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Conduction of Electrons in Quantum Wires of Circular Cross-Section

Pranati Purohit[1], Dilip Kumar Roy[2], Shankar Prasad Pati[3] and Sukadev Sahoo[4]

[1]Department of Applied Sciences, The North Cap University, HUDA Sector 23-A, Gurgaon - 122017, Haryana, India;pranatiprht@yahoo.co.in,
[2]Indian Institute of Technology- Delhi, Hauz Khas, Delhi – 110016,New Delhi, India; roydilip87@gmail.com
[3]School of Physics, Sambalpur University, Sambalpur – 768019,Odisha, India; prof_sppati@yahoo.co.in
[4]National Institute of Technology, Durgapur - 713209, West Bengal, India; sukadevsahoo@yahoo.com

Abstract

Objectives: Quantum wires are one-dimensional (1-D) material that exhibit length to width ratios of about 1000 or more. The properties of quantum wire are due to the electrons in them have quantized energy levels perpendicular to their lengths. Such quantum confinement effect exhibits discrete values of electrical conductance which are integral multiples of (e^2/h). **Methods/ Analysis:** In this paper we present a quantum mechanical analysis of evaluation of the electron energy eigen states and their corresponding eigen functions in a quantum wire of circular cross-section. **Findings:** The energy eigen values of quantum wires of different radii are calculated. **Applications:** On the basis of our preliminary analysis it has been observed that quantum wires can also be used as electronic energy filters.

Keywords: Energy filters, Quantum confinement, Quantum wire

1. Introduction

Quantum wire is a one-dimensional nanostructure having quantum confinement in two dimensions. This quantum confinement affects various physical properties of materials like structural, elastic, electronic, optical, electrical[1, 2] properties etc. and these effects have found many applications in various other disciplines[2-6]. Quantum wires can be made of organic molecular chains and of semiconductors such as InP, Si, GaN etc[7]. They have applications in nanomaterial science as interconnects and as functional units in fabricating devices with nano scale dimensions[8, 9]. Energy levels of a semiconductor nanostructure can be calculated by considering the electrons to be immersed in a potential well surrounded by a potential barrier[10]. Such structures can be cubes or spheres (quantum dot)[11], cylinder (quantum wire), potential well (quantum well). It is necessary to accurately evaluate the energy eigenvalues of the quantum wire for the design of the devices. With the potential barrier for experimental quantum wires being of finite heights, energy eigenvalues may be evaluated by applying numerical methods for solution of the relevant envelop function equation on the conventional technique. Gangopadhyay and Nag had calculated the energy eigenvalues in a square and a rectangular quantum wire with a finite barrier potential height[12].They extended their calculation for the triangular and arrowhead shaped quantum wires[13]. As it had been suggest in the tunneling concepts[14-16] that the electron eigenvalues and eigenfunctions remain unaffected within the quantum wells of different finite heights when the width of the barriers are of the order of several electron wavelengths (so that no tunneling can occur). In this paper we have presented a calculation for electrons emerged in a cylindrical potential well of infinite height and narrow cross-section (~nm^2) but of a larger length (~μm).

*Author for correspondence

2. Materials and Methods

2.1 Quantum Confinement Effect in a Cylindrical Quantum Wire

Presuming the electrons to be immersed in a barrier of infinite height, the time independent Schrodinger equation within the wire can be expressed as

$$\frac{-\hbar^2}{2m}\nabla^2 = E\psi \tag{1}$$

Where 'E' is the energy and 'm' is mass of electron, '$\hbar$' is reduced form of planks constant i.e. $\frac{h}{2\pi}$.

In cylindrical co-ordinates (as the quantum wire is of circular cross-section) it can be expressed as

$$\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial\psi}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\varphi^2}+\frac{\partial^2\psi}{\partial z^2}\right]=E\psi \tag{2}$$

Now if we write

$$\psi(\rho,\varphi,z)=R(\rho)\phi(\varphi)Z(z) \tag{3}$$

$R(\rho)$ is the radial part and $\phi(\varphi)Z(z)$ represents the axial part of the wave function.

Equation (3) reduces to

$$\frac{1}{R}\frac{\partial^2R}{\partial\rho^2}+\frac{1}{R\rho}\frac{\partial R}{\partial\rho}+\frac{1}{\phi\rho^2}\frac{\partial^2\phi}{\partial\varphi^2}+\frac{1}{Z}\frac{\partial^2Z}{\partial z^2}+\frac{2mE}{\hbar^2}=0 \tag{4}$$

Equation (4) can be rewritten as

$$\frac{1}{R}\frac{\partial^2R}{\partial\rho^2}+\frac{1}{R\rho}\frac{\partial R}{\partial\rho}+\frac{1}{\phi\rho^2}\frac{\partial^2\phi}{\partial\varphi^2}+\frac{1}{Z}\frac{\partial^2Z}{\partial z^2}=\frac{-2mE}{\hbar^2}$$
$$=-k^2 \tag{5}$$
$$=-\gamma^2-\omega^2$$

Where the total electron wave vector k can be expressed as

$$k^2=\frac{2mE}{\hbar^2} \tag{6}$$

Now, if γ and ω respectively represent axial and radial wave vectors, we may also write

$$\gamma^2=\frac{2mE_z}{\hbar^2} \tag{6a}$$

$$\omega^2=\frac{2mE_\rho}{\hbar^2} \tag{6b}$$

Where E_z is axial energy and E_ρ is radial energy.

This is so because $E=E_z+E_\rho$. Now from equation (5) we can isolate the axial part of the wave equation as

$$\frac{d^2Z}{dz^2}+\gamma^2Z=0 \tag{7}$$

Whose allowed solutions is

$$Z(z)=Ae^{\pm i\gamma z} \tag{8}$$

This represents a freely propagating wave along z– direction which is the longitudinal part of the wave function.

The transverse part of the wave function can also be isolated from (5) as

$$\frac{1}{R}\frac{\partial^2R}{\partial\rho^2}+\frac{1}{R\rho}\frac{\partial R}{\partial\rho}+\frac{1}{\phi\rho^2}\frac{\partial^2\phi}{\partial\varphi^2}=-\omega^2 \tag{9}$$

Rearranging (9) we write

$$\frac{\rho^2}{R}\frac{\partial^2R}{\partial\rho^2}+\frac{\rho}{R}\frac{\partial R}{\partial\rho}+(\omega^2\rho^2-m^2)+\left(\frac{1}{\phi}\frac{\partial^2\phi}{\partial\varphi^2}+m^2\right)=0 \tag{9a}$$

Where m is a pure number.

Now separating the ϕ part of the equation in (9a) we can write

$$\frac{d^2\phi}{d\varphi^2}+m^2\phi=0 \tag{10}$$

Whose solution is given by

$$\phi=Be^{\pm im\varphi} \tag{11}$$

This is the angular part of the wave function. The radial part of the wave equation is then given by

$$\frac{\rho^2}{R}\frac{\partial^2R}{\partial\rho^2}+\frac{\rho}{R}\frac{\partial R}{\partial\rho}+(\omega^2\rho^2-m^2)=0 \tag{12}$$

Rearranging (12) we write

$$\rho^2\frac{\partial^2R}{\partial\rho^2}+\rho\frac{\partial R}{\partial\rho}+(\omega^2\rho^2-m^2)R=0 \tag{12a}$$

This equation represents Bessel's function of integral order[17].Its solution is

$$R(\rho)=J_m(\omega\rho) \tag{13}$$

The total electronic wave function may then be expressed as

$$\psi(\rho,\varphi,z)=R(\rho)\phi(\varphi)Z(z)$$
$$=CJ_m(\omega\rho)e^{-i\gamma z}e^{\pm im\varphi} \tag{14}$$

This represents an electron wave of amplitude $J_m(\omega\rho)$ moving along Z-axis. From equation (5) we get

$$k^2=\omega^2+\gamma^2 \text{ or } \gamma^2=k^2-\omega^2 \tag{15}$$

We find from (15) that γ is real only if $k\geq\omega$. Only in such a case there can be free wave propagation along the axis of the cylinder. In other words

$$\text{i.e. } \frac{2\pi}{\lambda} \geq \frac{2\pi}{\lambda_p} \tag{16}$$

Where λ and λ_p represents the total and radial electron wave lengths respectively.This shows that electrons of wavelength $\lambda < \lambda_p$ can only propagate through the quantum wire, which suggests the possibility of a quantum wire to be used as an energy filter[18].

For m=0, equation (12a) becomes

$$\frac{\partial^2 R}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial R}{\partial \rho} + \omega^2 R = 0 \tag{17}$$

Let $s = \omega\rho$ so equation (17) becomes

$$\frac{\partial^2 R}{\partial s^2} + \frac{1}{s}\frac{\partial R}{\partial s} + R = 0 \tag{18}$$

This is Bessel's equation with m=0. Its general solution is

$$R_0 = C_1 J_0(s) + C_2 Y_0(s) \tag{19}$$

Where J_0 and Y_0 are Bessel functions of the first kind and of the order zero. Since, wave function R is always finite but Y_0 becomes infinite as $s \to 0$ as shown in Figure 1. We therefore cannot use Y_0 in (19) and we must choose $C_2 = 0$.

Clearly then $C_1 \neq 0$, otherwise $R = 0$. We may set $C_1 = 1$, when

$$R_0(\rho) = J_0(s) = J_0(\omega\rho) \tag{20}$$

3. Results and Discussion

At the boundary (surface) of the quantum wire $(\rho = a)$, we must then have for the radial part of the wave function:

$$R_a(a) = J_0(\omega a) = 0 \tag{21}$$

The Bessel's function $J_0(\omega a)$ has infinite number of zeroes.

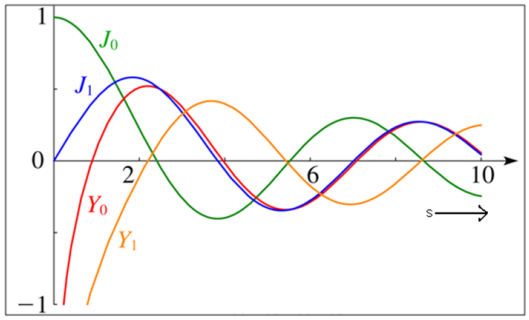

Figure 1. The plot of the Bessel Function of integral order[17]. $J_0(x), Y_0(x), J_1(x)$ and $Y_1(x)$.

Writing $s = \omega a$ the values of 's' for which $J_0(\omega a)$ is zero are represented as

s (nodes of the wave functions)= $\alpha_1, \alpha_2, \alpha_3, -----$

where $\alpha_1 = 2.4048$, $\alpha_2 = 5.5201$, $\alpha_3 = 8.6537$------- etc

We notice that these zeros are irregularly placed.

Let's write $\omega_n a = \alpha_n$

or $\omega_n = \frac{\alpha_n}{a}$, where n = 1,2,3----------

3.1 Calculation of the radial part of the eigen function

This is given by

$$R_{mn}(\rho) = J_m(\omega_n \rho) = J_m\left(\frac{\alpha_n}{a}\rho\right) \tag{22}$$

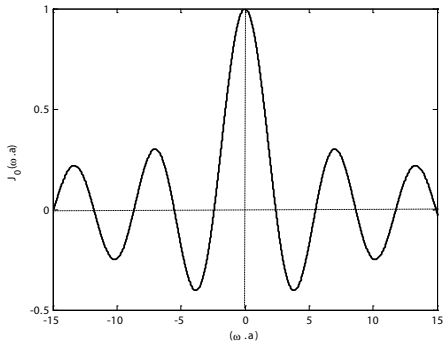

Figure.2. Bessel function of integral order $J_0(\omega a)$.

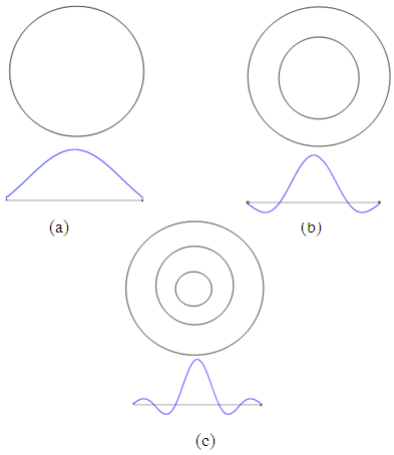

Figure 3. The first three radial parts of the wave function in a quantum wire for m=0. In the figure (a). i.e $R_{01}(\rho) = J_0\left(\frac{\alpha_1}{a}\rho\right)$, (b)i.e $R_{02}(\rho) = J_0\left(\frac{\alpha_2}{a}\rho\right)$ and (c) i.e $R_{03}(\rho) = J_0\left(\frac{\alpha_3}{a}\rho\right)$ plots are for the ground state, first-excited state, and the second excited state, respectively.

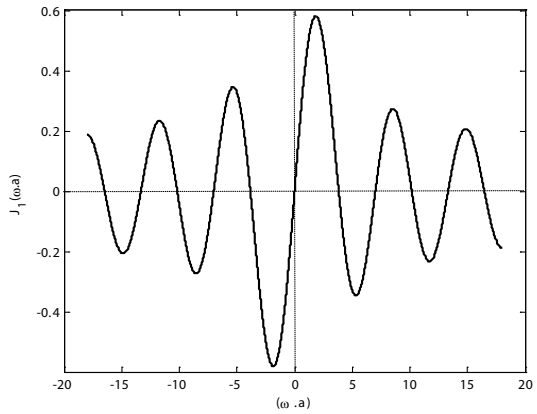

Figure 4. Bessel function $J_1(\omega a)$.

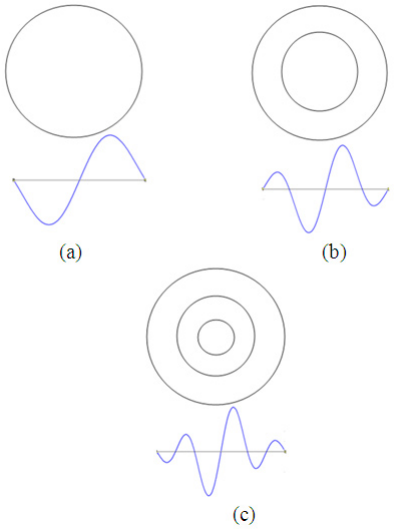

Figure 5. The first three radial parts of the wave function in a quantum wire for m=1. In the figure (a) i.e $R_{11}(\rho)=J_1\left(\frac{a_1}{a}\rho\right)$, (b)i.e $R_{12}(\rho)=J_1\left(\frac{a_2}{a}\rho\right)$ and (c)i.e $R_{13}(\rho)=J_1\left(\frac{a_3}{a}\rho\right)$ plots are for the ground state, first-excited state, and the second excited state, respectively.

This must vanish at $\rho=a$ (at the surface of the wire)

For $m=0$, $R_{0n}(\rho)=J_0\left(\frac{a_n}{a}\rho\right)$

For $m=1$, $R_{1n}(\rho)=J_1\left(\frac{a_n}{a}\rho\right)$

3.2 Calculation of energy eigen values for the radial parts of the wave function

The radial part of the energy eigenvalue is given by equation (6b) appended below

$$E_\rho=\frac{\hbar^2\omega^2}{2m} \tag{23}$$

Where E_ρ is the radial part of the energy. The energy eigenvalues of different eigenstates are tabulated in Table 1.

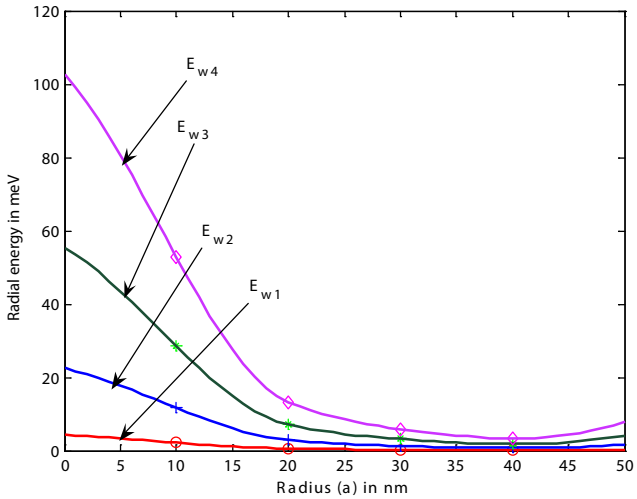

Figure 6. The radial energy eigen values vs. wire radius. The different curves correspond to different eigen states. The lower, middle and the top refer to the ground state, first-excited state and the second excited state respectively.

Table 1 Calculated values of $E_{\rho n}=\frac{\hbar^2\omega_n^{\,2}}{2m}$ in meV for the quantum wire of circular cross-section. $E_{\rho 1}, E_{\rho 2}$, $E_{\rho 3}$ refer to the ground state, first-excited state, and second- excited state energies, respectively. These values are calculated for quantum wires of different radii.

Radius of the wire in nm	For α_1 = 2.4048	For α_2 = 5.5201,	For α_3 = 8.6537
	$E_{\rho 1}=\frac{\hbar^2\omega_1^{\,2}}{2m}$ in meV	$E_{\rho 2}=\frac{\hbar^2\omega_2^{\,2}}{2m}$ in meV	$E_{\rho 3}=\frac{\hbar^2\omega_3^{\,2}}{2m}$ in meV
10	2.2	11.6	28.5
20	0.549	2.89	7.11
30	0.244	1.29	3.16
40	0.123	0.729	1.78

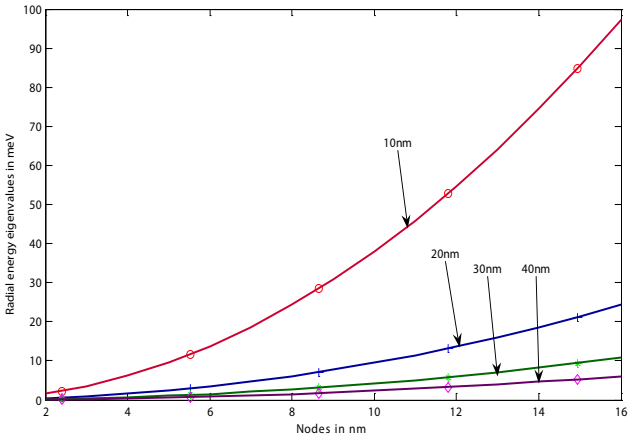

Figure 7. The radial energy eigenvalues of quantum wire of circular cross-section is plotted against the number of nodes (α_m) representing different energy eigenstates. The different curves correspond to quantum wires of different radii.

Table 2 Variation of radial quantized – energies in a quantum wire with circular cross-section as a function of α_m. It is observed that irrespective of the radius of the wire as we move from ground level to different higher level their energies increases.

α_m in nm (nodes)	Radial quantized energy E_ρ in meV			
	Quantum wire of radius 10nm	Quantum wire of radius 20nm	Quantum wire of radius 30nm	Quantum wire of radius 40nm
2.40	2.2	0.549	0.244	0.137
5.52	11.6	2.89	1.29	0.724
8.65	28.5	7.11	3.16	1.78
11.79	52.8	13.2	5.87	3.30
14.93	84.7	21.2	9.41	5.29

4. Conclusion

The paper presents a quantum mechanical analysis of the evaluation of the electron energy eigenstates and their corresponding energy eigenfunctions by solving Schrödinger's time independent wave equation in a quantum wire of varying radius using cylindrical co-ordinates. The results of our calculations are presented in Figures 1-7. We know that $E_z = E - E_p$, where E_z is the axial electron energy, E is the total energy and E_p is the radial component of energy. As E is increased electron conduction through the wire cannot begin (i.e. E_z cannot exist) as long as $E < E_\rho$. Conduction is only possible if

$$E\left(=\frac{\hbar^2k^2}{2m}\right) > E_\rho\left(=\frac{\hbar^2\omega^2}{2m}\right) \text{ i.e. } k \geq \omega \text{ or } \frac{2\pi}{\lambda} \geq \frac{2\pi}{\lambda_\rho}$$

This implies electrons of wavelengths $\lambda < \lambda_\rho$ will be able to propagate through the wire. This is the principle of energy filter.

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