Transfer-matrix theory of the energy levels and electron tunneling in heterostructures under an in-plane magnetic field

K.-M. Hung and G. Y. Wu
Department of Electrical Engineering, National Tsin-Hua University, Taiwan, Republic of China
(Received 5 August 1991)

We present a unified treatment, within the transfer-matrix approach, of the energy levels and electron tunneling in heterostructures under an in-plane magnetic field. Parabolic cylinder functions are used to expand the electronic wave functions. The theory is applied to a double-barrier resonant-tunneling structure made of GaAs and $Ga_{1-x}Al_xAs$. A few low-lying conduction subbands and wave functions are calculated. The transmission coefficients and tunnel currents are also presented.

I. INTRODUCTION

In recent years, semiconductor heterostructures, proposed by Esaki and Tsu,[1] have become a field of great interest. They are studied as low-dimensional electronic systems, with potentially useful applications ranging from optoelectronics to high-speed devices. Especially interesting physical phenomena may arise when these structures are subjected to transverse magnetic fields. For example, the subjects of magneto-optics and magnetotunneling heterostructures have been widely investigated both theoretically and experimentally.[2–14]

From a theoretical point of view, since the presence of the transverse magnetic field breaks the tetragonal symmetry of the heterostructure problem, the in-plane-field case is more complicated than the case without the presence of magnetic field or the case with a field in the longitudinal direction. With the symmetry in the problem lowered by the field, theories of magneto-optics and magnetotunneling in the in-plane-field case usually resort to heavy numerical computations or sometimes are burdened with unnecessary, inappropriate approximations. Consider, for example, theories of the energy levels of heterostructures in a transverse magnetic field. These theories mostly employ the variational method. In a pioneering work, Ando calculated with this method the magnetic energy levels in a Si/SiO_2 inversion layer.[3] Later Xia and Fan carried out similar calculations for a superlattice structure.[4] In the calculation they expanded the wave function by a set of basis functions, represented the Hamiltonian operator in matrix form, and diagonalized the matrix to obtain both the energy eigenvalues and eigenfunctions. However, to achieve reasonable accuracy in computing the wave function, they needed to increase the number of the basis functions in proportion to the characteristic layer width of the structure. Since the CPU time consumed in diagonalizing the Hamiltonian goes roughly as the cube of the matrix dimension, the computational requirements in the variational method may become prohibitively expensive in the case of wide-layer structures.

In contrast, several theoretical approaches have been taken to study the physics of magnetotunneling through heterostructures in a transverse magnetic field. For example, Brey, Platero, and Tejedor applied the transfer-Hamiltonian technique to this problem.[5] But the main limitation of this technique is that of being a perturbation theory. On the other hand, Eaves, Stevens, and Sheard used the WKB method to study tunneling through a single barrier.[6] Later, Zaslavsky *et al.* applied the same method to resonant tunneling in a double-barrier structure.[7] However, the WKB approximation fails in the case of thin-layer structures.

Therefore, in the in-plane-field case, the need arises of developing a theory capable of treating magnetic energy levels and magnetotunneling exactly and efficiently, for arbitrary layer thickness. An interesting question is whether one can derive a theory along the lines of the transfer-matrix method that Tsu and Esaki originally developed for the problem of electron tunneling in a multibarrier structure.[15] This method involves solving the Schrödinger equation in each layer of the structure. In connecting the wave function through the interface, a 2×2 matrix at each interface is formed by matching the wave function and its derivative at the interface. From the product of these matrices, one can obtain the transmission probability of an electron tunneling through the entire structure. The transfer-matrix method is exact and efficient. It has also proved to be time saving and successful in superlattice band-structure theories.[16–18]

In this paper we report unified treatment, within the transfer-matrix method, of the energy levels and electron tunneling in heterostructures under a transverse magnetic field. In Sec. II we describe the theory of the energy levels. In Sec. III we describe the theory of electron tunneling. In Sec. IV we present our results on the energy levels, wave functions, transmission coefficients, and tunnel currents in a double-barrier structure. In Sec. V we give a summary and draw some conclusions.

II. THEORY OF ENERGY LEVELS

We consider the $GaAs/Al_xGa_{1-x}As$ heterostructure placed in crossed electric and magnetic fields with its growth direction along the z axis. The structure extends from $z=0$ to a. The magnetic field $\mathbf{B}$ is taken to be uniform and directed along the positive x direction; the electric field $\mathbf{E}_s$ is taken to be uniform and directed along the

z axis. For the magnetic vector potential we write $\mathbf{A}=(0,-Bz,0)$. We consider only magnetic energy levels in the conduction band and write the Hamiltonian as

$$H=\frac{1}{2m^*}[P_x^2+(P_y-eBz)^2+P_z^2]+V(z)+eE_s z \ , \tag{1}$$

within the effective-mass approximation, where m^* is the conduction-band effective mass and $V(z)$ is the heterostructure potential, including the effect of the conduction-band offset. Note that although the spin-field interaction $\mu_x B$ has been dropped from the Hamiltonian, its inclusion would not complicate the theory since that amounts to only adding a constant to the Hamiltonian. Moreover, in the GaAs/Al_xGa_{1-x}As case, the magnitude of this term is negligible compared with the other terms in the Hamiltonian.

Since the Hamiltonian in Eq. (1) is translationally invariant along both the x and y directions, the wave numbers k_x and k_y are good quantum numbers which may be used to label the wave function of the electron. Hence we can separate the spatial variables and write the wave function as a product,

$$\Psi_{k_x,k_y,\nu}(x,y,z)=\exp(ik_x x)\exp(ik_y y)\Phi_\nu(z) \ , \tag{2}$$

where ν further labels the energy eigenvalues. Putting the wave function in the wave equation $H\Psi=E\Psi$, we obtain the energy eigenvalue equation

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}+\frac{\hbar^2}{2m^* l^4}(z-z_0)^2+V(z)\right]\Phi_\nu(z) = \left[E_\nu(z_0,k_x)-eE_s z_0-\frac{\hbar^2 k_d^2}{2m^*}-\frac{\hbar^2 k_x^2}{2m^*}\right]\Phi_\nu(z) \ , \tag{3}$$

where $l\equiv\sqrt{\hbar/eB}$ is the magnetic length, a measure of the cyclotron-resonance orbital size; $z_0\equiv l^2(k_y-k_d)$ is the center coordinate of the orbital motion, with $k_d\equiv m^*E_s/\hbar B$, the drift momentum of the electron along the y axis in the crossed magnetic and electric fields. The energy eigenvalue $E_\nu(z_0,k_x)$ represents a conduction subband and has a quadratic k_x dependence:

$$E_\nu(z_0,k_x)=E_\nu(s_0,\ k_x=0)+\frac{\hbar^2 k_x^2}{2m^*} \ . \tag{4}$$

By further making the variable change $z\rightarrow\xi=\sqrt{2}(z-z_0)/l$, we rewrite Eq. (3) as

$$\frac{d^2}{d\xi^2}\Phi_\nu(\xi)-(\tfrac{1}{4}\xi^2+\nu)\Phi_\nu(\xi)=0 \ , \tag{5}$$

where the eigenvalue

$$\nu=\left[E_\nu(z_0,k_x)-eE_s z_0-\frac{\hbar_2 k_d^2}{2m^*}-\frac{\hbar^2 k_x^2}{2m^*}-V(z)\right]\Big/\hbar\omega_c \ , \tag{6}$$

with $\omega_c\equiv eB/m^*$ the cyclotron-resonance frequency. The standard solution to Eq. (5) is a linear combination of parabolic cylinder functions $U_\nu(\xi)$ and $V_\nu(\xi)$ or of their mirror images $U_\nu^*(\xi)$ and $V_\nu^*(\xi)$, with $U_\nu^*(\xi)\equiv U_\nu(-\xi)$ and $V_\nu^*(\xi)\equiv V_\nu(-\xi)$, when $V(z)$ is constant. Properties of parabolic cylinder functions are listed in Ref. 19. Here we briefly mention their analytic properties at $\xi=\pm\infty$, important for our application: $U_\nu(\xi)\rightarrow 0[U_\nu^*(\xi)\rightarrow 0]$ as $\xi\rightarrow+\infty$ (as $\xi\rightarrow-\infty$), whereas $V_\nu(\xi)[V_\nu^*(\xi)]$ diverges at $\xi=+\infty$ (at $\xi=-\infty$). Thus, in their analytic properties at large distances, parabolic cylinder functions and their mirror images behave asymptotically like the exponential functions $\exp(\pm\kappa\xi)$.

For the wave function inside the structure, we use both $U_\nu(\xi)$ and $V_\nu(\xi)$ [both $U_n^*(\xi)$ and $V_\nu^*(\xi)$] to expand it for $\xi>0$ ($\xi<0$). We stress that $V_\nu(\xi)$ and $V_\nu^*(\xi)$, though asymptotically divergent at large distances, have to be kept for expanding the wave function in each layer. Outside the structure, however, only $U_\nu(\xi)$ $[U_\nu^*(\xi)]$ is to be used for the wave function at $\xi>0$ ($\xi<0$). The wave function so represented satisfies the boundary condition $\Psi(z\rightarrow\pm\infty)=0$, which is required in our case since the electron is confined by the in-plane magnetic field.

To solve Eq. (3) on the whole domain $(-\infty,+\infty)$, we divide the space into many thin slabs, each of which with a nearly constant $V(z)$. In particular, we take the boundary points d_m, with $m=1,2,\ldots,n$, in the following order: $d_1\ (=-\infty)<d_2\ (=0)<\cdots<d_i\ (=z_0)<\cdots<d_{n-1}\ (=a)<d_n\ (=+\infty)$. Solving Eq. (3) in each slab, we obtain the wave function as follows:

$$\Psi=\begin{cases} A_1 U_{\nu_1}^*(\xi), & d_1<z<d_2 \\ A_j U_{\nu_j}^*(\xi)+B_j V_{\nu_j}^*(\xi), & d_{j\geq 2}<z<d_{j+1\leq i} \\ A_k U_{\nu_k}(\xi)+B_k V_{\nu_k}(\xi), & d_{k\geq i}<z<d_{k+1\leq n-1} \\ A_n U_{\nu_n}(\xi), & d_{n-1}<z<d_n \ , \end{cases} \tag{7}$$

where ν_m in each slab is calculated according to Eq. (6). To connect the wave function in one slab to that in the adjacent slab, we match Ψ and $(1/m^*)(\partial\Psi/\partial z)$ at the slab interface and form a 2×2 transfer-matrix equation for each interface:

$$\begin{bmatrix} A_m \\ B_m \end{bmatrix}=\begin{bmatrix} T_{11}^{[m]} & T_{12}^{[m]} \\ T_{21}^{[m]} & T_{22}^{[m]} \end{bmatrix}\begin{bmatrix} A_{m+1} \\ B_{m+1} \end{bmatrix} \ . \tag{8}$$

This allows us to relate the expansion coefficients of the wave function at the leftmost slab to those at the rightmost slab:

$$\begin{bmatrix} A_1 \\ 0 \end{bmatrix}=\underline{T}^{[1]}\underline{T}^{[2]}\cdots\underline{T}^{[n-1]}\begin{bmatrix} A_n \\ 0 \end{bmatrix} =\underline{T}\begin{bmatrix} A_n \\ 0 \end{bmatrix} \ , \tag{9}$$

which requires that the matrix element

$$T_{21}=0 \ . \tag{10}$$

Solving Eq. (10) results in the energy eigenvalues and eigenfunctions.

III. THEORY OF ELECTRON TUNNELING

We assume that the $GaAs/Al_xGa_{1-x}As$ structure is subjected to a transverse magnetic field **B** and a longitudinal electric field $\mathbf{E}_s$. Furthermore, for definitiveness, we take both fields to vanish outside the device region $(0,a)$. For the vector potential associated with the magnetic field, we write $\mathbf{A}=(0,0,0)$ for $z<0$, $\mathbf{A}=(0,-Bz,0)$ for $0<z<a$, and $\mathbf{A}=(0,-Ba,0)$ for $z>a$. We stress that the vector potential outside the structure, although only a constant, must be considered, since phases of the incident, reflected, and transmitted waves all depend on it. We consider electron transport in an n-type $GaAs/Ga_xAl_{1-x}As$ heterostructure and treat only the tunneling via the conduction band. In solving for the wave function of the tunneling electron, we follow the procedures outlined in Sec. II, but with minor modifications: Within the region of the structure, we still represent the wave function by a linear combination of the parabolic-cylinder functions, whereas outside the structure, we expand the wave function in plane waves. However, care should be taken in writing down the plane waves as discussed in the following.

At the left electrode where $z\in(-\infty,0)$, the Hamiltonian is that of a free electron,

$$H=\frac{P_x^2}{2m^*}+\frac{P_y^2}{2m^*}+\frac{P_z^2}{2m^*}\ , \tag{11}$$

and the wave function in this region is made of the plane waves incident onto and reflected from the structure,

$$\Psi(x,y,z)=\exp(ik_x x)\exp(ik_y y)\times[\exp(ik_z^l z)+R\exp(-ik_z^l z)]\ , \tag{12}$$

where $k_z^l=[2m^*(E-E_x-E_y^l)]^{1/2}/\hbar$ with E the total energy of the electron, $E_x\equiv\hbar^2k_x^2/2m_*$, and $E_y^l\equiv\hbar^2k_y^2/2m_*$. Note that RR^* represents the reflection coefficient of the electron.

On the other hand, at the right electrode where $z\in(a,+\infty)$, the Hamiltonian is

$$H=\frac{P_x^2}{2m^*}+\frac{(P_y-eBa)^2}{2m^*}+\frac{P_z^2}{2m^*}-eV_a\ , \tag{13}$$

where V_a is the applied bias. The wave function of the electron in this region is the transmitted plane wave:

$$\Psi(x,y,z)=T\exp(ik_x x)\exp(ik_y y)\exp(ik_z^r z)\ , \tag{14}$$

where $k_z^r=[2m^*(E+eV_a-E_x-E_y^r)]^{1/2}/\hbar$, with $E_y^r\equiv(\hbar k_y-eBa)^2/2m^*$. Note that $(k_z^r/k_z^l)TT^*$ represents the transmission coefficient, which, together with the reflection coefficient RR^*, satisfies the identity $RR^*+(k_z^r/k_z^l)TT^*=1$, the law of probability conservation.

Now, following the procedure described in Sec. II, we slice the structure into many thin slabs, relate the wave function at the left electrode to that at the right electrode, and obtain

$$\begin{bmatrix}1\\R\end{bmatrix}=\underline{T}_1\underline{T}_2\cdots\underline{T}_{n-1}\begin{bmatrix}T\\0\end{bmatrix}\ . \tag{15}$$

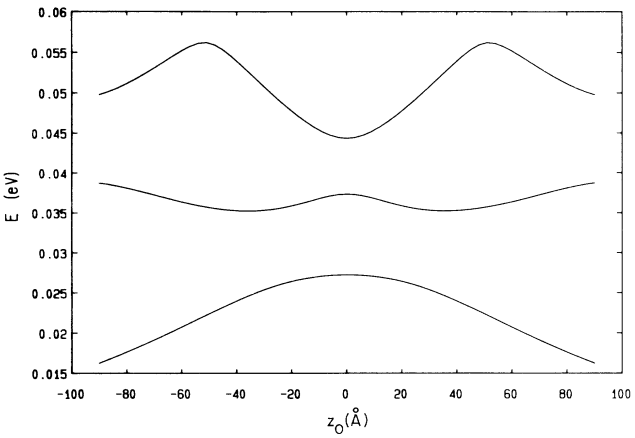

FIG. 1. Three lowest-energy subbands for the double-barrier structure. The magnetic field is taken to be 10 T. The electric field is taken to be zero. k_x is zero.

From the above equation one can then calculate the values of T and R and the tunnel current.

IV. RESULTS

We apply the theories outlined in Secs. II and III to a specific example and calculate the energy levels, wave functions, transmission coefficients, and tunnel currents in the double-barrier $GaAs/Al_{0.3}Ga_{0.7}$ As/$GaAs/Al_{0.3}Ga_{0.7}As/GaAs$ structure. The barrier is 28 Å wide and the well is 80 Å wide. The conduction-band offset is taken from Ref. 20. For the conduction-band effective mass, we use $0.067m_0$ in both the barrier and well. The origin of z is chosen to be at the well center.

We take $k_x=0$ in the energy-level calculation. In Fig. 1 we present a few low-lying energy subbands for the double-barrier structure. The magnetic field is taken to be 10 T. The curves are symmetrical with respect to $z_0=0$ as a result of inversion symmetry of the structure. In Fig. 2 we present the wave functions of the states at the edges of the subbands shown in Fig. 1. The wave

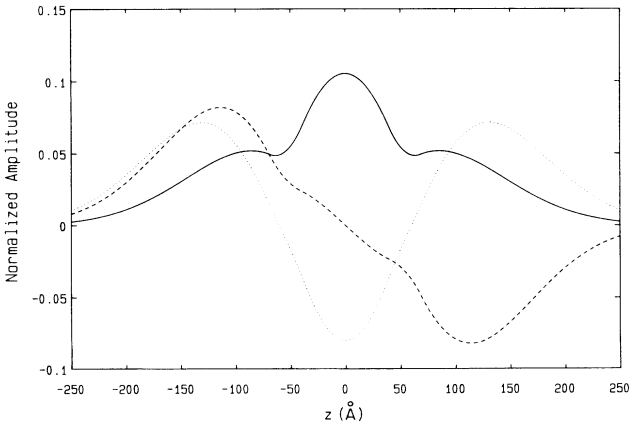

FIG. 2. Wave functions of the $z_0=0$ states at the low-lying subbands shown in Fig. 1. Solid curve, the lowest subband; dashed curve, the second subband; dotted curve, the third subband.

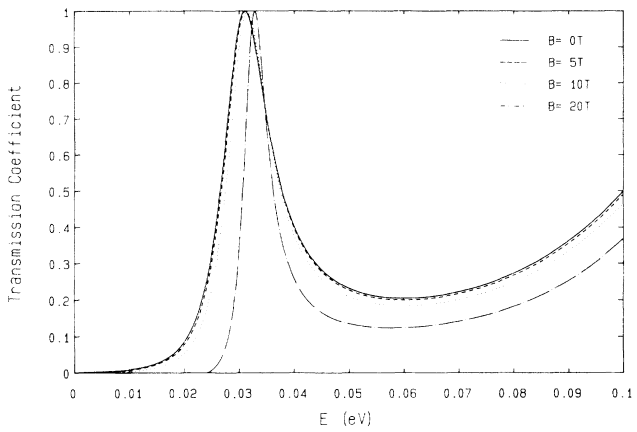

FIG. 3. Transmission coefficients as functions of E for the double-barrier structure at zero bias. Four magnetic fields are considered, namely 0, 5, 10, and 20 T. k_x and k_y are both taken to be zero.

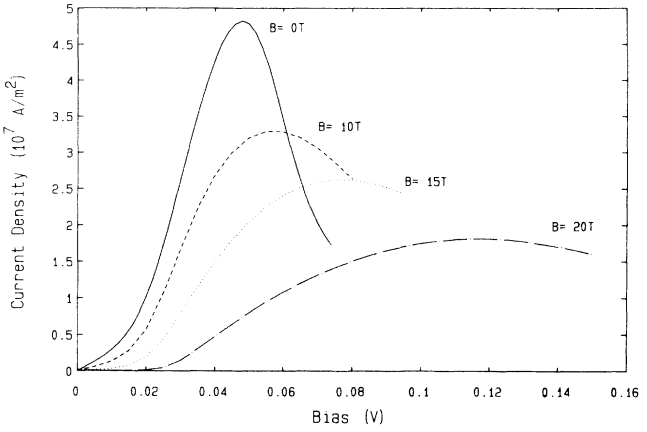

FIG. 4. Tunnel currents for the double-barrier structure. Four magnetic fields are considered, namely 0, 10, 15, and 20 T.

functions are all localized. They show zero, one, and two nodal points, respectively.

We again take $k_x=0$ in the calculation of transmission coefficients. In Fig. 3 we show the transmission coefficients as functions of the energy E for the double-barrier structure at zero bias. Four magnetic fields are considered, namely 0, 5, 10, and 20 T. k_y is taken to be zero. As shown in the figure, the energy where the transmission peaks increases with increasing magnetic field. On the other hand, the peak narrows and the transmission reduces overall with the magnetic field. In Fig. 4 we show the tunnel currents for the four magnetic fields 0, 10, 15, and 20 T. The peak current drops and the whole curve flattens out with increasing magnetic field. The voltage where the current peaks shifts to a higher value with increasing magnetic field.

V. SUMMARY AND CONCLUSIONS

In summary, we have presented a unified treatment of the energy levels and electron tunneling in heterostructures under an in-plane magnetic field. The transfer-matrix approach is employed. We have demonstrated the convenience of using parabolic cylinder functions for expanding the wave function. The treatment presented here is not only exact, but also efficient for the heterostructure problem, valid for all arbitrary layer widths. We have applied the theory to a double-barrier structure made of GaAs and $Al_{0.3}Ga_{0.7}As$ and calculated the energy levels, wave functions, transmission coefficients, and tunnel currents. Finally, we note that since the presented theory can treat any potential profile $V(z)$, it is therefore applicable to a self-consistent calculation in which the Coulomb interaction among the electrons needs to be included.

ACKNOWLEDGMENTS

We would like to acknowledge the support of the National Science Council of the Republic of China through Contract No. NSC80-0417-E-007-13.

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