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Density of states in an electrically biased quantum well

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Abstract. Density of states in a quantum well has been studied in the presence of an electric field applied perpendicular to the growth direction. We have shown that an extra quantization is introduced to the motion of the electron due to the discrete energy levels known as Wannier–Stark ladder states and the nature of density of electronic states changes from quasi two-dimensional to quasi one-dimensional.

Keywords. Quantum well; electric field; density of states; Wannier–Stark ladder.

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1. Introduction

Since the last two decades the electronic properties of quantum well (QW) in the presence of electric field have been studied with increasing interest [1–8] owing to their numerous device applications. Due to small dimensions of these devices, a small bias of even 0.1 V will produce a field of 10^8 V/m in the devices. The referred studies are mainly concerned with the application of the electric field in the QW along the growth direction. The field when applied along the growth direction produces a shift in the quasi-bound levels of the QW. The quasi-bound Stark states for the QW were calculated [1,2,5,8] and it was reported that the ground state energy for both the infinite and finite QW decreases with the increase of intensity of electric field whereas the first excited level raises [1,2,8]. This shows that the field along the growth direction changes the degree of quantum confinement along the growth direction. The detailed investigation on the tunneling of electrons through the QW in the presence of electric field has indicated that the density of states (DOS) in resonance is Lorentzian and the tunneling probability and the carrier lifetime are very much field-dependent [3,6,8].

The electric field along growth direction does not alter the motion of the electron in the interface plane where the motion is still governed by the Bloch electronic states. As a result the motion remains confined in two dimensions (in the plane of interface). On the other hand, the magnetic field along the growth direction quantizes the motion of electrons on the interface, giving rise to Landau levels. The most remarkable implication of this type of quantization is quantized Hall effect. Now, if the electric field is applied normal to the growth direction, i.e. parallel to the interface (say x-direction), then the quantum quasi-bound states along the growth direction are no longer affected by the electric field. But, along x-direction, the crystalline Bloch states are destroyed and the extended states are replaced by the quantized Wannier–Stark ladder states. The localization thus occurs along the growth direction due to the barrier potential in the QW and along a direction perpendicular to the growth direction by virtue of the field quantization. The electron motion thus is confined to only one direction that is perpendicular to both the growth direction and the field direction. In such a system the electronic and optical properties are expected to change significantly. These changes of properties, in principle, are seemed to resemble that of a one-dimensional system like quantum wire. In this work we have shown that the nature of DOS transforms to that of quantum wire when the electric field is applied normal to the growth direction of QW. To bring out the finer points of our study, it is worthwhile to review the condition that makes the electron motion quantized in an applied electric field.

2. Wannier–Stark ladder states in infinite and finite crystals

In a plane perpendicular to the growth direction in a QW the electrons behave almost like those in bulk crystals. In 1960, Wannier [9] predicted that being subjected to a uniform electric field, the continuous energy bands in a bulk crystal pass to a discrete, evenly spaced levels forming a ladder-like spectrum. The ladder-like spectrum in the presence of the field has come to be known as the Wannier–Stark ladder (WSL). The wave functions corresponding to these discrete levels are localized in successive unit cells of the crystal. The localization of the electrons in the QW in a direction perpendicular to the growth direction will lead to the occurrence of negative differential conductivity and opens up new avenues for application in devices. The application of the electric field $\vec{E}$ contributes a linear term $e\vec{E}\cdot\vec{r}$ to the Hamiltonian. If the field is applied perpendicular to a crystal plane, the field direction coincides with one of the reciprocal lattice directions. In view of Bloch's acceleration theorem, the electric field will excite an oscillation in the reciprocal space with a time period, $\tau = \hbar G/eE$ where G is the fundamental reciprocal lattice vector along the direction of the field. The oscillation can occur only when the electrons do not suffer any collision during the period, τ. The oscillation leads to a discrete ladder-like energy spectrum along the reciprocal lattice direction coinciding with the field direction. The condition for the occurrence of WSL in infinite crystals can be given as $\tau < \tau_m$, where τ_m is the relaxation time for all the scattering mechanism available in the crystal. This condition puts a lower limit on the field strength $\vec{E}$ for the occurrence of WSL as $E \geq h/ea\tau_m$, where a is the lattice periodicity of the crystal lattice along the field direction. The oscillation would

lead to the splitting of each continuous band in the field direction to a set of discrete, equally spaced ladder-like energy levels. The high field limit for the existence of WSL is being determined by the onset of interband Zener tunneling which will produce broadening of the WSL levels and thereby again switching over to a continuous energy spectrum. These are the conditions for the existence of WSL states in an infinite crystal. The existence of WSL in finite crystals is subject to some more conditions like: $eEa > \frac{1}{2}(\Delta\varepsilon_{\max})_n$, where $(\Delta\varepsilon_{\max})_n$ is the maximum level separation in the nth band in the absence of the electric field. This extra condition yields the value of the electric field in the finite crystal for which the levels around the center of the band starts forming a partial WSL. The WSL states are localized within a length (ga), where, $g = \varepsilon_{\rm bw}/eEa$, $\varepsilon_{\rm bw}$ being the width of the nth band.

3. Theoretical consideration for energy spectrum and density of states (DOS)

We consider a QW (figure 1), obtained by alternatively stacking layers of one semiconductor material, $Al_xGa_{1-x}As$ and another semiconductor material, GaAs. These two materials, GaAs and $Al_xGa_{1-x}As$, have similar band structures but different energy gaps. The low gap material (GaAs) forms the well region flanked by the high gap material ($Al_xGa_{1-x}As$) on both sides. Figure 2 depicts how the conduction band and valence band offsets bring forth the potential profile for the QW. The height of the potential barrier and the well width are considered as V_0 and b. Now, two-fold quantum confinement in a QW can be accomplished by the application of electric field in a direction perpendicular to the growth direction of the QW. The conduction band along the (1 0 0) direction which is perpendicular to the growth direction of the QW both in field-free and electrically biased situations is shown in figure 3. In the presence of the field, the band bends and the localization of the wave functions becomes more and more pronounced, leading to the occurrence of discrete WSL. Let us consider here that the growth of the QW is along z-direction and the electric field is applied along x-direction. Theoretically, the QW is considered through a superposing potential on the host crystal. The equation of motion of the system with the superposing potential $V(z)$ along the z-direction, the crystal potential, V_C and the field along x-direction appears as

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_C + V(z) - eEx\right)\psi(\vec{r}) = \varepsilon\psi(\vec{r}), \tag{1}$$

where

$$\begin{aligned} V(z) &= V_0 \quad \text{when } |z| \geq b/2; \\ &= 0 \quad \text{when } |z| \prec b/2. \end{aligned} \tag{2}$$

The equations of motion of the electron along the three directions can be separated as

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_C(x) - eEx\right)\psi_1 = \varepsilon_x\psi_1, \tag{3a}$$

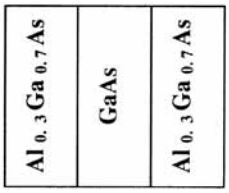

Figure 1. Schematic diagram of a QW formed by stacking a semiconductor (GaAs) sandwiched between the layers of other semiconductor ($Al_{0.3}Ga_{0.7}As$).

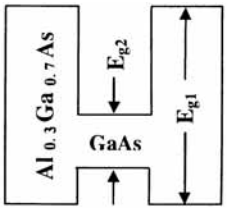

Figure 2. The conduction band and valence band offset profiles for the QW.

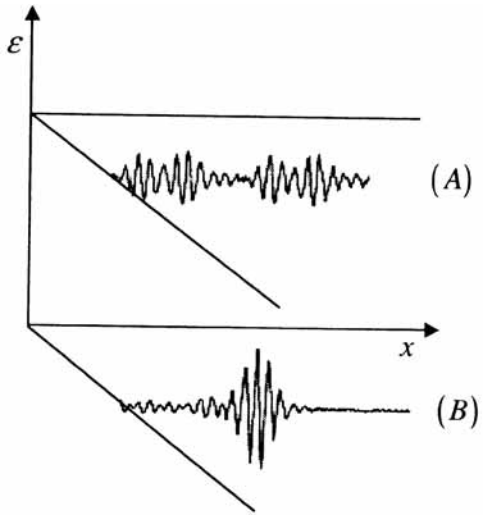

Figure 3. Bending of energy bands and localization of wave function in the presence of electric field. Wave function in field-free QW (A) and localized in an electrically biased QW (B) are shown.

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + V_C(y)\right)\psi_2 = \varepsilon_y\psi_2, \tag{3b}$$

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V_C(z) - V(z)\right)\psi_3 = \varepsilon_z\psi_3, \tag{3c}$$

where total energy $\varepsilon = \varepsilon_x + \varepsilon_y + \varepsilon_z$. The effect of the periodic crystal potential of the host crystal can be incorporated through the use of effective mass in the Schrödinger equation. Equations (3b) and (3c) in the effective mass formalism appear as

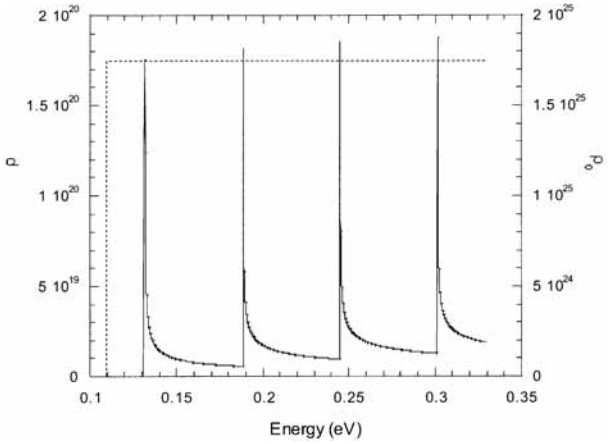

Figure 4. Density of states of $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ QW. Solid line represents ρ (with electric field perpendicular to the growth direction) and dotted line represents ρ_0 (without electric field). Break-down fields for Si and GaAs are 3×10^5 V/cm and 4×10^5 V/cm respectively.

$$\left(-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2}\right)\psi_2 = \varepsilon_y\psi_2, \tag{4a}$$

$$\left(-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} - V(z)\right)\psi_3 = \varepsilon_z\psi_3. \tag{4b}$$

Subjecting the wave function ψ_3 to the boundary conditions with the effective mass approximation under the framework of envelope function [10], we get the following two transcendental equations for the potential profile given by eq. (2) by solving eq. (3c):

$$\tan\sqrt{\frac{m_1^*\varepsilon_z^+ b^2}{2\hbar^2}} = \sqrt{\frac{m_1^*}{m_2^*}\left(\frac{V_0-\varepsilon_z^+}{\varepsilon_z^+}\right)} \quad \text{for even states,} \tag{5a}$$

$$\cot\sqrt{\frac{m_1^*\varepsilon_z^- b^2}{2\hbar^2}} = \sqrt{\frac{m_1^*}{m_2^*}\left(\frac{V_0-\varepsilon_z^-}{\varepsilon_z^-}\right)} \quad \text{for odd states.} \tag{5b}$$

Here, ε_z^+ and ε_z^- correspond to the energy eigenvalues of the even and odd states respectively. Here, m_1^* and m_2^* represent respectively the effective masses of the electron in the well and barrier regions. Then ε_z is obtained from the numerical analyses of the transcendental eqs (5a) and (5b).

The analytical solution of Schrödinger equation along x-direction as in eq. (3a) for infinite crystals [7] leads to a discrete, equally spaced WSL levels in the energy spectrum. The nth energy band splits into a set of discrete energy levels, $\varepsilon_{n\nu}$ and it is represented by the expression

$$\varepsilon_{n\nu} = \bar{\varepsilon}_n(\vec{k}) + eEX_{nn}(\vec{k}) + \nu eEa, \tag{6}$$

where $\varepsilon_{n\nu}$ is the νth level in the nth band and $eEX_{nn}(\vec{k})$ is the intraband shift of the levels of the nth band due to the presence of the electric field. Here eEa stands for the separation between the consecutive levels of the WSL. In eq. (6), $X_{nn}(\vec{k})$ appears as

$$X_{nn}(\vec{k}) = i\langle n, \vec{k}| \exp(i\vec{k}\cdot\vec{r})\frac{\partial}{\partial k_x}\exp(-i\vec{k}\cdot\vec{r})|n, \vec{k}\rangle,$$

where $|n, \vec{k}\rangle$ is the Bloch function corresponding to the $\vec{k}$ state of the nth band while $\bar{\varepsilon}_n$ and $\bar{X}_{nn}$ are the averages in the sense

$$\bar{f} = \frac{1}{G}\int_{-G/2}^{G/2} f(k)\,\mathrm{d}k.$$

Here, we consider the crystal to be finite of length L along (1 0 0) direction and the finiteness of the crystal is also incorporated through the periodic boundary condition, $\psi_1(x) = \psi_1(x + L)$, which is most suitable for the study of the bulk properties. The crystal potential, V_C, is represented by alternate rectangular wells and rectangular potential barriers with the well centered at the lattice sites. The ratio of the barrier width to the lattice periodicity and the barrier height of the lattice potential are chosen by trial and error method which gives correct energy gap and the correct value of effective mass for the holes in the valence band edge and the electrons in the conduction band edge of the crystal. The Schrödinger eq. (3a) is solved numerically by adopting Galerkin's technique. For the purpose we have considered the trigonometric functions $\sin(2\pi jx/L)$ and $\cos(2\pi jx/L)$ as the trial functions and the wave function ψ_1 in terms of the trial functions can be written as

$$\psi_1 = \frac{a_0}{\sqrt{2}} + \sum_{j=1}^{M}\left(a_{(2j-1)}\,\sin\frac{2\pi jx}{L} + a_{2j}\,\cos\frac{2\pi jx}{L}\right).$$

The wave function as given above can be the solution of eq. (3a) only if it satisfies the relations

$$\int_0^L \frac{\partial\psi_1}{\partial a_i}\left(-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2} - eEx - \varepsilon_x\right)\psi_1\,\mathrm{d}x = 0, \quad i = 0, 1, \ldots, (2M+1).$$

These relations lead to $(2M + 1)$ simultaneous equations in the form

$$\underline{A}\vec{a} = \varepsilon_x\vec{a}, \tag{7}$$

where $\underline{A}$ is a real symmetric matrix of order $(2M + 1)$ and $\vec{a}$ is a column matrix with $(2M+1)$ elements. The eigenvalues along the (1 0 0) direction in the presence of the field is obtained through the diagonalization of the matrix $\underline{A}$. The matrix is diagonalized using QL algorithm and Householder tridiagonalization method [11]. The energies are obtained both in the absence and presence of the field. In our numerical approach we have obtained the energy levels for three bands by taking suitable value for M in the summation. The energy levels obtained through the

numerical approach for the finite crystal in the presence of the field clearly show that each band consists of a discrete equally spaced WSL and the energy levels obtained broadly agree with the energy spectrum relation (6) obtained for infinite crystals. The value of ε_x calculated through the numerical method is mentioned in the result.

Without electric field the motion of electron in the QW is two-dimensional. It is well-known that in the two-dimensional systems the DOS remains constant with respect to energy. In our system, in the absence of the field, the electron motion along the z-direction is confined by the QW and results in a quasi two-dimensional system. The DOS becomes constant for each quantum level of the QW and can be given [12] as

$$\rho_0 = \frac{m_1^*}{\pi\hbar^2}\theta(\varepsilon - \varepsilon_z). \tag{8}$$

Here the step function $\theta(\varepsilon - \varepsilon_{zn}) = n$ if $\varepsilon \leq \varepsilon_{zn}$ where ε_{zn} is the nth level of the QW, which is along the z-direction.

When the electric field is applied, the motion of the electron becomes further quantized in the x-direction. So we get one-dimensional electronic motion in the y-direction. The energy of the electron in this direction becomes $(\varepsilon - \varepsilon_x - \varepsilon_z)$. Then the DOS for this one-dimensional system can be obtained as

$$\rho = \frac{1}{\pi}\sqrt{\frac{m_1^*}{2\hbar^2}}\frac{1}{\sqrt{\varepsilon - \varepsilon_x - \varepsilon_z}}. \tag{9}$$

Thus, the DOS of the electrically biased QW diverges like $(\varepsilon - \varepsilon_x - \varepsilon_z)^{-1/2}$.

4. Numerical analysis

We solve the transcendental equations (4) and (5) numerically to get the energy of the quantized bound state occurred along the growth direction (ε_z) for the $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ QW system. The effective masses of $Al_{0.3}Ga_{0.7}As$ and GaAs are $0.0919m_0$ and $0.067m_0$ respectively where m_0 is the free electron mass. On the framework of envelope functions [10], the barrier height is proposed to be equal to conduction band discontinuity that is considered to be 88% of the difference between the band gaps of two materials [13]. The band gaps of $Al_{0.3}Ga_{0.7}As$ and GaAs are respectively 1.7981 eV and 1.424 eV. Thus, the value of V_0 becomes 0.329208 eV. By construction, the zero of the QW coincides with the conduction band minimum of GaAs. We take the well width (b) as 40 Å and get only one bound state for our present system occurred at the energy $\varepsilon_z =$ 0.109789617 eV.

The motion is also quantized along x-direction by the discrete WSL states that have been obtained by the diagonalization of the matrix $\underline{A}$ in eq. (7). For the purpose we have considered the length along x-axis such as to consist of 63 cells. The crystal periodicity is considered as 5.6533 Å which is the same as that of the GaAs crystal. In the numerical approach, we have considered three band calculations and as a result the matrix $\underline{A}$ on diagonalization gives 189 eigenvalues which group into

three bands. A discrete WSL occurs for each band. The WSLs of the different bands superpose on each other. Hence the discrete levels occur both below and above the minimum of the conduction band for the applied electric field of 1 MV/cm. As the energy levels above the minimum of the conduction band always play the crucial role in the electronic properties, we take the minimum of the conduction band in the field-free case as the reference point and consider those WSL that are above the reference level to describe the quantized energy levels (ε_x).

5. Results and discussion

The WSL levels having positive energies in the vicinity of the reference point, which are physically significant, correspond to the valence band. Then with respect to the minimum of the conduction band in the field-free QW as reference point, we get the following values of ε_x (in eV): 0.02194, 0.07846, 0.13501, 0.19158, 0.24808, 0.30459, and 0.36115. These states have energies less than the barrier height of the QW and thus restrain the electron to the QW regime.

Finally, by substituting the values of ε_z and ε_x into eq. (9) we get the DOS (ρ) in presence of electric field whereas the DOS (ρ_0) without electric field is obtained from eq. (8). In figure 4, we plot them as a function of energy. Figure 4 depicts the following features:

(i) In the absence of electric field, the QW under consideration corresponds to only one quantum state. So the DOS (ρ_0) in this case has only one step at 0.109789617 eV. However, if we consider higher energy then the number of steps will increase depending on the condition, $\varepsilon \geq \varepsilon_{zn}$.

(ii) With the electric field, the DOS (ρ) shows some resonance-type peaks, while it varies with respect to energy. It is well-known that one-dimensional system like quantum wire is always depicting DOS to be of resonance peak type [12]. When the electric field is applied, an extra degree of quantization is added to the electronic motion making it one-dimensional. As a result, the step-like nature of DOS is destroyed. The resonance-type peaks also correspond to the divergent behavior of DOS as shown in eq. (9).

(iii) While comparing the magnitude of ρ_0 to that of ρ, we see that the localization caused due to the electric field results in the decrease in the DOS corresponding to the same energy.

6. Conclusion

We have studied DOS of a QW in the presence of electric field applied perpendicular to the growth direction. We observed that the motion of electron is transformed from two-dimensional to one-dimensional and the DOS exhibits resonance-type peaks.

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