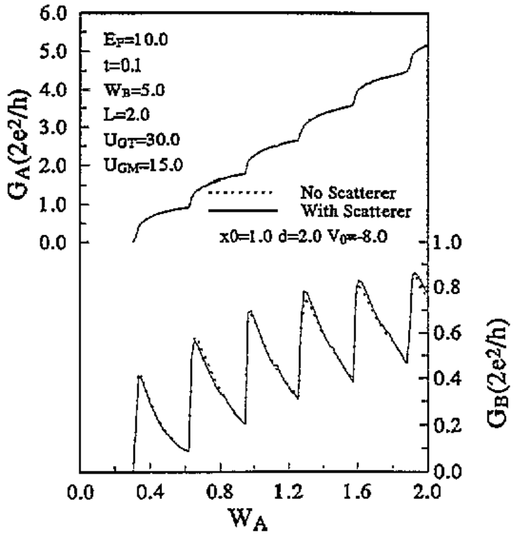

Figure 3. Conductances with the presence of an impurity outside the tunnelling barrier (in waveguide B).

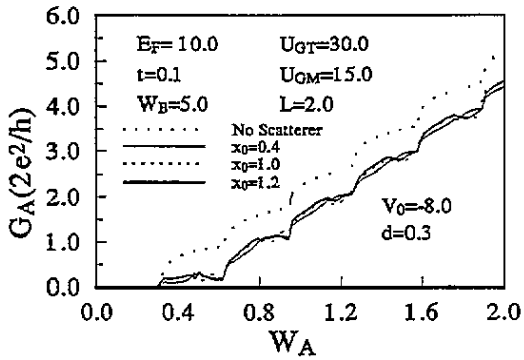

Figure 4. Conductances versus W_A for scatterers of different x_0, the longitudinal position.

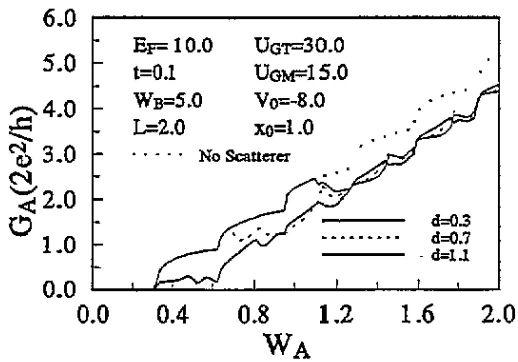

Figure 5. Conductances versus W_A for scatterers of different d, the distance from the tunnelling barrier.

The effects of a scatterer on the conductance steps and the tunnelling current are shown in figure 2. The conductance steps and the tunnelling current of a clean waveguide are also shown for comparison. The degradation and distortion of conductance steps due to the presence of the impurity are obvious. The oscillation of the tunnelling current is changed so remarkably that it would be difficult to find any connection between the tunnelling current and the 1D DOS of the waveguide. Both the conductance and tunnelling current of a waveguide with an attractive impurity and that with a repulsive impurity are shown in figure 2. The effect of the repulsive impurity is quite similar to that of an attractive one. It means that, as a scatterer, a repulsive and an attractive impurity do not differ very much in their effects on the transport properties of a leaky electron waveguide.

If the impurity is located outside the tunnelling barrier, i.e. it is located in waveguide B in our model structure, its effects on the conductance steps or on the tunnelling current are negligible. The results are shown in figure 3. We have calculated many cases of different impurity locations and different scattering strength V_0; the results are almost the same as that of a clean waveguide. This is understandable since the possibility for electrons in waveguide B to be scattered back into waveguide A is quite small.

Effects of impurity position are shown in figure 4 and figure 5. In figure 4, all the impurities have the same distance from the tunnelling barrier but different x_0. All the conductance curves looked quite similar and the difference is unremarkable. In figure 5, all the impurities have the same x_0 but different distance from the tunnelling barrier. It is worthwhile mentioning that if $d > W_A$ the impurity is located outside the waveguide; it will not have a significant effect on the conductance or the tunnelling current. For a fixed d, if W_A increases from some value which is less than d, i.e. the scatterer is located outside the waveguide A, the conductance steps will not be distorted until W_A reaches or exceeds d. It can be easily seen in figure 5 that the curve of conductance versus W_A would look undistorted before W_A reaches d. This fact makes it possible to determine the lateral position of a scatterer experimentally [10] by measuring the conductance of a electron waveguide while it is difficult to determine the longitudinal position of the scatterer in this way.

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