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Conductivity steps of a thick square barrier in a transverse magnetic field

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Abstract. We calculate the tunnelling current and the differential conductivity of a thick square barrier in a transverse magnetic field. This field has the same extension as the barrier. We investigate the role of the quasi-levels localized at the barrier and appearing when the barrier is sufficiently wide. We choose the parameters suitable to describe low barriers in semiconductor heterostructures. The tunnelling current and the differential conductivity can exhibit steps in the applied voltages and Fermi levels.

1. Introduction

In a previous work [1], we have calculated the transmission coefficient for the tunnelling in a magnetic field confined within a thick square barrier. We assumed this barrier to separate two reservoires of electrons. A tunnelling current arises when a voltage is applied across the barrier. Our model can be considered an idealization of a real device in which the electrodes act as a source and a detector of the coherent quantum tunnelling across the barrier. In other words, we assumed that the transport within very long electrodes is governed by the Boltzmann equation, so that here the magnetic field only contributes to the overall electron mobility, i.e., semi-classically. On the other hand, the transport across the barrier is described by the Schrödinger equation for one particle. We think that this picture is physically meaningful provided the phase coherence length is comparable to the barrier width (see [9] pp 1013–5).

Moreover, we asssumed the mobility in the electrodes to be so large that the behaviour of the device is dominated overwhelmingly by the conductivity in the small region of the barrier. We evaluate this conductivity within the standard transfer Hamiltonian formalism which requires the knowledge of the transmission coefficient t. The inclusion of phase-breaking processes in the trasmission coefficient is an open question, an object of current research in the field [12, 13]. We ignore the phase breaking here but we try to take into account the mobility jump forcing the wavefunctions to be plane waves outside the barrier, i.e. we push to zero both the electric and the magnetic field outside it. This is a very crude way of describing the wiping out of quantum interference patterns but it guarantees that the particle fluxes entering and exiting the barrier are spatially uniform. At the same time, this approximation allows us to compute t using elementary quantum mechanics.

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In this paper we present a discussion of the conductivity in this system, both in two and three dimensions. The most striking consequence of the presence of a magnetic field within a barrier is the appearance of resonant states localized in the barrier. The transmission coefficient t depends on k and k_x, where k is the wave vector in the plane perpendicular to the magnetic field and k_x is its component parallel to the barrier. The x, y, z coordinates can be separated in the Landau gauge. The motion along the y axis can be described by an effective potential parametrized by k_x. There is a particular value of k_x, i.e. k_0, for which the barrier deformation due to the magnetic field produces a parabolic well, superimposed on the barrier, that is symmetric around its centre. At this value of k_x, it may happen that the transmission coefficient becomes unity at various values of k^2 which, in the case of a thick enough barrier, are very close to the corresponding harmonic oscillator levels of the non-truncated parabola (the Landau levels). When we move k_x away from k_0, the minimum of the parabolic well leaves the centre of the barrier and approaches its left or right edge. Correspondingly, the transmission falls down and the resonances disappear.

Therefore, only electrons moving in a particular direction in the (x, y) plane, fixed by k_0, traverse the barrier with probability one; these are the electrons whose energy is that of the Landau quasi-levels. When these kinematics conditions are not satisfied, the barrier becomes opaque: that is, a sort of conduction channels are formed. This behaviour resembles that of a two-dimensional electron gas in an external potential which has a saddle-shaped bottleneck. Using the Landauer formula for conductance [2], Buttiker [3] has shown that this constriction gives rise to a quantization of conductance. His analysis of a simple harmonic saddle point, based on that of Halperin and Fertig [4], indicates that as the energy of the electrons impinging on the barrier increases, the conductance increases by steps of height e^2/h. Moreover, a uniform magnetic field perpendicular to the plane causes a flattening and sharpening of these steps. There, the lateral constriction is the origin of the quantized transmission and attention is focused on the accuracy of the quantization. The smooth variation of the distance between the walls gives exponentially small corrections to the transmission [5, 6]; it has a negligible effect on quantization, while the magnetic field improves the quantization. Our model is, in some sense, complementary to Buttiker's model. We do not have any lateral constriction and the steps in the conductivity arise from the resonances induced by the confined magnetic field.

Starting from the expression of the current in terms of t, we calculate the differential conductivity as a function of the Fermi level E_F of the reservoir. When E_F is close to the energy of a Landau quasi-level, a new 'channel' opens and the conductivity exhibits a sudden growth. We have to work with conductivity and not with conductance, because we deal with a 'constriction' of a different origin. It is due to the magnetic field; in our system, the scattering retains its two-dimensional nature and it is not reducible to one-dimensional scattering, as it is in Buttiker's case.

We study the system both in three and two dimensions. In the three-dimensional case, the integration over k_z (along the magnetic field) smooths the steps that are better pronounced in the two-dimensional case, that is when the electron gas is confined in a plane perpendicular to the magnetic field.

A closer analysis shows that the maxima of t lie along some lines in the (k, k_x) plane, contained in the domain in which $t > 0$. These lines are born and die on the border of this domain. As k increases, a resonance appears at $k = k_3$; it reaches its maximum ($t = 1$) when $k = k_2$ and disappears at $k = k_1$, with $k_1 > k_2 > k_3$. When the voltage V polarizing the barrier is increased, the depth of the parabolic well within the barrier increases as well. Naively, one could expect better-pronounced effects. However, k_3 decreases at larger voltages and k_1 increases. Therefore, at a large polarization and gradually increasing k, a new resonance appears before the former one has run out. The effects of the resonances on the conductivity are additive and the stepped behaviour is lost at a sufficiently high voltage.

2. The transmission coefficient

In this section we briefly review our results on the transmission coefficient in the problem under discussion here [1]. A repulsive square barrier of height U_0 and width L separates the two half-spaces $y < 0$ and $y > L$. A magnetic field of intensity B acts within the barrier, in the region $0 < y < L$. A voltage V is applied across the barrier in such a way that a tunnelling current flows along the y axis towards $+\infty$. The energy is measured in units of $\hbar\omega_c$ ($\omega_c = eB/m^*c$ is the cyclotron frequency) and the length in units of $\lambda = (\hbar/2m^*\omega_c)^{1/2}$. The vector potential of the uniform magnetic field in the Landau gauge has the x component only; this allows the separation of the x, y, z coordinates. A description of the scattering process can thus be made in terms of an *effective one-dimensional potential* $u(y)$. The motion along the y axis is the motion of a particle of energy k_y^2 scattered by the potential

$$\begin{aligned} u(y) &= 0 && y < 0 \\ u(y) &= \frac{y}{4}(y - L) - y(k_x - k_0) + U_0 && 0 \leqslant y \leqslant L \\ u(y) &= -L(k_x - k_0) && y > L. \end{aligned} \tag{1}$$

This potential is an explicit function of U_0, L, k_x and depends on Ve via

$$k_0 = L/4 - Ve/L. \tag{2}$$

The combined effect of the magnetic field and polarization amounts to a constant shift of the potential on the right hand side of the barrier, while the barrier height is reduced by a parabolic well. We note that at $k_x = k_0$, $u(y)$ becomes symmetric with respect to the centre of the barrier $y = L/2$. Figure 1 shows $u(y)$ as a function of y and k_x. As k_x increases, the minimum of the parabola shifts from the left edge to the right edge of the barrier. In other words, there is a particular angle of incidence at which quasi-levels can arise in the effective barrier for the motion along y.

These quasi-levels are close to the harmonic oscillator levels of the non-truncated parabola:

$$k_y^2 = U_0 - \frac{L^2}{16} + n + \frac{1}{2}. \tag{3}$$

As k_x moves away from k_0, the shape of $u(y)$ changes and the quasi-levels given by (3) vanish.

All these features are found in the transmission coefficient

$$t = \frac{4k_y k_y'}{w_1^2 + k_y^2 w_2^2 + k_y'^2 w_3^2 + k_y^2 k_y'^2 w_4^2 + 2k_y k_y'} \tag{4}$$

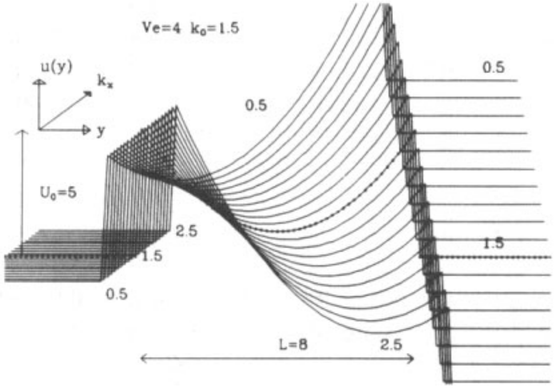

Figure 1. The effective potential u as a function of y and k_x for $U_0 = 5$, $L = 8$, $Ve = 4$. The heavy line refers to $k_x = k_0 = 1.5$, for which the effective potential is symmetric around its centre.

in which

$$\begin{aligned}
w_1 &= Y_1'(a,-y_0)Y_2'(a,L-y_0) - Y_2'(a,-y_0)Y_1'(a,L-y_0) \\
w_2 &= Y_1(a,-y_0)Y_2'(a,L-y_0) - Y_2(a,-y_0)Y_1'(a,L-y_0) \\
w_3 &= Y_1'(a,-y_0)Y_2(a,L-y_0) - Y_2'(a,-y_0)Y_1(a,L-y_0) \\
w_4 &= Y_1(a,-y_0)Y_2(a,L-y_0) - Y_2(a,-y_0)Y_1(a,L-y_0)
\end{aligned}$$

where Y is the parabolic cylinder function [7], and Y' is its derivative with respect to the argument. In addition, we have defined

$$y_0 = 2(k_x + Ve/L) \qquad a = U_0 - k^2 - e^2V^2/L^2 - 2k_xVe/L$$

and

$$k^2 = k_x^2 + k_y^2 \qquad k_y' = \sqrt{k_y^2 + L(k_x - L/4) + Ve}.$$

The transmission t depends both on k and k_x: the scattering in the (x, y) plane becomes directional in the presence of magnetic field. The dependence can be strong; this is seen in figures 2 (a) and 2 (b) where t is plotted as a function of k_x and k^2. Here, the transmission peaks correspond to the quasi-levels. As the energy k^2 of motion in the (x, y) plane increases, a resonance appears, reaches its maximum value 1 at $k_x = k_0$ and finally dies out. Other resonances can arise and disappear if the barrier is sufficiently wide. The higher the energy at which the resonance occurs, the larger its spread is. The transmission peaks run along some lines in the (k, k_x) plane within the domain in which $t > 0$. When $Ve < L^2/4$, this set is defined by the inequality

$$k_1 \leqslant k_x \leqslant k \qquad \text{for } k \geqslant k_0 \text{ with } k_1 = -\sqrt{k^2 + Ve} + L/2.$$

The full details can be found in our previous work [1].

Figures 3 (a) and 3 (b) show the trajectories of the first two resonances for two different voltages V. We see that at higher voltages, the energies of the resonances are lower, while the trajectories tend to rotate towards the k axis. The last feature implies that on increasing the voltage, the second resonance arises before the first has died. The ranges of k values spanned by each resonance do not overlap only when the polarization is sufficiently low. In what follows, we shall discuss the consequences of this on the tunnelling current.

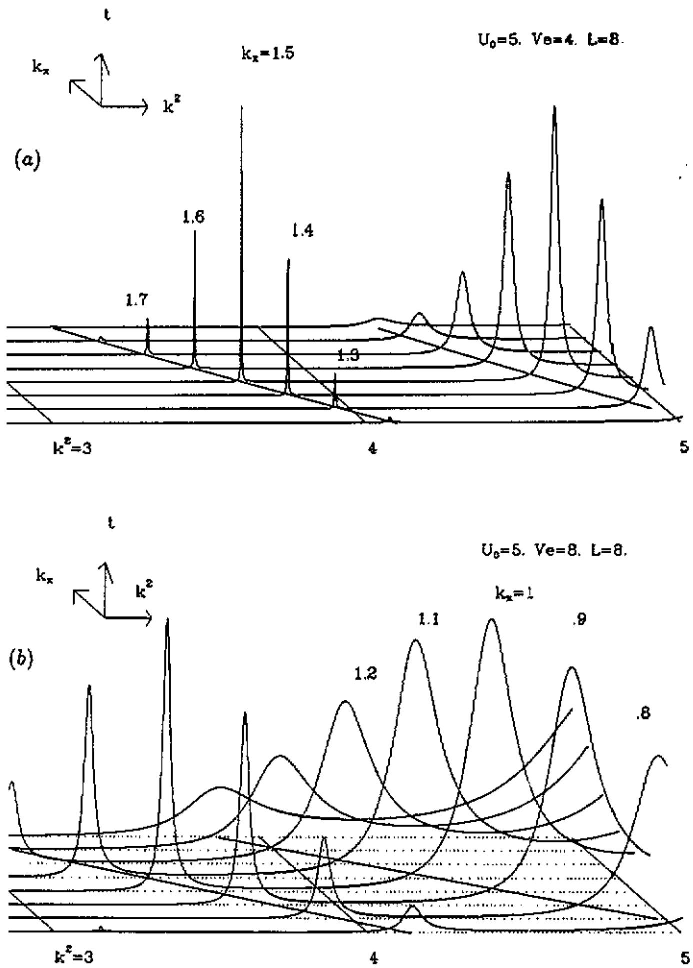

Figure 2. The transmission coefficient t as a function of k_x and k^2 for two values of Ve: (a) $Ve = 4$ and (b) $Ve = 8$. The numbers above the peaks indicate k_x values.

3. The tunnelling current and the differential conductivity

Assuming that the barrier separates two reservoires of electrons the transmission coefficient of equation (4) gives the following tunnelling current I per unit area:

$$I = 2I_0 \int_0^\infty \mathrm{d}E\,[f(E) - f(E - Ve)] \iint_{\mathcal{D}} \mathrm{d}k_x\,\mathrm{d}k_z t(\sqrt{E - k_z^2}, k_x) \tag{5}$$

where $I_0 = e\omega_c/8\pi^3\lambda^2$ is the reference density current and f is the Fermi distribution [8]. The integration domain $\mathcal{D}$ is the definition set of t as a function of k_x and k_z, whereas t in the set shown in figures 3 (a) and (b) t depends on the variables k_x and $k = \sqrt{E - k_z^2}$. Our bias is of the order of the Fermi energy E_F so that we are outside the range of linear response. Therefore, we do not use the Landauer formula giving the conductance in terms of the transmission coefficient [9]. Assuming that we are at

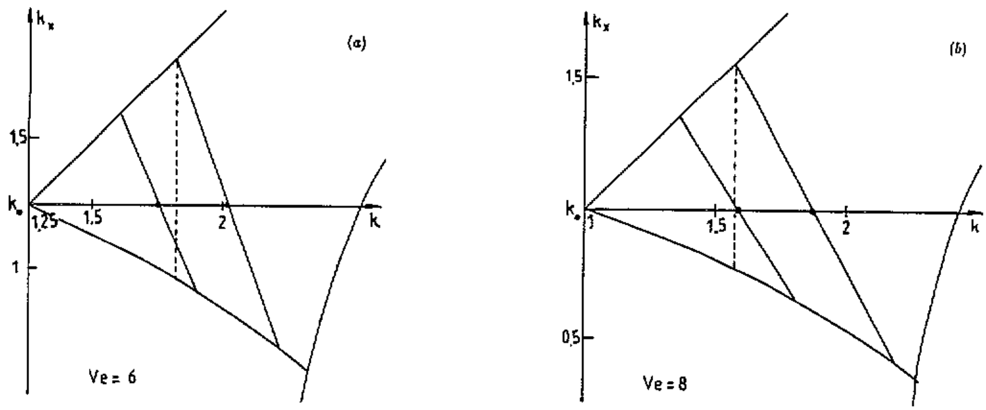

Figure 3. Trajectories of the resonances in the domain $t > 0$, in the k versus k_x plane.

$T = 0°$ K, the inverse tunnelling current is zero for $Ve > 0$ and equation (5) becomes:

$$I = 2I_0 \int_{E_m}^{E_F} \mathrm{d}E \iint_{\mathcal{D}} \mathrm{d}k_x\, \mathrm{d}k_z\, t(\sqrt{E - k_z^2}, k_x)$$

in which

$$E_m = (E_F - Ve)\, \Theta(E_F - Ve)$$

where Θ is the step function. We note that, as a consequence of the reciprocity, the reduction to an equivalent one-dimensional scattering process makes sure that the inverse process has the same transmission coefficient [10].

When the polarization is small, or the barriers are sufficiently wide, k_0 is positive. If $E_F < k_0^2$, the current is zero. For $E_F > k_0^2$ the energy of levels participating in the conduction lies between E_F and E_m. The current density is given by

$$\frac{I}{I_0} = \mathcal{F}(k_0, E_F) - \Theta(E_m - k_0^2)\mathcal{F}(k_0, E_m) \tag{6}$$

where

$$\mathcal{F}(k_0, \epsilon) = 4 \int_{k_0}^{\sqrt{\epsilon}} \mathrm{d}k\, k\sqrt{\epsilon - k^2} \int_{k_1}^{k} \mathrm{d}k_x t(k, k_x) \tag{7}$$

and $k_1 = L/2 - \sqrt{k^2 + Ve}$.

If k_0 negative, the current is given by

$$\frac{I}{I_0} = \mathcal{F}(0, E_F) - \Theta(E_m)\mathcal{F}(0, E_m)$$

provided the definition of k_1 is changed to

$$k_1 = -k \qquad \text{for } k \leqslant |k_0|$$
$$k_1 = L/2 - \sqrt{k^2 + Ve} \qquad \text{for } k \geqslant |k_0|.$$

However, the resonances play a role in the tunnelling process only when the barrier is sufficiently wide, so that hereafter we limit ourselves to the case $k_0 > 0$.

To obtain the differential conductivity g, let us begin the evaluation

$$\frac{\partial \mathcal{F}(k_0, E_m)}{\partial(Ve)} = 4 \int_{k_0}^{\sqrt{E_m}} \mathrm{d}k \left(k\sqrt{E_m - k^2}\frac{\partial \mathcal{G}}{\partial(Ve)} - \frac{k}{\sqrt{E_m - k^2}}\mathcal{G} \right) \tag{8}$$

where

$$\mathcal{G} = \int_{k_1}^{k} \mathrm{d}k_x t(k, k_x)$$

and

$$\frac{\partial \mathcal{G}}{\partial(Ve)} = \int_{k_1}^{k} \mathrm{d}k_x \frac{\partial t(k, k_x)}{\partial(Ve)}.$$

The second term on the right-hand side of equation (8) vanishes when we evaluate $\partial\mathcal{F}/\partial(Ve)$ at E_{F}, so that we get

$$g = 4g_0 \left[\int_{k_0}^{\sqrt{E_{\mathrm{F}}}} \mathrm{d}k \;\; k\sqrt{E_{\mathrm{F}} - k^2}\frac{\partial \mathcal{G}}{\partial(Ve)} - \Theta(E_m - k_0^2) \int_{k_0}^{\sqrt{E_m}} \mathrm{d}k \left(k\sqrt{E_m - k^2}\frac{\partial \mathcal{G}}{\partial(Ve)} - \frac{k}{\sqrt{E_m - k^2}}\mathcal{G} \right) \right] \tag{9}$$

in which $g_0 = e^2/\hbar 8\pi^3\lambda^2$ is the reference conductivity.

The first contribution to the conductivity is due to the change in the barrier penetration probability with Ve, i.e., due to the terms containing $\partial\mathcal{G}/\partial(Ve)$. The term containing $\mathcal{G}$ yields an additional positive contribution because a higher bias increases the number of electron states that participate in tunnelling. The conductivity of a square barrier without the magnetic field is always the sum of such a term with the first terms [8]. On the contrary, when the magnetic field is turned on, the terms depending on E_m may vanish if k_0 is sufficiently large.

The derivative of t with respect to Ve is given by equation (4)

$$\frac{\partial t}{\partial(Ve)} = \frac{1}{t_2}\left(\frac{2k_y}{k_y'} - t\frac{\partial t_2}{\partial(Ve)} \right) \tag{10}$$

where

$$t_2 = w_1^2 + k_y^2 w_2^2 + k_y'^2 w_3^2 + k_y^2 k_y'^2 w_4^2 + 2k_y k_y'$$

and

$$\frac{\partial t_2}{\partial (Ve)} = 2w_1(-z_0 w_1' - z_1 w_2 - z_2 w_3) + 2k_y^2 w_2(-z_0 w_2' - 2w_1/L - z_2 w_4) + w_3^2 + 2k_y'^2 w_3(-z_0 w_3' - z_1 w_4 - 2w_1/L) + k_y^2 w_4^2 + 2k_y^2 k_y'^2 w_4(-z_0 w_4' - 2(w_3 + w_2)/L) + k_y/k_y'$$

where

$$z_0 = y_0/L \qquad z_1 = 2(y_0^2/4 + a)/L \qquad z_2 = 2((L - y_0)^2/4 + a)/L.$$

Here the primed w_i indicate partial derivatives with respect to the index a. We note that $\partial t/\partial(Ve)$ has an integrable singularity at $k_x = k_1$ because for this value of k_x, $k_y' = 0$. The analytical calculation is needed to take care of this singularity. We obtain

$$\int_{k_1}^{k} \mathrm{d}k_x \frac{\partial t}{\partial (Ve)} = F_1 \left(\sin^{-1} \frac{k - L/2}{k_1 - L/2} - \frac{\pi}{2} \right) + \int_{k_1}^{k} \mathrm{d}k_x \frac{F(k_x) - F_1}{k_y'}$$

where

$$F(k_x) = \frac{2k_x}{t_2^2} \left(t_2 - 2k_y'^2 \frac{\partial t_2}{\partial (Ve)} \right)$$

and

$$F_1 = F(k_1) = \frac{2k_y(k_1)}{t_2(k_1)}.$$

We thus obtain

$$\lim_{k_x \to k_1} \frac{F(k_x) - F_1}{k_y'} = -F_1^2.$$

Let us use to junctions like GaAs/Al_xGa_{1-x}As/GaAs to make a choice of the parameters. With an effective mass of 0.067 electron masses, we have

$$\hbar\omega_c = 1.7B\,[\text{Tesla}]\ \text{meV} \qquad \text{and} \qquad \lambda = \frac{180}{\sqrt{B\,[\text{Tesla}]}}\ \text{Å}.$$

Devices like this have been studied by Gueret *et al* [11] with barriers of heights $U_0 = 40$ meV and 83 meV and widths $L = 430$ Å, 250 Å, with a maximum magnetic field of 4 Tesla. The doping of GaAs places the Fermi level 12 meV above the conduction band minimum in each GaAs layer. At $V = 5$, 10 and 20 mV, the junction bias is low.

To emphasize the effect of the resonances on the current, we consider wider barriers with higher bias, and higher Fermi levels. Figure 4 shows the current as a function of E_F for various voltages. When the Fermi level is close to a resonance, a conduction channel opens and the current displays a sudden increase. This can be better seen

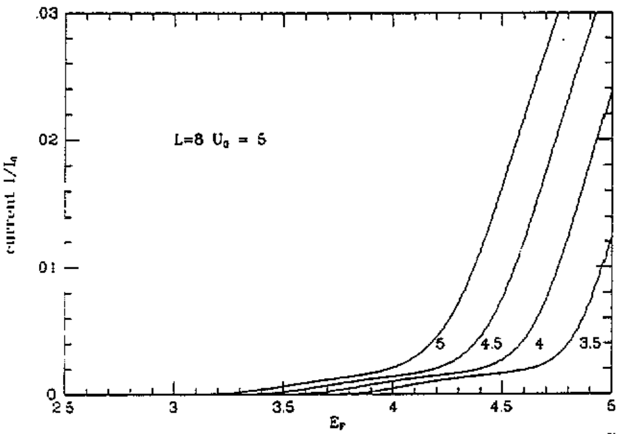

Figure 4. Current density in units of I_0 as a function of the Fermi energy. The numbers at the curves indicate the Ve values, for $U_0 = 5$ and $L = 8$.

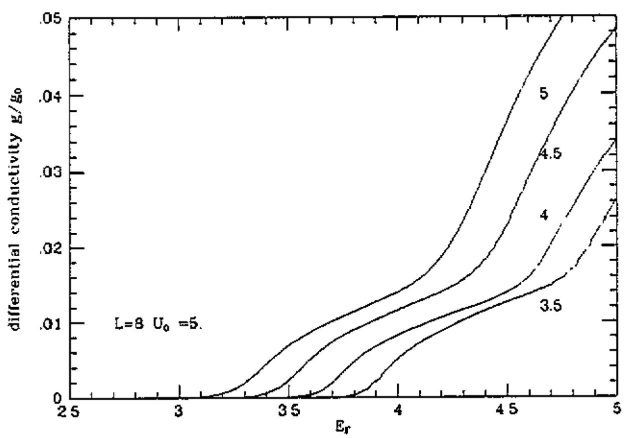

Figure 5. The differential conductivity in units of g_0 as a function of the Fermi energy, for the same values of parameters as in figure 4.

in the differential conductivity g that exhibits some smooth plateaus (figure 5). The resonances are located at approximately the points

$$k^2 \sim U_0 - Ve/2 + (Ve/L)^2 + n + \tfrac{1}{2} \tag{11}$$

obtained by adding k_0^2 to k_y^2 of equation (3). For the chosen values of parameters, we have only two resonances. The second one is close to the top of the barrier. Equation (11) implies that as Ve increases, the resonances move down in energy and the opening of a channel occurs at a smaller E_F. However, as noted before, when the bias becomes very large the effects of the resonances tend to overlap and the structures in the current are lost (see figure 6).

A comparison with experiment could be better done by calculating I and g as functions of Ve, at a fixed E_F. In figure 7, $\log I$ is plotted as a function of Ve at various E_F, while figure 8 shows the corresponding behaviour of $\log g$. The step due

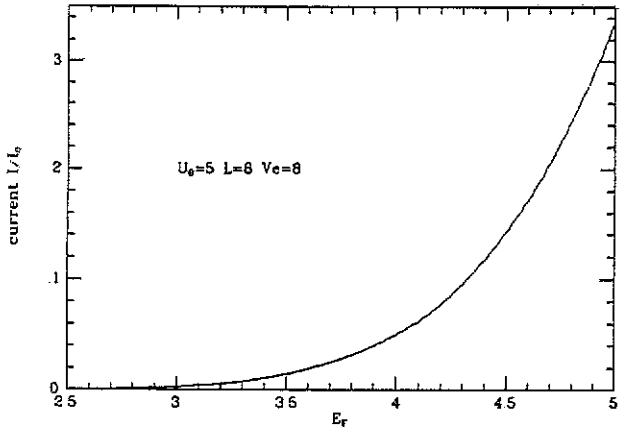

Figure 6. Current as a function of E_F at a large bias ($U_0 = 5$, $L = 8$). Note that the steps have disappeared.

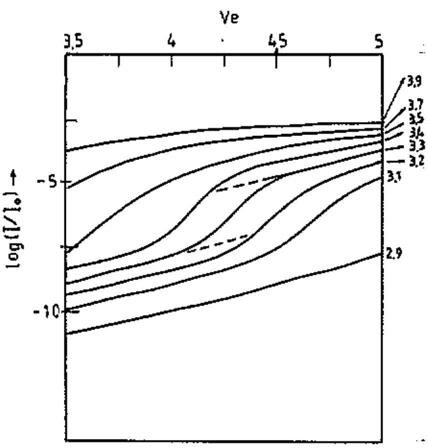

Figure 7. $\log(I/I_0)$ as a function of Ve ($U_0 = 5$, $L = 8$). The numbers alongside each curve give the values of E_F.

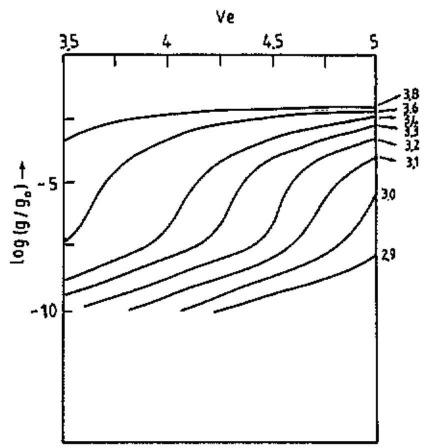

Figure 8. $\log(g/g_0)$ as a function of Ve ($U_0 = 5$, $L = 8$). The numbers alongside each curve give the values of E_F.

to the first resonance is evident both in $\log I$ and in $\log g$: for both quantities, the step amplitude is about two orders of magnitude. At higher E_F, the step appears at a smaller bias, because E_F comes closer to the value of k^2 given by equation (11) at lower Ve.

The previous discussion refers to a three-dimensional configuration. We expect that for a two-dimensional system the resonances play a more relevant role because there is now no smoothing effect of the integration over k_z. In two dimensions, all the former stuff is recovered by changing the definition of $\mathcal{F}$ in

$$\mathcal{F}(k_0, \epsilon) = 4 \int_{k_0}^{\sqrt{\epsilon}} \mathrm{d}k\, k \int_{k_1}^{k} \mathrm{d}k_x\, t(k, k_x)$$

and taking $I_0 = e\omega_c/4\pi^2\lambda$ as the reference current and $g_0 = e^2/4\pi^2\hbar\lambda$ and the refer-

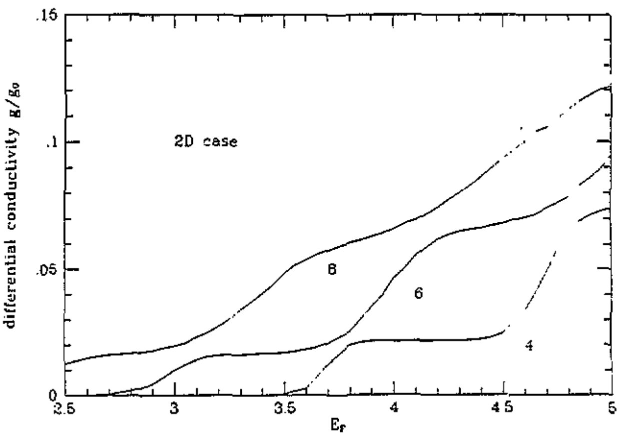

Figure 9. g/g_0 as a function of Ve in two dimensions ($U_0 = 5$, $L = 8$). As in figures 7 and 8, the numbers alongside the curves are the values of E_F.

ence conductivity. We limit ourselves to showing in figure 9 the behaviour of g as a function of E_F. The steps are sharper in two dimensions, but they tend to disappear again as the bias goes up.

4. Summary

We have investigated the tunnelling current flow across a thick, voltage biased square barrier in a transverse magnetic field. The magnetic field is confined within the barrier. A detailed study of the transmission coefficient shows that quasi-levels, resembling the Landau levels, appear when the barriers are sufficiently wide. These quasi-levels are found only for some values of the momentum on the plane perpendicular to the field and for its component parallel to the barrier. The barrier can be traversed with probability one, at certain directions of incidence, at energies lower than the maximum barrier height. Therefore, the magnetic field gives rise to a sort of dynamical constriction. We have shown that if a bias is applied to the barrier, the tunnelling current and the differential conductivity have a stepped behaviour, being functions of either the Fermi level or the applied voltage. We have performed the calculations both in three and in two dimensions. The steps are more evident in two dimensions. The deformation of the barrier due to the magnetic field produces effects that resemble those of an external potential causing a lateral constriction.

We carried out measurements on low, thick semiconductor barriers like those in $GaAs/Al_xGa_{1-x}As/GaAs$ heterostructures that have already been studied theoretically and experimentally by Gueret *et al* [11]. These authors measure the field dependence of the tunnelling current at different applied biases and compared it with a theoretical estimate. Their theory uses a WKB calculation of the transmission coefficient with the magnetic field confined within the barrier. They find the experimental data agree with the theory. We have used the same model to perform a complete calculation of the transmission coefficient without any restriction imposed on the barrier parameters. The stepped behaviour of the tunnelling current conductivity is obtained for the barrier parameters whose values are close to those studied by Gueret *et al.* With a magnetic field of 3 Tesla, the parameters of the barrier used in the figures are

$U_0 = 25$ meV and $L = 830$ Å. The corresponding values in [11] are $U_0 = 40$ value of $E_F = 12$ meV, the resonances cannot arise in their device.

At very low temperatures, the phase coherence length can exceed the barrier width. In this case we have to take into account the effect of the magnetic field in the region outside the barrier. In our opinion, a magnetic field leaking out of the barrier requires the barrier to be higher if structures are to be searched for in the transmission (see [1] p 2208).

Acknowledgments

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