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Massive wall confinement in cylindrical quantum wires

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Abstract: The energy spectrum of an electron in an annular cylindrical quantum wire has been studied and it shows that the complete electron confinement in the well region achieved through infinite potential walls and through massive walls at the interface boundaries of the well and the barrier regions give different sets of eigenvalues for any given energy subband of the wire. The massive wall approximation (MWA) is found to satisfy the boundary conditions which are fundamentally different as compared to usually applied infinite potential approximation (IPA); the conditions in the two cases are typically akin, respectively, to TE- and TM-mode like situations in electromagnetic waveguides with perfect metallic boundaries. The energy eigenvalues as a function of the radius 'a' of the inner cylindrical region has been found to have a decreasing trend with increase in 'a' for MWA in sharp contrast with IPA. The results pertaining to a simply connected wire are retrieved in the limit when 'a' tends to zero.

Keywords: Quantum wire, potential well, energy subbands.

1. Introduction

The low-dimensional structures, such as quantum wires, are the subjects of enormous interest nowadays. In these systems, quantization of energy spectrum due to the confinement of electrons in the transverse direction plays a crucial role in understanding various transport phenomena. Hence, there have been studies[1,2] of the confined energy states of an electron in cylindrical quantum wires under finite or infinite confining potential approximations. The calculations show that in a particular subband the energy eigenvalues are on

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the higher side when the electron is completely confined as compared to the situation when confinement is through finite potential.

When the band offset between the well and the barrier regions is assumed finite, the electron wavefunction $\psi(\vec{r})$ spreads out into the barrier region. But under extreme limit of infinite band offset, i.e. when there is an infinite potential wall at the boundary, the electrons are fully confined in the well region. In this paper, we employ an alternative approach of attaining complete confinement in which the effective-mass of the electron is assumed very high in the barrier region, i.e. there is a *massive wall* [3,4] at the interface of the well and the barrier regions.

The motion of an electron in a semiconductor heterostructure is governed by the effective-mass Schrödinger equation[3,5]. The boundary conditions across the interface are the continuity of $\psi(\vec{r})$ and $[\vec{\nabla}\,\psi(\vec{r})]/m^*(\vec{r})$ with $m^*(\vec{r})$ as the space-dependent effective-mass. When $m^*(\vec{r}) \to \infty$ in the barrier region, we obtain solution characterized by the boundary condition $\vec{\nabla}\,\psi(\vec{r}) = 0$ at the interface boundary whereas for the infinite potential approximation (IPA) $\psi(\vec{r}) = 0$; the former and the latter are typically akin to TE- and TM- type boundary conditions, respectively, for electromagnetic waveguides with perfect metallic boundaries. Furthermore, most of the transport models[6–8] assume the extreme quantum limit, i.e. the electron is supposed to occupy only the lowest subband. This approximation is untenable particularly when the subband spacing is of the order of k_BT or when the hot-electron effects induce intersubband scattering[9]. Hence the informations concerning the higher subbands are desirable for a realistic analysis of many of the transport properties.

This paper deals with the study of the energy eigenvalues pertaining to the excited states, apart from the ground state E_0, for an electron in an annular cylindrical space under finite potential approximation (FPA) as well as under the two distinct types of complete confinement approaches: the IPA and the MWA. The dependence of the energy eigenvalues on the radius of the inner cylindrical region as well as on the confining potentials, and the ratio of the mass of the well and the barrier regions have been investigated. Under appropriate limiting conditions, our results are found to be consistent with those of Constantinou and Ridley[1], and Masale et al.[2].

2. Solution

We consider a quantum wire in which an electron is free to move along the axial direction, assumed to be z-axis of the cylindrical polar coordinates, in an annular space between the cylindrical structures of inner and outer radii 'a' and 'b', respectively. The potential profile in the transverse plane is taken to be of the form

$$V(\vec{r}) = (\delta_{\ell,1} + \delta_{\ell,3}) V_\ell, \tag{1}$$

where $\ell = 1, 2$ and 3 represent the three regions for which $0 < r < a$, $a < r < b$ and $r > b$, respectively, and $\delta_{m,n}$ is the Kronecker delta function.

The solution of the effective-mass Schrödinger equation in the three regions are written as :

$$\psi_I(r, \theta, z) = A_m I_m(\kappa_1 r) \exp[i(m\theta + k_z z)];\ 0 < r < a, \tag{2}$$

$$\psi_{II}(r, \theta, z) = [B_m J_m(\kappa_2 r) + C_m Y_m(\kappa_2 r)] \exp[i(m\theta + k_z z)];\ a < r < b \tag{3}$$

and

$$\psi_{III}(r, \theta, z) = D_m K_m(\kappa_3 r) \exp[i(m\theta + k_z z)];\ r > b, \tag{4}$$

where A_m, B_m, C_m and D_m are constants, $J_m(x)$ and $Y_m(x)$ are the cylindrical Bessel functions of the first and the second kinds, $I_m(x)$ and $K_m(x)$ are the corresponding modified Bessel functions, and k_z is the z-component of the wave vector. Moreover,

$$\kappa_\ell = \left[\frac{2m_\ell}{\hbar^2}\left\{V_\ell + (-1)^\ell E\right\} + (-1)^{\ell+1} k_z^2\right]^{1/2} \tag{5}$$

where m_ℓ^* is the effective-mass of the electron in the ℓth region and E is the energy of the electron related to the total energy E_t by the relation $E_t = E + \hbar^2 k_z^2 / 2m_2^*$.

The application of the standard effective-mass boundary conditions at r=a and at r=b for all values of θ finally leads to the transcedental equation for determining the eigenvalues:

$$F_m(\kappa_1, \kappa_2) S_m(\kappa_2, \kappa_3) + G_m(\kappa_1, \kappa_2) T_m(\kappa_2, \kappa_3) = 0, \tag{6}$$

where

$$F_m(\kappa_1, \kappa_2) = \kappa_2 I_m(\kappa_1 a) Y_m'(\kappa_2 a) - \kappa_1 \frac{m_2^*}{m_1^*} I_m'(\kappa_1 a) Y_m(\kappa_2 a), \tag{7}$$

$$G_m(\kappa_1, \kappa_2) = \kappa_1 \frac{m_2^*}{m_1^*} I_m'(\kappa_1 a) J_m(\kappa_2 a) - \kappa_2 I_m(\kappa_1 a) J_m'(\kappa_2 a), \tag{8}$$

$$S_m(\kappa_2, \kappa_3) = \kappa_3 \frac{m_2^*}{m_3^*} K_m'(\kappa_3 b) J_m(\kappa_2 b) - \kappa_2 K_m(\kappa_3 b) J_m'(\kappa_2 a) \tag{9}$$

and

$$T_m(\kappa_2, \kappa_3) = \kappa_3 \frac{m_2^*}{m_3^*} K_m'(\kappa_3 b) Y_m(\kappa_2 b) - \kappa_2 K_m(\kappa_3 b) Y_m'(\kappa_2 b). \tag{10}$$

Now, in order to discuss the limiting behaviour we consider infinite potential walls at r=a as well as at r=b so that $V_1=V_3 \rightarrow \infty$ and $\kappa_1 = \kappa_3 \rightarrow \infty$. We then get from Eq.(6):

$$J_m(\kappa_2 a)Y_m(\kappa_2 b) - J_m(\kappa_2 b)Y_m(\kappa_2 a) = 0 \tag{11}$$

which is the eigenvalue equation for an electron fully confined in the well region due to infinite potential walls and is the same as that obtained by Masale et al[2]. However, if we take $m_1^* = m_3^* \rightarrow \infty$, then Eq. (6) gives

$$J'_m(\kappa_2 a)Y'_m(\kappa_2 b) - J'_m(\kappa_2 b)Y'_m(\kappa_2 a) = 0. \tag{12}$$

We observe that Eq. (11) involves the Bessel functions whereas Eq. (12) contains their derivatives. Hence, the two equations can be expected to lead to different sets of eigenvalues under identical geometrical conditions. Furthermore, the equations governing the eigenvalues for a simply connected cylindrical wire can be obtained from Eq. (6) by putting first a=0 and then letting $V_3 \rightarrow \infty$ for IPA or $m_3^* \rightarrow \infty$ for MWA. The corresponding equations under finite potential approximation (FPA), IPA and MWA are, respectively,

$$\kappa_2 m_3^* J'_m(\kappa_2 b)K_m(\kappa_3 b) - \kappa_3 m_2^* J_m(\kappa_2 b)K'_m(\kappa_3 b) = 0, \tag{13}$$

$$J_m(\kappa_2 b) = 0 \tag{14}$$

and

$$J'_m(\kappa_2 b) = 0. \tag{15}$$

Equations (13) and (14) had been obtained earlier by Constantinou and Ridley[1] whereas Eq. (15) has appeared in our study here.

3. Numerical results

The well region of the system is taken to be GaAs whereas both inner and outer barrier regions are of the material $Al_{0.3}Ga_{0.7}As$. The conduction-band offset of the well and barrier materials is 190 meV[1], and the effective-masses are taken as $m_2^*=5.73\text{x}10^{-32}$ kg and $m_1^*=m_3^*=1.4m_2^*$. We have set $k_z = 0$ and b=20 nm.

Figure 1 depicts the variation of the energies of the ground state, E_0, and four excited states as a function of the inner radius 'a'. It is observed that under both FPA and IPA all the energy eigenvalues increase with increase in 'a'. Similar results had earlier been obtained in case of a simply connected cylindrical wire[1]. However, under massive limit we find the trend just to be opposite; the ground state energy decreases with increase in 'a' and approaches the bottom of the conduction band of the well region[4,5]. On the other hand, each of the MWA excited states shows a maximum which shifts towards the higher value of 'a' as we go to the higher excited states. Also, the maximum region tends to develop into pronounced peaks for the higher states.

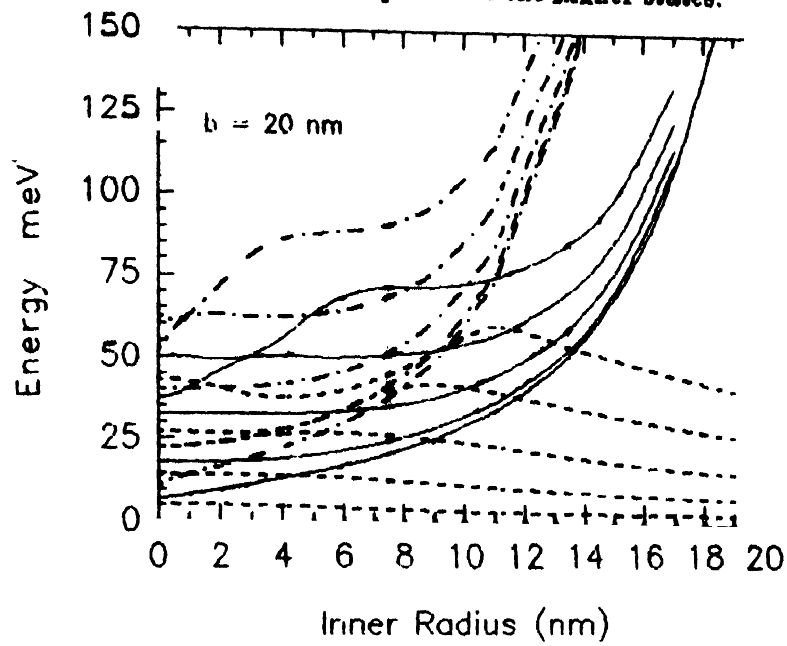

Figure 1. The energies of ground state and four excited states as a function of the inner radius of the annular quantum wire. Dash–dot curves – IPA, broken curves – MWA and solid curves – FPA.

Figure 2 shows the dependence of E_0 on the barrier potentials; inner and outer potentials have been varied independently. Here upper (lower) solid curve corresponds to V_3-infinite (V_3 = 190 mev) and V_1-variable whereas the broken upper (lower) curve is meant for V_1-infinite (V_1 = 190 mev) and V_3-variable. The topmost two curves differ a bit initially but approach a limiting value corresponding to the situation when $V_1=V_3=\infty$. Again, the lower two curves differ only slightly and the difference increases for the higher values of the variable potentials; the cross-over of the curves occurs at $V_1=V_3$ =190 meV. These results indicate that E_0 increases when the potential of one of the barrier regions is kept fixed, infinite or finite, and that on the other side of the well is increased.

The graph in the inset of Figure 2 shows the variation of E_0 with change in m_1^* and m_3^* with $(m_2^*/m_1^*) = (m_2^*/m_3^*) = m^*$; E_0 decreases with increase of $m_1^*(= m_3^*)$. We have set for this curve $V_1 = V_3$ =190 meV.

Summing up, we have shown that the energy spectra arising due to confining boundary conditions MWA and IPA are different; the two approximations

lead respectively to the zero-slope and the zero value for the wavefunction the boundaries.

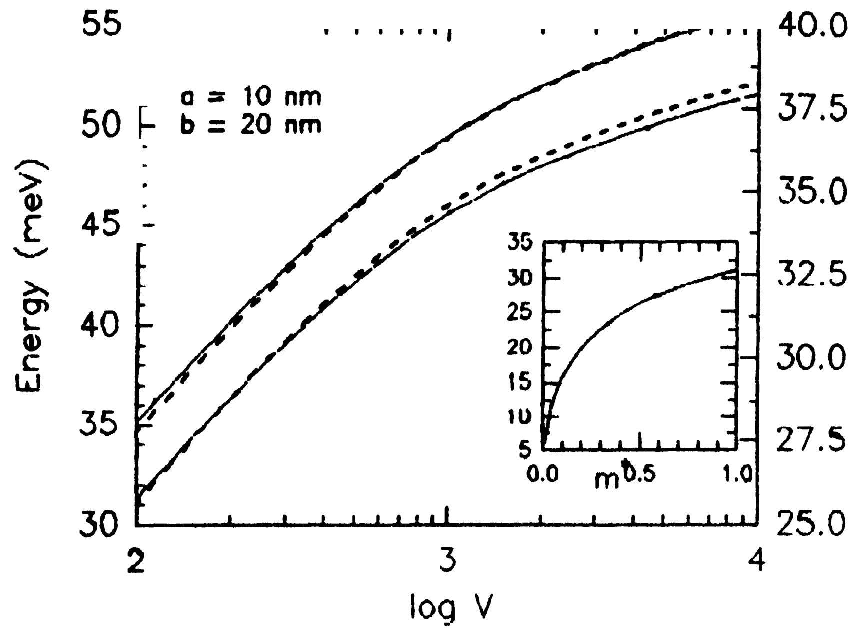

Figure 2. The ground state energy as a function of confining potentials. The inset shows the variation of the ground state energy as a function of the mass ratio m*. The left vertical scale is for V_1 or V_3 infinite whereas the right vertical scale is for V_1 or V_3 190 meV.

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