Exponentially Decaying Wave Functions and Energy Levels in Nano Particles and Hydrogen-Like Atoms

Kevin Davis[1], Emma Harris[2], Andrew Stewart[3], Rachel Wood[4], John Foster[5]

[*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, DharanAljanoub, Saudi Arabia

[4]Sudan University of Science & Technology-College of Science-Department of Physics - Khartoum - Sudan & International University of Africa- College of Science-Department of Physics -Khartoum-Sudan

[5]University of Bahri - College of Applied & Industrial Sciences Department of Physics - Khartoum - Sudan

ABSTRACT

The solution of radial Schrödinger equation for hydrogen like atoms is complex. One needs simple solution the behavior of nano particle needs also to be described. Nano spherical particles are isolated non interacting particles that obey quantum laws. Thus one expects their behavior to resemble that of particles in a box, or hydrogen like atoms. The spherical nano shape requires using spherical coordinate to solve Schrödinger Equation. The solution found that the wave function is diminishing outside the sphere, which agrees with observations. This solution is simpler than the conventional one, where it is a sum of sine and cosine function.

For the nano particle the energy is quantized and depends on the orbital quantum number. The energy expression resembles that of hydrogen like atoms.

The results show also that the absorption coefficient and the conductivity increases with the particle nano size for positively ionized conductors like Zn.

Keywords: *Nano, Spherical, Particle, Schrödinger equation, periodic structure, Energy Quantization.*

I. INTRODUCTION

The laws of quantum mechanics are used to describe the behavior of atoms. Quantum mechanical laws are based on wave-particle duality of atomic particles. The most popular widely used one is the so called Schrödinger equation, Schrödinger equation is based on Newton energy-momentum relation [1, 2]. It is widely used to describe atomic spectra as well as the behavior of elementary particles. Nano science is one of the most promising branches of physics. It deals with the behavior of particles having dimensions in the range of$(1 - 300\, nm)$. The ordinary material can be converted into a nano one by splitting them into isolated particles, being none interacting, does not obey classical laws [1, 2, 3]. This is related to the fact that such isolated particles are very small in scale, where quantum effects become important. They are described by the laws of quantum mechanics [4, 5]. Thus one expects their behavior to be different from bulk matter.

The advantages of nano material come from the ability to change the physical properties of the nano materials by changing their nano structure [6, 7]. Such ability is related to the sensitivity of quantum system to the structure of the particles. The description of nano of nano materials is based on the so called quantum dots [8, 9]. Many other approaches were used also [10, 11]. Unfortunately they cannot describe all nano science phenomena. Thus further developments and models are needed to get better understanding to nano materials. In a spherical coordinate is used to describe the behavior of nano spherical amorphous and crystalline particles.

II. THEORETICAL MODEL FOR SPHERICAL PARTICLE

It is well known that the wave function of the radial part of spherically symmetric system takes the form:

$$\ddot{u} - \frac{c_1}{r^2}u + k^2 u - \frac{2m}{\hbar^2}V = 0 \qquad (1)$$

Where

$$R = \frac{u}{r} \ddot{u} = \frac{\partial^2 u}{\partial r^2}$$
$$c_1 = \frac{2mc}{\hbar^2}$$
$$c = \frac{\hbar^2 l(l+1)}{2m}$$
$$c_1 = \frac{l(l+1)}{\hbar^2}$$

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

With l, E and m representing orbital angular momentum quantum number, energy, and mass.
Assume now that the potential applied on bounded electrons and free electrons to be that of hydrogen like atoms. In this case

$$V = -\frac{Ze^2}{4\pi\epsilon r}$$

Thus

$-\frac{2mv}{\hbar^2} = \frac{mZe^2}{2\pi\epsilon\hbar^2 r} = \frac{c_2}{r}$ (3)

$\ddot{u} - \frac{c_1}{r^2} + \frac{c_2}{r^2} + k^2 u = 0$ (4)

Equation (4) can be solved by suggesting the solution

$u = A \sin f + B \cos f$ (5)

Where

$$f = f(r)$$

Differentiating (5) with respect to r twice yields

$$\dot{u} = \dot{f} A \cos f - \dot{f} B \sin f$$
$$\ddot{u} = \ddot{f} A \cos f - \dot{f}^2 A \sin f - \ddot{f} B \sin f - \dot{f}^2 B \cos f$$

Rearranging yields

$\ddot{u} = -\left(\frac{B}{A}\ddot{f} + \dot{f}^2\right) A \sin f + \left(\frac{A}{B}\ddot{f} - \dot{f}^2\right) A \cos f$ (6)

A direct substitution of equation (6) in equation (3) gives

$-\left(\frac{B}{A}\ddot{f} + \dot{f}^2\right) A \sin f + \left(\frac{A}{B}\ddot{f} - \dot{f}^2\right) A \cos f = g(r) u$ (7)

Where

$g(r) = \frac{c_1}{r^2} - k^2 - \frac{c_2}{r}$ (8)

Thus

$-\left(\frac{B}{A}\ddot{f} + \dot{f}^2\right) A \sin f + \left(\frac{A}{B}\ddot{f} - \dot{f}^2\right) A \cos f = gA \sin f + gB \cos f$ (9)

Equating the coefficients of sin and cos on both sides yields

$-\left(\frac{B}{A}\ddot{f} + \dot{f}^2\right) = g$ (10)

$\left(\frac{A}{B}\ddot{f} - \dot{f}^2\right) = g$ (11)

Thus equations (10) and (11) can be subtracted from each other's to get

$-\frac{B}{A}\ddot{f} - \dot{f}^2 = g$ (12)

$\frac{A}{B}\ddot{f} - \dot{f}^2 = g$ (13)

$-\left(\frac{B}{A} + \frac{A}{B}\right)\ddot{f} = 0$ (14)

One of the possible solutions is to suggest

$\frac{B}{A} + \frac{A}{B} = 0$ $\frac{B}{A} = -\frac{A}{B}$ (15)

Thus one gets

$$B^2 = -A^2 \qquad B = \pm iA$$

$A = \pm iB$ (16)

Rearranging (12) and (13) then adding gives

$$-\ddot{f} = \frac{A}{B}\dot{f}^2 = \frac{A}{B}g$$
$$\ddot{f} - \frac{B}{A}\dot{f}^2 = \frac{B}{A}g$$

$-\left(\frac{A}{B} + \frac{B}{A}\right)\dot{f}^2 = \left(\frac{A}{B} + \frac{B}{A}\right)g$ (17)

$\dot{f} = -g = k^2 + \frac{c_2}{r} - \frac{c_1}{r^2}$ (18)

Consider now a solution

$f = c_3 \ln r + c_4 r$ (19)

Differentiating w,r,t r gives

$\dot{f} = \frac{c_3}{r} + c_4$ (20)

A direct substitution of (20) in (18) gives

$$\left(\frac{c_3}{r} + c_4\right)^2 = \frac{c_3^2}{r^2} + \frac{2c_3c_4}{r} + c_4^2$$

$= -\frac{c_1}{r^2} + \frac{c_2}{r} + k^2$ (21)

Equating the coefficients of r^{-2}, r^{-1} and free terms on both sides of (21) yields

$c_3^2 = -c_1 c_3 = \pm i\sqrt{c_1}$

$2c_3c_4 = c_2 c_4 = \frac{c_2}{2c_3}$ (22)

$c_4^2 = k^2 c_4 = \pm k$

According to equations (2) and (22)

$$\sqrt{\frac{2mE}{\hbar^2}} = \pm c_4 = \pm\frac{c_2}{2c_3} = \pm\frac{ic_2}{2\sqrt{c_1}}$$
$$E = -\frac{c_2^2\hbar^2}{4c_1 m}$$

$E = -\frac{c_2^2\hbar^2}{4l(l+1)m}$ (23)

In view of equation (3), equations (23) reads

$E = -\frac{mZ^2e^4}{4\epsilon^2\hbar^2 l(l+1)}$ (24)

With $l = 0, 1, 2, 3, \ldots$

This means that the energy is quantized for any nano spherical particle even when it is amorphous. It also shows that the energy of hydrogen atoms like is quantized

According to equations (2), (5), (16) and (19) the radial part of the wave function is gives by

$$R = \frac{u}{r}$$

Thus according to equations (5) and (19) beside (16)

$$R = \frac{B(\cos f + i \sin f)}{r} = B\frac{e^{if}}{r}$$

$$= B\left(e^{\ln r}\right)^{ic_3} e^{ic_4 r} \Big/ r$$

$$R = \frac{Br^{ic_3}}{r} e^{ic_4 r}$$

In view of equation (22)

$$R = Br^{ic_3 - 1} e^{ic_4 r} = Br^{\sqrt{c_1} - 1} e^{ic_4 r} \qquad (26)$$

Using equations (22) and (2) beside (3) gives

$$c_4 = \pm \frac{ic_2}{2\sqrt{c_1}} \qquad (27)$$

$$c_4 = \pm \frac{imZe^2}{4\pi\epsilon\hbar\sqrt{l(l+1)}} = \pm ic_5 \qquad (28)$$

To satisfy boundary conditions for nano isolated particles, it is suitable to take the plus sign of equation (28) to write (26) as

$$R(r) = Br^{\sqrt{c_1} - 1} e^{-(c_5 r)} \qquad (29)$$

Equation (29) conforms with the fact that outside the nano crystal no electrons exists because

$$R \to 0 \quad as \quad r \to \infty \qquad (30)$$

Such choice agree also with the fact that inside the nucleus, no particle exists, for $(r = 0)$

$$R(r) = 0 \qquad (31)$$

According to equation (29)

$$R(r) = r^{\sqrt{c_1} - 1} e^{-0} = r^{\sqrt{c_1} - 1} \to 0 \qquad (32)$$

This requires

$$\sqrt{c_1} - 1 > 0 \qquad \sqrt{c_1} > 1 \qquad (33)$$

This is quite reasonable since equation (2) gives

$$\sqrt{c_1} = \frac{\sqrt{l(l+1)}}{\hbar^2} > 10^{34} \qquad (34)$$

To diminish faster outside the sphere of radius$a$, one requires that for

$$r > a \qquad c_5 r > 1 \qquad (35)$$

$$R(r) \to 0 \qquad (36)$$

Thus

$$r > \frac{1}{c_5} \qquad (37)$$

Therefore

$$a \sim \frac{1}{c_5} \qquad (38)$$

In view of equations (2) and (22)

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 c_4^2}{2m} = -\frac{\hbar^2 c_5^2}{2m} \quad (39)$$

Since the energy is negative (see (24)) it follows that

$$E = -|E| = -\frac{\hbar^2 c_5^2}{2m} = -\frac{\hbar^2}{2ma^2} = -\frac{\hbar^2}{2ma^2} \quad (40)$$

III. DISCUSSION

Assuming nano particles has spherical shape; a useful expression for Schrödinger equation was obtained. The Schrödinger Equation was solved in spherical coordinate as shown by equation (1) (2) and (3) for spherical coulomb potential affecting electrons. The solution suggests the wave function to be a sum of sin and cosine function [see equation (5)]. The energy obtained is shown to be quantized, depending on the orbital quantum number as equation (24) indicates. The minus sign in the energy expression shows that the energy particles are bounded by attractive force. This describes orbital electrons as well as electrons moving near positively ionized atoms, like conductor atoms. The wave function in equations (29), (30), (31) and (32) reflects the fact that outside the atom and nano particle no electrons exist, as well as inside the nucleus. This agrees with the fact that (34).

$$\sqrt{c_1} > 1$$

This solution holds for hydrogen like atoms also. It is much simpler that the ordinary one. But the energy here depends on the orbital quantum number rather than the principal number.

It is also important to note that using the expression of the Bohr minimum radius

$$r_0 = \frac{\hbar^2 \epsilon}{\pi Z m e^2}$$

Equation (24) gives the energy gap to be

$$E_g = (E_{l+1} - E_l) \sim \frac{1}{r_0} \sim \frac{1}{a_0}$$

This conforms to equation (40). It also means that increasing nano crystal size decreases the energy gap, thus increases absorption coefficient α and conductivityσ, since

$$\sigma \sim \alpha$$

This theoretical result agrees with observations, where the increase of nano particle size increases absorption coefficient and conductivity, as pointed out by some researchers and confirmed experimentally.

IV. CONCLUSION

The Schrödinger Equation for spherical atoms or nano particles shows that no electrons exist outside the nano sphere; it also shows that the energy is quantized. The absorption coefficient of the nano particle increases upon increasing particle size which agrees with some observations. This solution can describe hydrogen like atoms easily. The energy here depends on the orbital quantum number rather than the principal quantum number.

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