

Onset voltage shift due to non-zero Landau ground state level in coherent magnetotransport

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Abstract

Coherent electron transport in double-barrier heterostructures with parallel electric and magnetic fields is analyzed theoretically and with the aid of a quantum simulator accounting for 3-dimensional transport effects. The onset-voltage shift induced by the magnetic field in resonant tunneling diodes, which was previously attributed to the cyclotron frequency w_c inside the well is found to arise from an upward shift of the non-zero ground (lowest) Landau state energy in the entire quantum region where coherent transport takes place. The spatial dependence of the cyclotron frequency is accounted for and verified to have a negligible impact on resonant tunneling for the device and magnetic field strength considered. A correction term for the onset-voltage shift arising from the magnetic field dependence of the chemical potential is also derived. The Landau ground state with its nonvanishing finite harmonic oscillator energy $\hbar w_c/2$ is verified however to be the principal contributor to the onset voltage shift at low temperatures.

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I. INTRODUCTION

One of the most fundamental results of quantum theory is the fact that the harmonic oscillator has a ground state with a *non-zero* energy $\hbar w_c/2$. This energy is usually ignored in most field calculations because it is merely a constant and it is therefore treated as a reference point in energy.

The quantum state of an electron in a constant and uniform magnetic field is described by a *harmonic oscillator* with cyclotron frequency w_c . Indeed from a classical mechanics point of view, this results from the fact that the electrons move through the device according to helicoidal trajectories, and that the projected motion along an arbitrary transverse axis is that of a simple harmonic oscillator. Varying the magnetic field changes the cyclotron frequency and is found in turns to induce a *shift of the onset voltage* in the IV characteristic of double barrier heterostructures. We demonstrate in this paper that this collective phenomenon in the electron current occurs due to the varying energy value $\hbar w_c/2$ of the ground-state of the harmonic-oscillator representing the electrons (see Fig. 3).

The famous Casimir effect¹ has the same origin in nature. Each mode of the electromagnetic field is represented by a harmonic oscillator. The finite ground state energy of an electromagnetic field between parallel metal plates depends on the separation of the plates, which is similar to the dependence upon the varying magnetic field in the system studied here. The Casimir effect which was predicted in 1948 was recently verified experimentally by Lamoreaux in 1996².

Other known examples are the Lamb shift³, and the unfreezing of liquid helium at extremely low temperatures. Nevertheless phenomena which have a direct relation with the nonvanishing, finite ground-state (zero-point) energy of the corresponding harmonic oscillator are very *few*. In this paper one more occurrence is demonstrated for magnetotransport in semiconductor heterostructures.

The magnetotransport phenomenon in multiple barrier heterostructures with a magnetic field applied parallel to the electric field was first investigated and reported in the pioneer-

ing work of Mendez, Esaki and Wang⁴. When both the magnetic field and electric field are perpendicular to the heterostructure interface⁵, the electron motion becomes quasi-one dimensional⁶, as the electron states in the plane perpendicular to the layered direction are quantized in discrete Landau levels. This dimensional reduction of the electron motion has a profound effect on the transmission probability and current-voltage characteristic when compared with the case of zero magnetic field.

The experimental work on GaAs/GaAlAs double barrier structures incorporating both a parallel electric field and a magnetic field showed some remarkable features, including a shift of onset voltage and enhanced peak-to-valley-ratio^{4,7}. However, these observations have not been fully accounted for from a theoretical standpoint, and such a theoretical analysis is needed to understand the underlying physical processes and inspire possible device applications.

Specifically in Ref. 4 the shift of onset voltage with increasing magnetic fields was predicted to be given by the energy $\hbar w_c/2$ associated with the cyclotron frequency inside the well region. In this paper we demonstrate instead that the onset voltage shift originates from an upward shift of the non-zero ground (lowest) Landau state energy in the perpendicular plane throughout the *entire* region of the quantum structure where coherent transport takes place, including the left contact, rather than only inside the well. We also derive and numerically calculate a correction term for the onset voltage shift which arises from the magnetic field dependence of the chemical potential. Finally we have verified using our 3D transport model that the spatial dependence of the cyclotron frequency has a negligible impact on resonant tunneling in the test device for the magnetic field strength considered.

From a fundamental physical point of view, the fact that the *nonvanishing* ground state energy $1/2 \cdot \hbar w_c$ reveals itself in a shift of the onset voltage is a very noticeable phenomenon. We account here for this abnormal feature with the aid of a quantum simulator **based on a 3-dimensional transport picture** which incorporates the Landau states in the perpendicular plane.

Undoped Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As double barrier structures with heavily doped

n^+ -GaAs left and right contact layers are considered. The donor doping density is $1 \times 10^{18}/\text{cm}^3$. The conduction-band profile without an applied voltage is shown in the inset of Fig. 1. The effective mass of the electrons for GaAs and $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ are given by $m^* = 0.067m, 0.092m$, respectively, where m is the electron rest-mass.

Two structures with a barrier and a well width of 34\AA (structure A) and 50\AA (structure B) respectively are examined. We assume that the donors in the contacts are completely ionized ($n = N_d$) due to the heavy doping density. A tight-binding band in the superlattice direction and a parabolic band in the perpendicular plane are used. Spin splitting in a magnetic field is ignored for simplicity. Finally we focus on the low temperature case, $T = 4.2\text{K}$.

II. THEORY

The electron Hamiltonian in the heterostructure in the most general case includes interaction terms which describe disorder scattering by phonons, impurities, interface roughness, etc. Since the electron mean free path at very low temperatures is relatively large compared to the heterostructure size under investigation ($w_c\tau \gg 1$), we can safely neglect scattering. Therefore, only the coherent, ballistic electron motion will be considered here and the Schrödinger equation to be solved is

$$H_e|\Psi\rangle = i\hbar\frac{d}{dt}|\Psi\rangle. \quad (1)$$

In the plane perpendicular to the superlattice direction, the electrons move classically in a circular path. In a quantum treatment the electron energy is quantized in Landau states⁸, which are given by the quantized harmonic oscillator states,

$$E_p = (L + 1/2)\hbar w_c(n), \quad (2)$$

where $w_c(n) = eB/m^*(n)$ is the cyclotron frequency in the magnetic field B at the lattice site n in the superlattice direction. In the following discussion we will see that the lowest

Landau state $L = 0$ is not just a reference point but gives an important contribution to the current flow in the double barrier heterostructure.

We expand the electron wave function in a basis consisting of generalized Wannier functions in the superlattice direction (x -direction)⁹ and of the Landau states in the (y, z) plane which result when the Landau gauge is chosen for the vector potential of the magnetic field,

$$|\Psi\rangle = \sum_{n,L} \int f(k_y, L, n) |k_y, L, n\rangle dk_y, \quad (3)$$

where $f(k_y, L, n)$ is the envelope function of the electron states. The matrix element for the heterostructure Hamiltonian between generalized Wannier-Landau states is⁹

$$\langle k_y, L, n | H_e | k'_y, L', n' \rangle = H_{e,nn'}(L) \delta_{L,L'} \delta(k_y - k'_y), \quad (4)$$

where

$$H_{e,nn'}(L) = H_{nn'} + (L + 1/2) \hbar \omega_c(n) \delta_{nn'}, \quad (5)$$

and

$$H_{nn'} = -\frac{\hbar^2}{2a^2 \sqrt{m^*(n)m^*(n+1)}} \delta_{n+1,n'} - \frac{\hbar^2}{2a^2 \sqrt{m^*(n)m^*(n-1)}} \delta_{n-1,n'} + \left[\frac{\hbar^2}{a^2 m^*(n)} + E_{con}(n) - eV_{app}(n) \right] \delta_{n,n'}. \quad (6)$$

Here $E_{con}(n)$ is the conduction band edge and $V_{app}(n)$ is the electrostatic potential at the lattice site n .

The transversal mass in the perpendicular part of the Hamiltonian matrix also varies along the longitudinal direction. We introduce a new Hamiltonian matrix which absorbs this n -dependent transversal part as

$$H_{e,nn'}(L) = \tilde{H}_{nn'}(L) + (L + 1/2) \hbar \omega_c(0) \delta_{nn'}, \quad (7)$$

where

$$\tilde{H}_{nn'}(L) = H_{nn'} + (L + 1/2) \hbar \omega_c(0) [m^*(0)/m^*(n) - 1] \delta_{nn'}. \quad (8)$$

Here $\tilde{H}_{nm'}$ depends on the perpendicular states L , incorporating 3-dimensional **band-structure** effects in the longitudinal motion of the electrons.

Thus the Schrödinger equation reduces to the following 3-dimensional envelope equation for $f(k_y, L, n)$:

$$i\hbar \frac{df(k_y, L, n)}{dt} = (L + 1/2)\hbar w_{c0} f(k_y, L, n) + \sum_m \tilde{H}_{nm} f(k_y, L, m), \quad (9)$$

where $w_{c0} = eB/m^*(0)$ is the cyclotron frequency at the left contact.

The incident electrons in the left contact occupy the sub-bands $E_{L_0} = E_{0x} + (L_0 + 1/2)\hbar w_{c0}$, where $E_{0x} = \hbar^2 k_x^2 / (2m^*(0))$. Since in the absence of scattering an incident ballistic electron conserves its Landau level L_0 and its total energy E_{L_0} , as it goes through the structure, the envelope function solution of Eq.(9) in Landau gauge takes the form

$$f(k_y, L, n) = e^{-iE_{L_0}t} f_0(n) \delta(k_y - k_{y0}) \delta_{LL_0}. \quad (10)$$

When Eq.(10) is substituted into the Schrödinger equation (9), we arrive at the time independent form

$$E_{0x} f_0(n) = \sum_m \tilde{H}_{nm} f_0(m) \quad (11)$$

Note that the longitudinal electron wave function $f_0(n)$ depends on the perpendicular Landau sub-band level L_0 , since the second term in the right hand side of Eq.(8) is a function of the Landau level. This is a 3-dimensional transport effect which was exactly implemented in our numerical analysis.

The electron currents for an incident and transmitted state (E_{0x}, L_0) are respectively,

$$\begin{aligned} j_{I0}(E_{0x}, L_0) &= ev_L(E_{0x}) \\ j_{T0}(E_{0x}, L_0) &= e|f_0(n_R)|^2 v_R(E_{0x}), \end{aligned} \quad (12)$$

where v_L, v_R are the electron velocities at the left and right contacts, and n_R is the lattice-site index of the right contact. The transmission probability from left to right contact is then defined as

$$T_{L \rightarrow R}(E_{0x}, L_0) = j_{T0}(E_{0x}, L_0) / j_{I0}(E_{0x}, L_0). \quad (13)$$

It is noted that the longitudinal transmission probability depends on the perpendicular state L_0 . Fig. 1 shows the transmission probability for different applied biases.

In order to calculate the total diode current, the chemical potential corresponding to a doping density n in the contacts in the presence of a magnetic field should be determined. The chemical potential has an oscillatory dependence on the magnetic field which is determined from the carrier density through the following integration relation,

$$n = N_d = (\sqrt{2m^*}/\pi\hbar)D \sum_{L_0=0}^{\infty} \int_0^{\infty} (1/\sqrt{E_{0x}}) f_{FD}(E_{0x}, L_0, \mu(B)) dE_{0x}, \quad (14)$$

where $D = \epsilon B/h$ is a degeneracy factor in the plane perpendicular to the superlattice direction and where the Fermi-Dirac function f_{FD} is given by

$$f_{FD}(E_{0x}, L_0, \mu) = \{\exp[(E_{0x} + (L_0 + 1/2)\hbar w_{c0} - \mu)/kT] + 1\}^{-1}. \quad (15)$$

The chemical potential μ is a complex function of the electron density n , magnetic field and temperature. Its numerical calculation shows that the chemical potential μ oscillates by a large quantity when the magnetic field B is strong; for example, there is a difference of 4.4 meV between its value at $B = 13$ and at $B = 17$ Tesla. It is important to account for this behavior to obtain an accurate value of the current.

Under strong magnetic fields, the density of electronic states (see Eq.(14)) drastically departs from the magnetic-field free case and in addition an upward shift $\hbar w_c(n)/2$ of electron's lateral energy with respect to the conduction band minimum occurs in the entire quantum region. As we will see below, the current integration over electronic states in the local emitter will strongly depend on the $\hbar w_{c0}/2$ shift via the Fermi-Dirac distribution function, Eq.(15). This will lead in turn to the onset voltage shift in the current-voltage curve.

The total diode current density is then

$$I_{tot} = (eD/\pi\hbar) \sum_{L_0=0}^{\infty} \int T_{L \rightarrow R}(E_{0x}, L_0) \cdot f_{FD}(E_{0x}, L_0, \mu(B)) dE_{0x} - [L \leftrightarrow R], \quad (16)$$

where the second term in the right-hand side is the backward contribution to the total current. In understanding the abnormal characteristics of the current, it is helpful to define an effective chemical potential $\mu_{eff}(B, L_0)$ dependent upon the Landau level L_0 as follows

$$\mu_{eff}(B, L_0) = \mu(B) - (2L_0 + 1)\hbar w_{c0}/2 \quad (17)$$

At extremely low temperatures such as 4.2 K, the Fermi-Dirac function becomes flat for energies below the chemical potential. To contribute to the total current, the longitudinal energy of electron states (E_{0x}, L_0) should satisfy $E_{0x} \leq \mu_{eff}(B, L_0)$.

As is indicated by Eq.(16) the resonant tunneling current through a double barrier structure generally depends on the details of the transmission probability, the density of electronic states (DOS) and the chemical potential μ (or Fermi energy). Among these, the DOS is much more affected by strong magnetic fields rather than the other properties. As the summation and factor $1/\sqrt{E_{0x}}$ in Eq.(14) indicate, the DOS severely changes due to the quantization of the lateral energy of electrons in the left (right) local contact. The electron states are then classified using the longitudinal sub-band index L_0 . At the temperature of 4.2 K, the longitudinal energy range depends on L_0 according to $E_{0x} \leq \mu_{eff}(B, L_0)$. Thus the effective chemical potential $\mu_{eff}(B, L_0)$ for a particular sub-band L_0 is defined to indicate the cutoff obtained in the longitudinal energy space.

Under such conditions, the current for an occupied sub-band L_0 reduces to

$$I_{tot, L_0} \approx (eD/\pi\hbar) \int_0^{\mu_{eff}} T_{L \rightarrow R}(E_{0x}, L_0) dE_{0x} - [L \leftrightarrow R], \quad (18)$$

where the minimum of the conduction band at the left contact has been set to zero. Therefore, the area of the transmission probability determines the contribution of each occupied sub-band to the total current. Fig. 2 shows the currents calculated for structure A and B. As the voltage is increased, the lowest L_0 sub-band contributes to the current first with higher Landau levels contributing at higher voltages.

III. RESULTS

We note here two important features in the results obtained. First, a shift of the onset voltage depending on the magnetic field strength is observed⁴. It is sharper for the structure with thicker barriers. Second, the current peaks are enhanced in regions of strong fields in both structures⁷. For a thicker barrier (structure B) this current increase is quite remarkable over a wide range of B field.

Let us analyze why these features occur in the presence of a magnetic field. As the applied voltage increases, the quasi-resonant energy E_r (see the inset of Fig. 1) is lowered. At the same time, the conduction band profile has a decreased symmetry due to its tilt. It results that the height and width of the peak transmission probability near E_r decreases, as can be verified in Fig. 1. The energy width of the transmission probability is narrower in RTD structures with a thicker barrier. Therefore the transmission probability is much sharper for structure B than for structure A. These properties explain the increased sharpness of the current threshold and the downward decline of the current plateau in structure B (see Fig. 2).

Let us consider the lowest Landau sub-band $L_0 = 0$, whose effective chemical potential is $\mu_{eff}(B, 0) = \mu(B) - \hbar w_{c0}(B)/2$. In the absence of a magnetic field, the onset voltage for RTD diodes with symmetric barriers and for $eV_D = E_{f,L} - E_{f,R}$ positive is well-known to be approximately given by

$$V_{D,on}/2 = E_r - E_{f,L} = E_r - \mu(0), \quad (19)$$

where $E_{f,L}$ is the Fermi energy level for the electron carriers on the left contact. In the presence of a magnetic field $\mu(0)$ is just replaced by $\mu_{eff}(B, 0)$ and E_r can be assumed to remain unchanged. Indeed the dependence of E_r upon the magnetic field B which arises from the variation of the mass along the superlattice direction (see Eq.(8)) was verified to be negligible in the structures studied. As a result the shift $\Delta V_{D,on}$ of the onset voltage is approximately given by

$$\Delta V_{D,on}/2 = [V_{D,on}(B) - V_{D,on}(0)]/2 \simeq [\mu(0) - \mu(B)] + \hbar w_{c0}(B)/2, \quad (20)$$

which is equal to the difference in effective chemical potential. Fig. 3 indicates that the dominant contribution to the onset voltage shift originates from the non-zero energy $\hbar w_{c0}/2$ of the Landau ground (lowest) state which is a unique feature. Note also that the superposed oscillation in $\Delta V_{D,on}$ has the same origin, namely the oscillation of the chemical potential, as in other phenomena such as de Haas-van Alphen effect¹⁰.

Finally let us look at the increase of the current peak (see Fig. 2). The current density Eq.(18) has a weight factor proportional to the degeneracy D . As discussed, the sharpness of the transmission coefficient depends on the structure parameters such as the barrier widths as well as the conduction-band barrier heights. The enhancement of the current peaks in presence of magnetic field depends on the width of the transmission coefficient peak near the quasi-resonant energy E_r . Therefore, a structure with a sharper transmission probability has a more enhanced peak.

The RTD diode current in Fig. 2 for structure B increases step by step for a weaker magnetic field, with plateaus slowly declining downward. However for a strong magnetic field at $B = 20$ Telsa where the two lowest Landau levels of the emitter are occupied, its diode current rises to its maximum peak value in just one step. For structure A (B) in a strong field of $B = 20$ Telsa, an enhancement of the current peak by 10(37) % is observed.

IV. CONCLUSION

In this paper we have analyzed coherent electron transport in double-barrier heterostructures with parallel electric and magnetic fields **with the aid of a quantum simulator accounting for 3-dimensional transport**. The presence of a magnetic field affect severely the electron transport in a resonant tunneling diode causing a shift of the onset voltage.

Our analysis establishes that the onset-voltage shift induced by the magnetic field arises from an upward shift of the non-zero ground (lowest) Landau state energy in the *entire* quantum region where coherent transport takes place. Note that quantum region therefore

includes the left contact rather than only the well as previously reported⁴. Actually in this work the left contact is used as the cyclotron energy reference. Indeed our 3-dimensional **transport** analysis accounts for the spatial dependence of the cyclotron frequency which is, however, verified to have a relatively small impact on resonant tunneling in the device analyzed for the magnetic field strength considered. A larger correction term for the onset-voltage shift arising from the magnetic field dependence of the chemical potential is also derived.

The comprehensive 3D analysis reported in this paper reveals that the Landau ground state with its nonvanishing finite harmonic oscillator energy $\hbar\omega_c(0)/2$ is indeed the principal contributor to the onset voltage shift at low temperatures. Finally it is also shown in this paper how the abnormal increase of the current peak depends on the external magnetic field as well as the structure parameters of the double barrier heterostructure.

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FIGURES

FIG. 1. The inset shows the conduction band profile of the resonant-tunneling structure. The transmission probability with increased voltage at $T = 4.2K$, magnetic field $B = 10$ Telsa, and the Landau state $L_0 = 0$ for structure A and B. The solid, dotted, and dashed lines are calculated for $V_D = 0.18, 0.23, 0.28$ V for structure A and $V_D = 0.07, 0.12, 0.17$ V for structure B, respectively.

FIG. 2. The current-voltage characteristic at $T = 4.2K$ for the structure A and B in presence of magnetic fields. The solid, dotted, dashed, dot-dashed, double dot-dashed lines are for $B = 0, 5, 10, 15, 20$ Telsa, respectively, for both structures.

FIG. 3. The solid line is the shift of onset voltage at $T = 4.2K$ in structure B for increasing magnetic field. The dashed line shows the contribution in Eq.(20) of the energy $1/2\hbar w_c$ of the Landau ground (lowest) state.





