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The energy due to confinement of one-dimensional cylindrical quantum wire

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Abstract. We have determined the energy due to confinement of one-dimensional cylindrical quantum wire by solving Schrödinger's equation. By considering some boundaries conditions, the Schrödinger's equation has been transformed to the second-order linear differential equation. From this transformation, the wave function and the expression of the energy due to confinement are easily described. We obtained the energy due to confinement of 1D-CQW is inversely proportional to the square of the wire's radius. Smaller wires have stronger energy due to confinement than bigger ones.

1. Introduction

It has long been understood that narrow dimension materials have unique properties different from the bulk materials due to quantum effect [1-5]. The unique properties of nanomaterial make them potentially used for electronic and optoelectronic nanodevices application [6-10]. However, to realize this goal, the quantum properties, in particular confinement effect of electrons within nanomaterial must be further understood.

Schrödinger's equation is a versatile mathematical tool in quantum mechanics. By solving this equation, some Eigenvalue such as energy and positional probability of particle can be determined. Consequently energy due to confinement of one-dimensional quantum wire can also be obtained. In fact, inside quantum wire electrons are confined across two directions, whereas within two-dimensional quantum well electrons are confined in one direction and then no electrons are confined within a bulk material [11]. This means that within a quantum wire electrons are just allowed to move in one direction and are confined across two directions. As a result energies of electrons are having discrete values due to confinement effect.

Based on quantum mechanical point of view energies of particle can be determined if the wave function of the particle is identified. The wave function of particle can then be obtained by solving Schrödinger's equation. In practice, the algorithm using Schrödinger's equation is simple enough with



just two general steps. First, find the wave function of the particle by solving Schrödinger's equation by applying some boundaries conditions. Secondly, find the energy of the particle by solving the wave function of the particle. Therefore, in this work we determined the energy due to confinement of one-dimensional cylindrical quantum wire by solving the Schrödinger's equation.

2. Schrödinger's equation in infinitely one-dimensional quantum wire

Confinements of electrons due to the reduced dimensions would lead to dramatic change in the properties and behaviour of the material [11, 12]. The dimensionality of material refers to the number of degrees of freedom in the electron motion and the number of directions for electron confinement. Consequently by changing the dimensionality of a material will change the degrees of freedom as well as the number of confinement directions of electron inside those materials. In a quantum wire, electrons are confined across two directions [11], thereby electrons are just allowed to move in one direction. As a result energy of electrons are also confined across two directions then is called electron has the energy due to confinement. In the Cartesian coordinate, Schrödinger's equation for constant effective mass (m^*) can be expressed as,

$$-\frac{\hbar^2}{2m^*}\nabla^2\psi(x, y, z) + V(x, y, z)\psi(x, y, z) = E\psi(x, y, z) \quad (1)$$

To simplify the problem, we assumed that inside the quantum wire, potential is zero ($V = 0$), while potential outside the wire is infinitely large. The schematic illustration of one-dimensional cylindrical quantum wire is shown in figure 1.

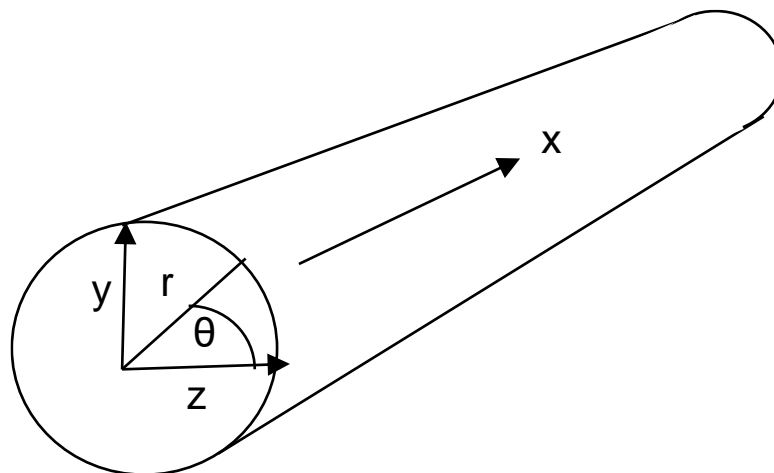


Figure 1. Schematic illustration of one-dimensional cylindrical quantum wire

As a result of the confinement electron across two directions within the wire, the total potential $V(x, y, z)$ can be written as the sum of two-dimensional confinement potential plus potential along the wire [12], while the Eigen function can then be written as a product of the function along the wire and the function of components as shown in equation (2) and (3).

$$V(x, y, z) = V(x) + V(y, z) \quad (2)$$

$$\psi(x, y, z) = \psi(x)\psi(y, z) \quad (3)$$

We considered that the relationship among r , y and z can be written as $y = r \sin \theta$, $z = r \cos \theta$, and $r = \sqrt{y^2 + z^2}$. Then $V(y, z)$ and $\psi(y, z)$ can be expressed as function of r , therefore we obtained:

$$V(x, y, z) = V(x) + V(r) \quad (4)$$

$$\psi(x, y, z) = \psi(x)\psi(r) \quad (5)$$

We substituted both equation (4) and (5) into (1), therefore it is obtained:

$$-\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(x)\psi(r) + (V(x) + V(r))\psi(x)\psi(r) = E\psi(x)\psi(r) \quad (6)$$

We write the energy as a sum of terms associated with the two components of the motion:

$$-\frac{\hbar^2}{2m^*} \left(\psi(r) \frac{\partial^2 \psi(x)}{\partial x^2} + \psi(x) \frac{\partial^2 \psi(r)}{\partial y^2} + \psi(x) \frac{\partial^2 \psi(r)}{\partial z^2} \right) + \psi(r)(V(x)\psi(x) + \psi(x)V(r)\psi(r)) = (E_x + E_r)\psi(x)\psi(r) \quad (7)$$

Now, it is possible to separate equation (7) into two single equations as expressed in equation (8) and (9):

$$-\frac{\hbar^2}{2m^*} \frac{\partial^2 \psi(x)}{\partial x^2} + (V(x)\psi(x)) = E_x \psi(x) \quad (8)$$

$$-\frac{\hbar^2}{2m^*} \left(\frac{\partial^2 \psi(r)}{\partial y^2} + \frac{\partial^2 \psi(r)}{\partial z^2} \right) + V(r)\psi(r) = E_r \psi(r) \quad (9)$$

We have assumed that within the wire potential is zero, so that equation (8) and (9) become:

$$\frac{\partial^2 \psi(x)}{\partial x^2} = -\frac{2m^* E_x}{\hbar^2} \psi(x) \quad (10)$$

$$\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(r) + (E_r)\psi(r) = 0 \quad (11)$$

One of the solutions that satisfied to the equation (10) is a sinusoidal wave in the form of $\exp(ik_x x)$ with the expression of the energy is given by equation (12).

$$E_x = \frac{\hbar^2 k_x^2}{2m^*} \quad (12)$$

Meanwhile, the energy due to confinement of quantum wires can be obtained by solving equation (11). Once more, consider that the potential inside the wire is zero ($V = 0$), while outside the wire is infinitely large. Hence, outside the wire, $\psi(r) = 0$ (probability of finding the particle is zero) then equation (11) becomes:

$$\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(r) + (E_r)\psi(r) = 0 \quad (13)$$

By simple mathematical manipulation and considering the relationship among r , y and z , we obtained:

$$\frac{\hbar^2}{2m^*} \left(\frac{\partial^2 \psi(r)}{\partial r^2} + \frac{1}{r} \frac{\partial \psi(r)}{\partial r} \right) + (E_r)\psi(r) = 0 \quad (14)$$

$$\frac{\partial^2 \psi(r)}{\partial r^2} + \frac{1}{r} \frac{\partial \psi(r)}{\partial r} + \frac{2m^*}{\hbar^2} (E_r)\psi(r) = 0 \quad (15)$$

Equation (15) can then be solved by using second-order linear differential equation [13]. A second-order linear differential equation has the form of:

$$a \frac{\partial^2}{\partial r^2} \psi(r) + b \frac{\partial}{\partial r} \psi(r) + c \psi(r) = 0 \quad (16)$$

with $a = 1$, $b = \frac{1}{r}$ and $c = \frac{2m^* E_r}{\hbar^2}$

One of the solutions that satisfy to the equation (16) is a function $\psi(r) = e^{-\beta r}$ with β is a constant. We choose the constants $-\beta$ (negative) to ensure that $\psi(r)$ is finite when r approaches infinity. If the value of $\psi(r)$ is infinite, this condition has no physical meaning so that the β constant must be negative. Then by using this solution, equation (16) becomes:

$$(a\beta^2 - b\beta + c)e^{-\beta r} = 0 \quad (17)$$

$$(a\beta^2 - b\beta + c) = 0 \quad (18)$$

Then β can be found by using the quadratic formula as follow:

$$\beta_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad (19)$$

$$\beta_{1,2} = \frac{\frac{1}{r} \pm \sqrt{\left(\frac{1}{r^2} - 4 \cdot \frac{2m^* E_r}{\hbar^2}\right)}}{2} \quad (20)$$

$$\beta_{1,2} = \frac{1}{2r} \pm \frac{1}{2} \delta, \text{ with } \delta = \sqrt{\left(\frac{1}{r^2} - \frac{8m^* E_r}{\hbar^2}\right)} \quad (21)$$

It can be seen that Equation (21) poses three possible solutions i.e. $\frac{1}{r^2} - \frac{8m^* E_r}{\hbar^2} > 0$, $\frac{1}{r^2} - \frac{8m^* E_r}{\hbar^2} = 0$, and $\frac{1}{r^2} - \frac{8m^* E_r}{\hbar^2} < 0$. The general solution for the first condition ($\frac{1}{r^2} - \frac{8m^* E_r}{\hbar^2} > 0$) is expressed in Equation (24)

$$\psi_1(r) = Ae^{\beta_1 r} + Be^{\beta_2 r}, \text{ with } \beta_1 = \frac{1}{2r} + \frac{1}{2} \delta \text{ and } \beta_2 = \frac{1}{2r} - \frac{1}{2} \delta \quad (22)$$

$$\psi_1(r) = Ae^{\left(\frac{1}{2r} + \frac{1}{2} \delta\right)r} + Be^{\left(\frac{1}{2r} - \frac{1}{2} \delta\right)r} \quad (23)$$

$$\psi_1(r) = e^{\frac{1}{2}r} \left[Ae^{\frac{\delta r}{2}} + Be^{-\frac{\delta r}{2}} \right] \quad (24)$$

We can see that equation (24) is not function that associate to the osilation wave, therefore it is not desired solution. We expect, when the potential is zero ($V = 0$) the solution must be function of osilation wave. The general solution of second condition ($\frac{1}{r^2} - \frac{8m^* E_r}{\hbar^2} = 0$) is shown in equation (26)

$$\psi_2(r) = (C + Dr)e^{\beta r} \text{ with } \beta = \frac{1}{2r} \quad (25)$$

$$\psi_2(r) = (C + Dr)e^{\frac{1}{2}r} \quad (26)$$

It clearly be seen that $\psi_2(r)$ is also un-expected solution because it is a linear fuction. Then, the solution of the third condition is shown in equation (28). It can be seen that equation (28) expresses the fuction of osilation wave, it is an expected solution that we are looking for.

$$\psi_3(r) = Ee^{\left(\frac{1}{2r} + \frac{i\gamma}{2}\right)r} + Fe^{\left(\frac{1}{2r} - \frac{i\gamma}{2}\right)r} \text{ with } \gamma = \sqrt{\left(\frac{8m^* E_r}{\hbar^2} - \frac{1}{r^2}\right)} \text{ and } \beta_{1,2} = \frac{1}{2r} \pm \frac{i\gamma}{2} \quad (27)$$

$$\psi_3(r) = e^{\frac{1}{2}r} \left[Ee^{\frac{i\gamma r}{2}} + Fe^{-\frac{i\gamma r}{2}} \right] = Ge^{\frac{i\gamma r}{2}} + He^{-\frac{i\gamma r}{2}} \quad (28)$$

Then, to simplify the problems suppose that $G = H$, therefore

$$\psi_3(r) = H(e^{\frac{i\gamma r}{2}} + e^{-\frac{i\gamma r}{2}}) \quad (29)$$

$$\psi_3(r) = H \left(\left[\cos\left(\frac{\gamma r}{2}\right) + i \sin\left(\frac{\gamma r}{2}\right) \right] + \left[\cos\left(\frac{\gamma r}{2}\right) - i \sin\left(\frac{\gamma r}{2}\right) \right] \right) \quad (30)$$

$$\psi_3(r) = 2H \cos\left(\frac{\gamma r}{2}\right) = 2H \cos(kr) \text{ with } k = \frac{\gamma}{2} \quad (31)$$

Based on equation (31), it can be seen that the maximum value of $\psi_3(r)$ occurred if $\cos(kr) = 1$, consequently $kr = 0$, then $r = 0$. We can see that the maximum value of $\psi_3(r)$ is located in center of the wire. By using the condition $\psi(r) = 0$ at $r = R$, as well as consider the value of γ , we obtain the expression of energy due to confinement as shown in equation (34):

$$\cos(kr) = 0 \quad (32)$$

$$k = \frac{(n-1/2)\pi}{R}, \quad n = 1, 2, 3, \dots \quad (33)$$

$$E_r = \frac{\hbar^2}{8m^*} \left(\frac{1}{r^2} + \frac{4(n-1/2)^2 \pi^2}{R^2} \right) \quad (34)$$

Plot of the energy due to confinement of indefinitely one-dimensional cylindrical quantum wire is showed in figure 2.

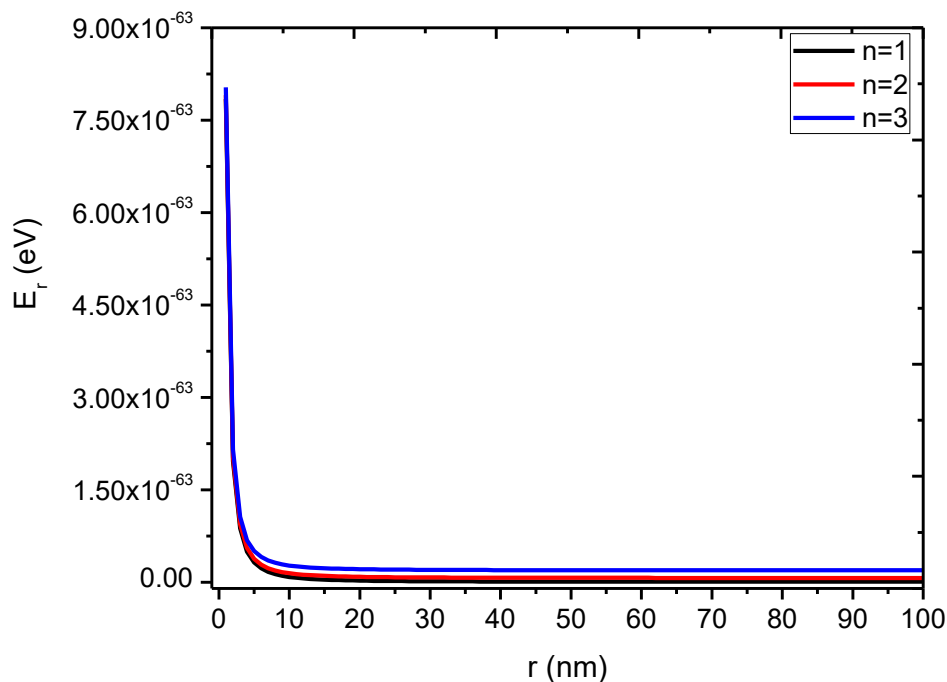


Figure 2. The energy due to confinement of one-dimensional cylindrical quantum wire

Based on Equation (34) and figure 2, it can be seen that the energy due to confinement of cylindrical quantum wire so strongly dependent on size (radius) of wire. Wire with smaller radius has higher energy due to strong confinement. Hence, this results confirmed that the control of size of a quantum wire is an important aspect that must be done to fabricate one-dimensional material such as nanowire with strong quantum confinement. Therefore, the amazing nanodevices application can be realized.

3. Conclusion

The expression of energy due to confinement of one-dimensional cylindrical quantum wire has been successfully obtained by solving Schrödinger's equation. We obtained those energy is inversely proportional to the square of the wire's radius. The smaller wire shows stronger energy due to confinement than bigger one.

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