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1991 J. Phys.: Condens. Matter 2 8953

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Quantum tunnelling of electrons through a GaAs– $\text{Ga}_{1-x}\text{Al}_x\text{As}$ superlattice in a transverse magnetic field: an analytical calculation of the transmission coefficient

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Received 28 March 1990, in final form 6 June 1990

Abstract. The transmission coefficient for tunnelling through double barriers and superlattices of GaAs– $\text{Ga}_{1-x}\text{Al}_x\text{As}$, under transverse-magnetic-field action, has been calculated using a transfer matrix model. In this work, the one-dimensional effective-mass equation has been first solved analytically by means of the confluent hypergeometric functions as envelope functions.

Since the advent of exacting epitaxial growth techniques, particularly molecular-beam epitaxy and metallo-organic chemical vapour deposition, realization of superlattices and quantum well structures has become possible. The superlattices, as originally proposed by Esaki and Tsu [1], have found wide application in many new devices, such as photodetectors [2–5], transistors [6, 7] and light emitters [8]. The most thoroughly studied material system has been GaAs– $\text{Ga}_{1-x}\text{Al}_x\text{As}$ owing to the relative ease of its fabrication as well as its close lattice matching. Several experimental measurements have recently confirmed the presence of resonant tunnelling in single- and double-quantum-well structures [9–12]. Optical absorption measurements [13] have also independently verified the formation of superlattice minibands arising from the coupling of adjacent quantum states.

The theories to explain the resonant tunnelling phenomena generally can be divided into three different approaches: the use of the Wentzel–Kramers–Brillouin (WKB) approximation [14, 15] (which is valid if the barrier energy varies slowly compared with the scale of the electron wavelength); a Monte Carlo solution of the semiclassical Boltzmann transport equation [16, 17] (in which case a quasi-particle of electron is assumed); the transfer matrix approach which gives the transmissivity of the structure as a function of the energy directly. The WKB approximation is not valid in the devices of greatest interest, those with narrow barriers, because the potential changes rapidly in these structures. For the WKB method to be valid, the change in the wavelength in the potential energy relative to the kinetic energy must be small, i.e. the wavelength must be small compared with the distance over which the momentum changes appreciably. This situation is not satisfied in the structures in which barriers are narrow, especially at low incident carrier energies. The Monte Carlo method is useful because it includes phonon scattering but does not easily lend itself to the calculation of the structure

transparency. In the transfer matrix model, Tsu and Esaki [18] first provided a theoretical description of the electron tunnelling current density in a multilayer structure. Their approach involves the solution of the Schrödinger equation in each region of the device under the assumption that the effective mass is constant throughout, and phonon scattering can be neglected. The tunnelling transmission coefficient is then determined by the transfer matrix method. A 2×2 matrix at each interface is formed by matching the continuity of the wavefunctions and their derivatives. Successive multiplication of these matrices then couples the incident wavevector to the outgoing wavevector of the heterostructure stack.

The present availability of high-quality semiconductor heterostructures and high magnetic fields has stimulated many experimental studies of magnetotransport in low-dimensional electronic systems. A particular topic of increasing current interest concerns the effect of a transverse magnetic field on the tunnel current because the electrons are forced to execute cyclotron motion while tunnelling through the barrier in the plane perpendicular to the field [19–24]. In this paper, such an effect on the tunnelling probability of a charged particle through a double barrier (DB) and superlattice of GaAs–Ga_{1-x}Al_xAs has been investigated in the transfer matrix approach, but using the exact solution of the associated one-dimensional effective-mass equation.

Let us consider a beam of particles, with kinetic energy E and effective mass m_1 (m_b inside the barrier), incident on a rectangular potential barrier of height V_0 and width d . According to quantum theory, the electron, even if its energy is lower than V_0 , can traverse the barrier by quantum mechanical tunnelling. The effect of an applied magnetic field \mathbf{B} on the tunnel current in this structure is expected to be largest when the field is acting perpendicular to the current direction [19]. This has a simple classical analogue: when the electron is moving perpendicular to \mathbf{B} , the Lorentz force $-|e|\mathbf{v} \times \mathbf{B}$ is a maximum. In the case in which $\mathbf{B} \parallel \mathbf{x}$ and z is the heterostructure growth direction, the Hamiltonian of the system is given by [25]

$$H = -(\hbar^2/2m_j)\nabla^2 + e^2 B^2 z^2/2m_j c^2 - (ie\hbar Bz/m_j c)(\partial/\partial y) + V_0(z) \quad (1)$$

where $j = w, b$ and V_0 represents the barrier potential profile. We have chosen the gauge $\mathbf{A} = (0, -Bz, 0)$. By using plane waves in the x and y direction (and neglecting spin effects), one finds that the envelope function $\psi(z)$ describing the motion along the z direction satisfies the equation $H_0\psi(z) = E\psi(z)$, where E is the particle energy and the effective-mass Hamiltonian is given by

$$H_0 = -(\hbar^2/2m_j)(d^2/dz^2) + \frac{1}{2}m_j\omega_j^2(z - z_0)^2 + V_0(z) \quad (2)$$

where the free-particle motion along x has been ignored. Here we have used the definitions $\omega_j = eB/m_j c$ and $z_0 = -\hbar k_y c/eB$. When $V_0 = \text{constant}$, equation (2) reduces to the familiar harmonic oscillator Hamiltonian, the solutions of which are the equidistant Landau levels having the same energy $\hbar\omega_j(n + \frac{1}{2})$ for any k_y -value. In the presence of a step-like potential $V_0(z)$ the translational invariance along z is broken and the eigenvalues of (2) depend on z_0 , the coordinate of the classical cyclotron orbit centre [26]. The observed reduction in the tunnel current in a single barrier placed in a magnetic field [26] can be easily understood in terms of the increase in the effective barrier height due to the diamagnetic term in (2). If one assumes that the magnetic field is confined to the barrier region, then the last two terms in (2) can be viewed as giving an effective potential barrier.

Therefore our calculation is performed in a straightforward way by solving exactly the Schrödinger equation in each region (barrier and well) and applying the continuity

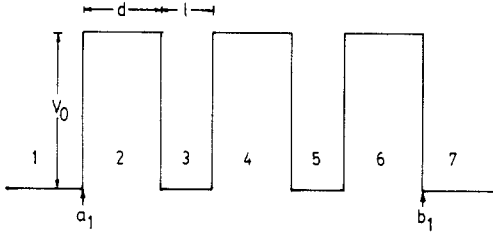


Figure 1. Typical potential structure for resonant tunnelling experiments at $B = 0$ applied magnetic field. In this work, $V_0 = 0.3$ eV, $l = 25$ Å, $d = 50$ Å, $m_w = 0.067$ and $m_b = 0.087$.

of the logarithmic derivative at each boundary. A representative multilayer stack is diagrammatically drawn in figure 1 where d and l are the barrier and well widths, respectively. We shall assume that the transverse magnetic field is confined from region 2 to $2n$ both included in (a_1, b_1) . The solution of the Schrödinger equation in region 1 is a linear combination of an incident and a reflected plane wave:

$$\psi_1(z) = \exp(ik_1z) + R \exp(-ik_1z) \quad (3)$$

where R is a constant, $k_1 = \sqrt{2m_1E}/\hbar$ and m_1 is the effective mass in the narrow gap of the GaAs layer. Equation (2) can be solved analytically in pair (barrier) and odd (well) regions as

$$\psi_{b,w}(z) = A_{b,w}f_{b,w}(z) + B_{b,w}g_{b,w}(z) \quad (4)$$

where $A_{b,w}$ and $B_{b,w}$ are $4(n-1)$ arbitrary constants and

$$f_{b,w}(z) = U(a_{b,w}, \frac{1}{2}, \zeta^2) \exp(-\frac{1}{2}\zeta^2) \quad (5a)$$

$$g_{b,w}(z) = M(a_{b,w}, \frac{1}{2}, \zeta^2) \exp(-\frac{1}{2}\zeta^2). \quad (5b)$$

U and M are confluent hypergeometric functions [27] (see appendix), and

$$a_b = [1 - (2/\hbar\omega_b)(E - V_0 + \hbar^2k_y^2/2m_b)] \quad (6a)$$

$$\zeta^2 = (Be/\hbar c)(z + c\hbar k_y/eB)^2 \quad (6b)$$

where m_b (m_w) is the electron effective mass in the barrier (well), V_0 is the barrier height and $\omega_b = eB/m_b c$. In the well-like regions,

$$a_w = [1 - (2/\hbar\omega_w)(E + \hbar^2k_y^2/2m_w)] \quad (7)$$

and $\omega_w = eB/m_w c$. In region $2n + 1$ we again have a plane wave [28]:

$$\psi_{2n+1} = \tau \exp(-ik_{(2n+1)}z) \quad (8)$$

where τ is a new constant. If we apply the usual boundary conditions at the well–barrier interfaces, this yields in matrix form

$$\begin{pmatrix} 1 \\ R \end{pmatrix} = \mathbf{N}(z) \begin{pmatrix} \tau \\ 0 \end{pmatrix} \quad (9)$$

where the matrix $\mathbf{N}(z)$ is

$$\mathbf{N}(z) = \frac{1}{2ik_1} \begin{pmatrix} ik_1 & 1 \\ ik_1 & -1 \end{pmatrix} \mathbf{S}(z) \begin{pmatrix} 1 & 1 \\ ik_{(2n+1)} & -ik_{(2n+1)} \end{pmatrix} \quad (10)$$

and

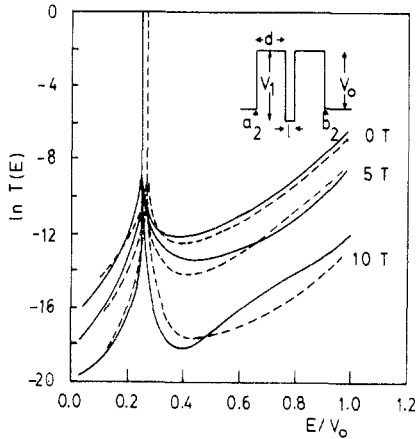


Figure 2. DB transmission probability $T(E, n = 2)$ for different values of the magnetic field: —, this work; ---, from [25]. The potential energy profile used at $B = 0$ is shown in the inset ($d = 200 \text{ \AA}$, $l = 30 \text{ \AA}$, $m_w = 0.067$, $m_b = 0.087$, $V_0 = 0.04 \text{ eV}$ and $V_1 = 0.11 \text{ eV}$).

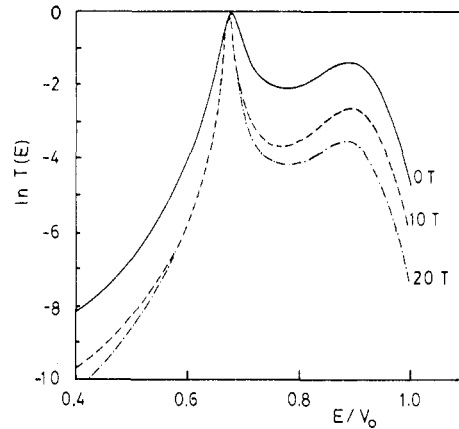


Figure 3. Transmission probability $T(E, n = 3)$ for different values of the applied transverse magnetic field: —, $B = 0 \text{ T}$; ---, $B = 10 \text{ T}$; - · -, $B = 20 \text{ T}$. The potential profile used at $B = 0 \text{ T}$ is the same as in figure 1.

$$\mathbf{S}(z) = \mathbf{S}_b(z=0)\mathbf{S}_b^{-1}(z=d)\mathbf{S}_w(z=d)\mathbf{S}_w^{-1}(z=d+1)\mathbf{S}_b(z=d+1) \dots \mathbf{S}_b^{-1}[z=nd+(n-1)l] \quad (11)$$

where the transfer matrices

$$\mathbf{S}_{b,w}(z) = \begin{pmatrix} f_{b,w}(z) & g_{b,w}(z) \\ f'_{b,w}(z) & g'_{b,w}(z) \end{pmatrix}. \quad (12)$$

The transmission probability $T(E)$ can be found from (9) as $T(E) = k_1 N_{11}^2(z)/k_{(2n+1)}$ [28]. Therefore,

$$T(E) = (4k_1/k_{(2n+1)})\{[(\alpha + k_1)/\delta k_{(2n+1)}]^2 + [\gamma/(k_1 - k_{(2n+1)})\beta]^2\} \quad (13)$$

where $\alpha, \beta, \gamma, \delta$ are the elements of the $\mathbf{S}(z)$ matrix.

Let us consider explicitly one-electron tunnelling through a DB structure placed in a transverse magnetic field. It is well known that resonant tunnelling [29] occurs at an incident particle energy E_0 where there is a quasi-local level within the barriers. The transmission probability has a sharp peak near $E = E_0$ and the thickness of the confining barriers mainly affects the width of the peak, the latter being related to the lifetime for escape out of the well [24]; this peak gives in turn the dominant contribution to the tunnelling current through the DB. We have used in our calculation the same barrier potential profile for GaAs–Ga_{1-x}Al_xAs as in [25] (shown in the inset of figure 2). The magnetic field is assumed to be confined [30] in the barrier region (in the (a_2, b_2) interval of the inset of figure 2). The transmission probability $T(E)$ for the DB (where E is the incident particle energy) has been calculated with $n = 2$. Figure 2 shows the logarithm of $T(E)$ (obtained in this work) plotted for several values of the applied magnetic field B and compared with the WKB transmission probability, under the magnetic field action, obtained by Ancilotto [25]. He computed two linearly independent (numerical) solutions of the Schrödinger equation in the interval (a_2, b_2) , matching them with the plane-wave

solutions, and using the same electron effective masses inside the well and barriers. The curves shown in figure 2 refer to the particular case $z_0 = -\hbar k_y c / eB = 0$ (symmetric effective barrier) where $T(E)$ is a maximum. We have chosen $z_0 = 0$ (as in [25]) in order to compare appropriately both methods of calculation. An average over this coordinate yields the expected reduction, in the tunnelling current, proportional to $\exp(-B^2)$ for DB heterostructures [31] (figure 2). We have superimposed the $B \neq 0$ curves on the $B = 0$ curve; actually they should be slightly shifted as in [25]. Note that the value of $T(E)$ at resonance is not affected by the magnetic field, but the overall shape of the transmission coefficient reflects the expected reduction in current along the heterostructure axis [19].

As another example, we have calculated the $T(E)$ -value for a GaAs-Ga_{0.7}Al_{0.3}As superlattice with $n = 3$ (two wells and three barriers), $d = 50 \text{ \AA}$ (barrier) and $l = 25 \text{ \AA}$ (well). The required confluent hypergeometric functions have been exactly obtained as shown in the appendix. In this case we have taken different electron effective masses for wells and barriers as our expressions allow us to do. Figure 3 shows the transmission probability T (in logarithmic scale) versus the energy E of the incident particle, for several values of the applied magnetic field. At $B = 0$ we find that one recovers the well known structure of two peaks of $T(E)$ for two wells and three barriers [32]. The strong reduction in the tunnel current in figures 2 and 3 with increasing B is a consequence of the change in the momentum in the current direction induced by the Lorentz force (from a semiclassical point of view). If the magnetic field is confined to the barrier region, then the last two terms in (2) can be viewed as giving an effective potential barrier that increases with increasing B (so decreasing the transmission coefficient). However, a strong enhancement of the transmission coefficient at resonance takes place and the electron can easily complete its orbit through the barriers without being scattered so that the resonance peak will always be equal to unity at resonance although the field B increases. The combination of the latter two effects explains the fact that the main peak in figures 2 and 3 narrows when the field increases.

In summary, we have calculated the transmission coefficient $T(E)$ for tunnelling through DB heterostructures and superlattices under transverse magnetic fields in a transfer matrix model. The one-dimensional effective-mass equation has been solved first analytically by means of the confluent hypergeometric functions as envelope functions. These have been shown to be a powerful tool for the analysis of several physical properties. We have found the expected reduction in current along the heterostructure axis due to the Lorentz force as reflects the shape of $T(E)$. Finally, let us mention that our method gives exact results in narrow-barrier structures when the WKB approximation is not valid. The present work can be extended to energies above the barrier because confluent hypergeometric functions account for these states too; this will be the subject of a future work.

Acknowledgments

This work has been supported in part by the Gobierno Autónomo de Canarias. The authors also wish to thank Dr Muñoz for several helpful comments and remarks.

Appendix

The confluent hypergeometric functions $M(a, b, x)$ and $U(a, b, x)$ obtained as analytical solutions of equation (2) can be found in [27], where x is the variable. These functions are defined as follows:

$$M(a, b, x) = 1 + ax/b + (a)_2 x^2 / (b)_2 2! + \dots + (a)_n x^n / (b)_n n! + \dots \quad (\text{A1})$$

$$U(a, b, x) = [\pi / \sin(\pi b)] [M(a, b, x) / \Gamma(1 + a - b) \Gamma(b) - x^{1-b} M(1 + a - b, 2 - b, x) / \Gamma(a) \Gamma(2 - b)] \quad (\text{A2})$$

where $(a)_n = a(a+1)(a+2)\dots(a+n-1)$, $a_0 = 0$, and analogously for $(b)_n$. Taking the values of a, b, x from (5a) and (5b) and expanding (A1) and (A2) in a series of Bessel functions J_n of fractional order, we find that

$$f(z) = z^{1/2} \sum_{n=0}^{\infty} \alpha_n \left(\frac{Bz}{k_l} \right)^n J_{n-1/2}(k_l z) \quad (\text{A3})$$

$$g(z) = z^{1/2} \sum_{n=0}^{\infty} \beta_n \left(\frac{Bz}{k_l} \right)^n J_{n+1/2}(k_l z) \quad (\text{A4})$$

where $\alpha_0 = 1$, $\alpha_1 = 0$, $\alpha_2 = \frac{1}{4}$, $(n+1)\alpha_{n+1} = (n - \frac{1}{2})\alpha_{n-1} + (2a - \frac{1}{2})\alpha_{n-2}$, $\beta_0 = 1$, $\beta_1 = 0$, $\beta_2 = \frac{3}{4}$, $(n+1)\beta_{n+1} = (n + \frac{1}{2})\beta_{n-1} + (2a - \frac{3}{2})\beta_{n-2}$ and $k_l = \sqrt{2m_l(E - V_0)}$. Adding a large number of terms in the expansions (A3) and (A4) until we obtain convergence in the series, we can compute $f(z)$ and $g(z)$ exactly. We can recover from (A3) and (A4) the well known envelope functions in the absence of external fields ($B \rightarrow 0$) for a finite quantum well: two plane waves. Note that in (A3) and (A4) for high B -values ($B > 30$ T) we must take a very large number of terms in the expansions to obtain convergence, needing longer computer time than for low B -values (in which case the calculation is straightforward and very fast). However, other theoretical methods such as that of WBK, involve the computation of two linearly independent numerical solutions of the Schrödinger equation requiring a long computer time for all B -values. Otherwise, the confluent hypergeometric functions account for any size of barriers, particularly for narrow barriers when the WBK method fails.

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