IOSR Journal of Applied Physics (IOSR-JAP)
e-ISSN: 2278-4861.Volume 11, Issue 2 Ser. II (Mar. – Apr. 2019), PP 65-69
www.iosrjournals.org

Energy Quantization of Electrons for Spherically Symmetric Atoms and Nano Particles According to Schrödinger Equation

[1]Amna E. Musa, [2]Ghada E. S. Elammeen, [3]Hassaballa M. A. Mahmoud, [4]Elharam E. Mohammed, [5]Mubarak Dirar Abdallah, & [6]Sawsan Ahmed Elhouri Ahmed

[1]University of Hafr AlBatin – Department of Physics – Faculty of Science –Hafr AlBatin, Saudi Arabia
[2] King Khalid University – College of Science& Arts, Ahud, Rufeda, Saudi Arabia
[3]King Khalid University – Department of Physics – College of Science & Arts, Dharan Aljanoub, Saudi Arabia
[4]Gazan University, University College in Al Arada, Physics Department, Saudi Arabia
[5]Sudan University of Science &Technology-College of Science-Department of Physics & International University of Africa- College of Science Department of Physics- Khartoum-Sudan
[6]University of Bahri - College of Applied & Industrial Sciences Department of Physics-Khartoum- Sudan
Corresponding Author: Amna E. Musa

Abstract: *Schrödinger Equation for spherical atoms and nano particles was used to describe the behavior of electrons and phonons by treating them as strings oscillating thermally and under the action of external force. The solution shows that for thermally excited phonons and electrons the energy and frequency are quantized .For electrons excited by external force the energy and frequency are also quantized. The energy in both cases resembles the zero point energy for harmonic oscillator of the quantum system. The solution also describes free as well as bounded electrons. The results obtained agree with previous models and observations.*

***Key words**: Schrödinger Equation, spherical symmetry, string theory, phonon, energy quantization*

Date of Submission: 18-03-2019 Date of acceptance: 02-04-2019

I. Introduction

The history of quantum dates and starts from the plank hypothesis that light and electromagnetic waves behaves as particles or discrete quanta with energy proportional to frequency [1]. This hypothesis was proposed to explain black body radiation spectrum. This encourages De Broglie to propose that particles like electrons can behave also as waves [2]. The wave-particle dual nature of atomic and subatomic particles represents the black bone and corner stone of quantum mechanics. Quantum laws describe the time evolution of the system either in terms of the wave function in the so called Schrödinger picture or in terms of the operators in the so called Heisenberg picture [3]. The Schrödinger picture describes slowly moving particles which obey Newton laws by Schrödinger equation. High speed relativistic particles are described by Klein-Gordon equation for spin less particles or by Dirac equation for particles having spin [4].These quantum laws describe a wide variety of physical phenomena. These include the atomic spectra, magnetic and electron spin resonance, radioactivity. One of the most widely used applications is that concerned with the behavior of atoms specially the atomic spectra. This behavior is described by hydrogen like atom model in which are assumed to be spherically symmetric. Thus Schrödinger equation is solved in spherical coordinates [5]. This solution predicts that energy and orbital angular momentum are both quantized. This model succeeded in explaining many subatomic phenomena, like atomic spectra, magnetic and spins resonance [6]. But unfortunately this model is complex and cannot describe some nano particles behaviors. This requires searching for simple solution that can incorporate new trends like string model [7, 8, 9] that can successfully compatible with observation.

Atomic String Model for Spherically Symmetric Atoms

Solving Schrödinger Equation in spherical coordinate the radial part for zero potential gives

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial r^2}+\frac{c}{r^2}=Eu$$

$$\frac{\partial^2 u}{\partial r^2}-\frac{\hbar^2}{2m}\frac{cu}{r^2}=-\frac{2Emu}{\hbar^2}=-k^2u$$

$\ddot{u}-\frac{c_1}{r^2}u=-k^2u$ (1)

The wave function is given by

$$\psi(r,\theta,\phi)=R(r)Q(\theta,\phi)$$

Where the radial part is given by

$R=\frac{u}{r}$ (2)

And

$c_1=\frac{2m}{\hbar^2}c$ (3)

$k^2=\frac{2mE}{\hbar^2}$ (4)

$c=\frac{\hbar l(l+1)}{2m}$ (5)

$c_1=\frac{l(l+1)}{\hbar^2}$ (6)

For $(l=0, c_1=0)$ the solution takes the form

$\ddot{u}=-k^2u$ (7)

$u=A\sin kr+B\cos kr$ (8)

$$\dot{u}=kA\cos kr-kB\sin kr$$

$\ddot{u}=-k^2(A\sin kr+B\cos kr)$ (9)

To find the constant parameters, one uses some boundary conditions. For a point particle like electrons in free space, the radius a is vanishingly small, i.e.

$a\to 0$ (10)

The existence of the electron in free space for

$r\geq a$ (11)

Is equal to zero, i.e.

$|u(a)|^2=0 \qquad u(a)=0$ (12)

According to equation (8)

Since $(a\to a)$ for electrons thus

$u(a)=A\sin ka+B\cos ka=0$ (13)

$$\sin ka\approx\sin 0=0$$

$\cos ka\approx\cos 0=1$ (14)

It follows that

$$0+B=0$$

$B=0$ (15)

Thus using equation (15), equation (8) becomes

$u=A\sin kr$ (16)

To obtain k, consider spherical nano particle having radius a, such that just outside it no particle exist. In this case

$|u(r)|^2=0 \qquad u(r)=0 \quad r\geq 0$ (17)

$u(a)=A\sin ka=0$ (18)

This condition can be satisfied when

$$ka=2n\pi$$

$k=\frac{2n\pi}{a}$ (19)

This condition can be satisfied by bearing in mind that nano particles are isolated from each other, such that no subatomic particle from them exists in vicinity or close proximity.

In the presence of potential, for $(l\neq 0, c\neq 0)$equation (1) becomes

$\ddot{u}-\frac{2m}{\hbar^2}(V-E)u=\frac{2mc}{\hbar^2}\frac{u^2}{r}$ (20)

In view of equations (3) and (4)

$\ddot{u}+k^2u-\frac{c_1}{r^2u}-\frac{2m}{\hbar^2}Vu=0$ (21)

For strings oscillating the radius r, the potential is given by

$V=\frac{1}{2}kr^2=\frac{1}{2}mw_0^2r^2$ (22)

Thus

$\frac{2m}{\hbar^2}V = \frac{mk}{\hbar^2}r^2 = \frac{m^2 w_0^2}{\hbar^2}r^2 = c_2 r^2$ (23)

Thus equation (21) reads

$\ddot{u} - \frac{c_1}{r^2}u - k^2 u - c_2 r^2 u = 0$ (24)

One can solve this equation by trying a solution

$u = e^f \, \dot{u} = \dot{f}e^f \, \ddot{u} = \left(\ddot{f} + \dot{f}^2\right)e^f$ (25)

Inserting equation (25) in (24) yields

$\ddot{f} + \dot{f} - \frac{c_1}{r^2} + k^2 - c_2 r^2 = 0$ (26)

Consider the solution

$$f = c_3 \ln r - c_4 r^2$$

$$\dot{f} = \frac{c_3}{r} + 2c_4 r$$

$\ddot{f} = -\frac{c_3}{r^2} + 2c_4$ (27)

A direct substitution of equation (27) in (26) gives

$$-\frac{c_3}{r^2} + 2c_4 + \left(\frac{c_3}{r} + 2c_4 r\right)^2 - \frac{c_1}{r^2} + k^2 - c_2 r^2 = 0$$

$-\frac{c_3}{r^2} + 2c_4 + \frac{c_3^2}{r^2} + 4c_3 c_4 r + 4c_4^2 r^2 - \frac{c_1}{r^2} + k^2 - c_2 r^2 = 0$ (28)

Equating the coefficients of r^{-2}, r^2 and free terms, one gets

$-c_3 + c_3^2 - c_1 = 0$ (29)

$2c_4 + k^2 + 4c_3 c_4 = 0$ (30)

$4c_4^2 - c_2 = 0$ (31)

One can find c_3 by using the identity

$$c_3 = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$c_3 = \frac{1 \pm \sqrt{1 + 4c_1}}{2}$ (32)

Where

$a = 1 \qquad b = -1 \qquad c = -c_1$ (33)

$k^2 = -2c_4(1 + 2c_3)k^2 = -2c_4(1 + 2c_3)$ (34)

$c_4 = \pm\frac{1}{2}\sqrt{c_2}$ (35)

In view of equation (23) equation (34) gives

$c_4 = \pm\frac{1}{2}\frac{mw_0}{\hbar}$ (36)

Thus according to equations (25) and (27)

$$c_3 \ln r + c_4 r^2$$

$u = u(r) = 0$ (37)

$u = c_3 r e^{c_4 r^2}$ (38)

This solution is not physically acceptable as far as it gives zero probability at the center of the nano particle. To avoid this situation assume that the micro particles oscillate due to thermal agitation, in this case the equation of motion is given by

$m\ddot{x} = -\nabla P$ (39)

Where

$$x = x_0 e^{+w_0 t} \, \ddot{x} = -w_0^2 x$$

$P = nRTIV$ (40)

Therefore

$-mw_0^2 x = -\nabla P$ (41)

When these particles are affected by a force F, such that

$F = -\nabla V$ (42)

Where V is the potential energy.

In this case the equation of motion is given by

$m\ddot{x} = -\nabla P + F = -\nabla P - \nabla V = -mw_0^2 x - \frac{\partial V}{\partial x}$ (43)

Consider now the solution

$x = x_0 e^{+iwt} \, \ddot{x} = -w^2 x$ (44)

Hence, equation ( ) reads

$$-mw^2 x = -mw_0^2 x - \frac{\partial V}{\partial x}$$

$m(w^2 - w_0^2)\int x dx = \frac{1}{2}m(w^2 - w_0^2)x^2 = \frac{1}{2}kx^2 = \frac{1}{2}kr^2$ (45)

Thus equation (23) can be rewritten in the form

$$\frac{2m}{\hbar^2}V = \frac{mk}{\hbar^2}r^2 = \frac{m^2}{\hbar^2}(w^2 - w_0^2)r^2 = c_2 \qquad (46)$$

According to equation (35) when the field frequency w is less than the natural one w_0, one gets

$$c_4 = \pm\frac{1}{z}\sqrt{c_2} = \pm\frac{m}{2\hbar^2}\sqrt{(w^2 - w_0^2)} \qquad (47)$$

$$c_4 = \pm i\sqrt{\left(w_0^2 - w^2\right)}\left(\frac{m}{2\hbar}\right)$$

$$c_4 = \pm c_5 i \qquad (48)$$

To obtain physical acceptable solution which does not give zero probability at the origin of the nano solution, one should choose

$$l = 0 \qquad c_1 = 0 \qquad (49)$$

In equation (6), then insert it in equation (32) to get

$$c_3 = \frac{1\pm\sqrt{1}}{2} = \frac{1\pm 1}{2} \qquad (50)$$

By selecting the minus sign, one gets

$$c_3 = 0 \qquad (51)$$

Thus according to equation (37)

$$u = e^{c_4 r^2} = e^{\pm c_5 r^2 i} \qquad (52)$$

When the nano spherical particle is in the form of a crystal with periodic structure, the wave function satisfies block condition

$$u(r+d) = u(r) \qquad (53)$$

Where d is the distance between two adjacent points. Thus

$$e^{ic_5(r+d)^2} = e^{ic_5 r^2} \qquad (54)$$

$$e^{ic_5[(r+d)^2 - r^2]} = 1$$

$$e^{ic_5(r+d+r)(r+d-r)} = 1$$

$$e^{ic_5(2r+d)d} = 1 \qquad (55)$$

Very near to the origin

$$r \to 0 \qquad (56)$$

$$e^{ic_5 d^2} = 1$$

$$\cos c_5 d^2 + i\sin c_5 d^2 = 1 \qquad (57)$$

$$\cos c_5 d^2 = 1$$

$$\sin c_5 d^2 = 0 \qquad (58)$$

This equation can be satisfied, when

$$c_5 d^2 = 2n\pi \qquad c_5 = \frac{2n\pi}{d^2} \qquad (59)$$

$$n = 0, 1, 2, \ldots \qquad (60)$$

According to equations (34), (48), (51) and (56), one gets

$$c_5 = \pm i c_4 = \pm i\left(-\frac{1}{2}k^2\right) = \pm\left(\frac{mE}{\hbar^2}\right)i$$

$$E_n = \pm\frac{2n\pi\hbar^2}{m^2 d^2}i \qquad (61)$$

When

$$w_0 = 0$$

Equation (48) and (61) gives

$$E = \frac{1}{2}\hbar w \qquad (62)$$

But when

$$w = 0$$

$$E = \frac{1}{2}\hbar w_0 \qquad (63)$$

This represents thermal phonons with minimum energy which represents rest mass energy. In view of equation (61) and (63) the phonon energy is quantized.

II. Discussion

Equation (1) describes the equation of motion of spherically particles or system with no potential. The wave function in equation (16) and the expressions of the wave number and energy in equations (19) & (4) resembles that of particle in a box.

If one considers electrons inside the nano particle or atom as strings as equation (23) shows, the solution can be suggested to be exponential. To simplify the solution electrons are assumed to be having zero momentum (see equation (49)).The electrons which act as strings are oscillating thermally and by external oscillating agent such that the two forces apposes each other as shown by equation (46). The solution shows that, when thermal forces dominate, the wave function is constant, which means that the electrons are regularly distributed inside the nano particles. This agrees with observations. .When thermal energy dominates the energy is quantized and imaginary. This agrees with some models which suggest that frictional energy is imaginary .Friction causes collision which generates thermal energy. However when external force dominate, equations (48) & (61) show that the electron energy is that of harmonic oscillator. These equations give either positive energy representing free electrons or negative energy standing for bounded electrons.

III. Conclusion

For spherically symmetric atoms or nano particles the string model shows that the electrons are regularly distributed inside them. The energy is quantized and is imaginary for thermally oscillating strings and is also quantized and resembles that of ordinary harmonic quantum oscillator when the external force acts only. The energy is positive or negative describing either free or bounded electrons.

Reference

[1]. David. J. Griffith, Introduction to Quantum Mechanics (Prentice Hall, New Jerssy, 2005).
[2]. L. I. Schiff, Quantum Mechanics (McGraw Hill, Tokyo, 2009).
[3]. Schawbl, F, Quantum Mechanics, 3rd Edition (springer, Berlin, 2005).
[4]. Dyson, F. J, Advanced Quantum Mechanics, 2nd Edition (world Scientific, Singapore, 2006).
[5]. R. P. Feynman and A. R. Hibbs, Quantum Mechanics and Path Integrals (McGraw Hill, Inc, New York, 1965).
[6]. E. Nelson, Quantum Fluctuation (Princeton University Press, Princeton, 2005).
[7]. Einas M. A, Mubarak> D, Sawsan A. E, Quantum Energy Wave Function Equation and Harmonic Oscillator, International J. of Adw. Res. In Sci. Eng. And Tech. V2, I 12, December 2015.
[8]. Mobarak I. T, Mubarak D., Asim A. M, Sawsan A. E, Lutfi M. A, Quantum Relativistic Equation and String Mass Quantization, Int. J. of Science & Research, Tagabo, 4. (10): October 2015.
[9]. Lutfi, M. A, Mubarak D., Amel A., Rawia A. A, Sawsan A. E, Schrödinger Quantum Equation From Classical and Quantum Harmocin Oscillator, Int. J. of Sciences & Research, Algadir, 5(2): February, 2016.

IOSR Journal of Applied Physics (IOSR-JAP) is UGC approved Journal with Sl. No. 5010, Journal no. 49054.

Amna E. Musa " Energy Quantization of Electrons for Spherically Symmetric Atoms and Nano Particles According to Schrödinger Equation." IOSR Journal of Applied Physics (IOSR-JAP) , vol. 11, no. 2, 2019, pp. 65-69.