Global Journal of Science Frontier Research: F
Mathematics and Decision Sciences
Volume 19 Issue 1 Version 1.0 Year 2019
Type : Double Blind Peer Reviewed International Research Journal
Publisher: Global Journals
Online ISSN: 2249-4626 & Print ISSN: 0975-5896

General Solution of the Schrödinger Equation with Potential Field Quantization and Some Applications

By Hasan Hüseyin Erbil
Ege University

Abstract- A simple procedure has been found for the general solution of the time-independent Schrödinger Equation (SE) with the help of quantization of potential area in one dimension without making any approximation.Energy values are not dependent on wave functions. So, to find the energy values, it is enough to find the classic turning points of the potential function. Two different solutions were obtained, namely, symmetric and anti symmetric in bound states. These normalized wave functions are always periodic. It is enough to take the integral of the square root of the potential energy function to find the normalized wave functions. If these calculations cannot be made analytically, they should then be performed by numerical methods. The SE has been solved for a particle in many one-dimension and the spherical symmetric central potential well, the relativistic theory of Dirac as examples.

Keywords: *potential quantization, schrödinger equation, potential wells of any form, energy values of bound states, dirac equation, tunneling theory, transmission coefficient, α-decay theory, scattering theory.*

GJSFR-F Classification: *MSC 2010: 32W50*

Strictly as per the compliance and regulations of:

General Solution of the Schrödinger Equation with Potential Field Quantization and Some Applications

Hasan Hüseyin Erbil

Abstract- A simple procedure has been found for the general solution of the time-independent Schrödinger Equation (SE) with the help of quantization of potential area in one dimension without making any approximation.Energy values are not dependent on wave functions. So, to find the energy values, it is enough to find the classic turning points of the potential function. Two different solutions were obtained, namely, symmetric and anti symmetric in bound states. These normalized wave functions are always periodic. It is enough to take the integral of the square root of the potential energy function to find the normalized wave functions. If these calculations cannot be made analytically, they should then be performed by numerical methods. The SE has been solved for a particle in many one-dimension and the spherical symmetric central potential well, the relativistic theory of Dirac as examples. Their energies and normalized wave functions were found as examples. These solutions were also applied to the theories of scattering, tunneling and alpha decay. The results obtained with the experimental values were compared with the calculated values. The calculated results were consistent with measured experimental results.

Keywords: potential quantization, schrödinger equation, potential wells of any form, energy values of bound states, dirac equation, tunneling theory, transmission coefficient, α-decay theory, scattering theory.

I. Introduction

Mechanical total energy (E) is the sum of kinetic energy (T) and potential energy (U). That is $E = T + U$. If $E = U$ then $T = 0$.If $E > U$ *then* $T > 0$; If $E < U$ *then* $T < 0$ (it is not possible, classically).In quantum mechanics, the total energy is equal to the eigen value of the total energy operator$\hat{H}$ (Hamiltonian). One dimension Hamiltonian operator is given as follows: $\hat{H} = -\frac{\hbar^2}{2\,m}\frac{d^2}{dx^2} + U(x)$. This operator is hermitic and its eigen values are real numbers. The equation of eigen values of this Hamiltonian is given as follows (time-independent Schrödinger Equation, SE):

$$\hat{H}\,\psi(x) = \left[-\frac{\hbar^2}{2\,m}\frac{d^2}{dx^2} + U(x)\right]\psi(x) = E\,\psi(x) \qquad (1)$$

The eigen value E can have two values, $-E$ and $+E$, $(E > 0)$,so from equation(1), the following differential equation is obtained:

$$\frac{d^2\psi(x)}{dx^2} + [k^2 - m_1^2\,U(x)]\,\psi(x) = 0, \qquad (2)$$

Where, $k^2 = -m_1^2\,E$ for $-E$ and $k^2 = m_1^2\,E$ for $+E$; $m_1^2 = 2\,m/\hbar^2$ (3)

Author: Ege University Science Faculty Izmir Turkey. e-mail: Hhuseyin.Erbil@Gmail.Com

Although we succeed in solving the time-independent SE for some quantum mechanical problems in one dimension, an exact solution is not possible in complicated situations. We must then resort to approximation methods. For the calculation of stationary states and energy eigenvalues, these include the variation method, the method of Nikiforov-Uvarovthe supersymmetric quantum mechanics, the Wentzel-Kramers-Brillouin (WKB) and the super symmetric WKB approximations, and the perturbation theory. Perturbation theory is applicable if the Hamiltonian differs from an exactly solvable part by a small amount. The variation method is appropriate for the calculation of the ground state energy if one has a qualitative idea of the form of the wave function. The WKB method is applicable in the nearly classical limit. The exact general solution of the differential equation given in Equation(2) has not been achieved yet. This is problem a very challenging problem for theoretical physicists.

In this study, we followed a simple procedure for the exact general solution of the time-independent SE in one dimension without making any approximation. We have applied this simple procedure to various quantum mechanical problems: one-dimension potentials, spherically symmetric potentials, relativist equation of Dirac, tunneling effect, theory of alpha decay, scattering theory and presented some examples.

This text was prepared based on the reference [1]. For this reason, most references in [1] are not given here again.

II. Solution of the Time-Independent SE in one Dimension

Let us rewrite the time-independent SE in one dimension given in Equation(2):

$$\frac{d^2\psi(x)}{dx^2} + [k^2 - m_1^2\, U(x)]\, \psi(x) = 0 \tag{4}$$

Here, E (in k) and U(x)arerespectively the total and effective potential energies of a particle of mass m. Two kinds of solutions to the SE correspond precisely to bound and scattering (unbound) states. When $E < U(-\infty)$ and $U(+\infty)$, solutions correspond to bound states; when $E > U(-\infty)$ or $U(+\infty)$,the solutions correspond to scattering states. In real life, many potential functions go to zero at infinity, in which case the criterion is simplified even further: when $E < 0$, *bound states occur; when* $E > 0$scattering states occurs. In this section, we shall explore potentials that give rise to both kinds of states. We will solve Equation(4)]in two steps as follows.

a) The first Step

Inspired by the theorem given in [2], we consider the following integral function:

$$S(x) = \int U(x)dx. \tag{5}$$

If f(x) = S(x)in this theorem, we get:

$$F(\varepsilon) = \int_{-\infty}^{+\infty} S(x)\, y(x - x_0, \varepsilon)\, dx \tag{6}$$

From this function for$\varepsilon = 0$, the following is obtained:

$$\lim_{\varepsilon\to 0} F(\varepsilon) = F(0) = \lim_{\varepsilon\to 0} \int_{-\infty}^{+\infty} S(x)\, \delta(x - x_0)\, dx = S(x_0) = S \tag{7}$$

Now, let us take the potential and wave functions respectively as follows:

$$S = \int_{x_1}^{x_2} U(x)\, dx;\ U(x) = S(x_0)\, \delta(x - x_0) = S\, \delta(x - x_0) \text{and} \psi(x) = F(x) \tag{8}$$

Ref
1. Erbil, H. H., Turkish Journal of Physics, 42, 2018, 527-572.

Here, $\delta(x-x_0)$ is Dirac function. x_1 and x_2 are the roots of the equation $E = U(x)$, that is the apsis of the classical turning point of the potential function. If we take $x_0 = (x_1 + x_2)/2$ and $d = x_2 - x_1$, $(x_2 > x_1)$, then we find $x_1 = x_0 - d/2$, $x_2 = x_0 + d/2$. (See Figure1).If we take these functions, the SE given in Equation(4) becomes as follows:

$$\frac{d^2F(x)}{dx^2} + k^2F(x) = m_1^2 S\,\delta(x - x_0)\,F(x) \qquad (9)$$

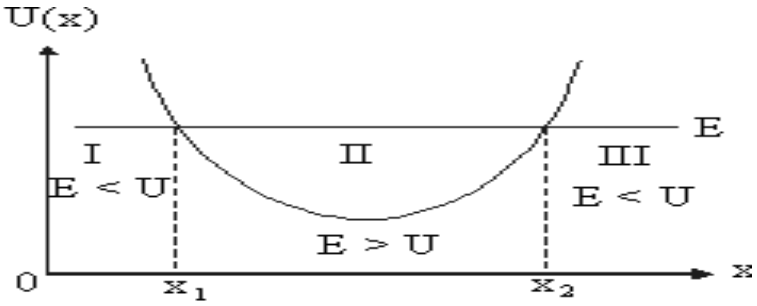
Notes

To evaluate the behavior of $F(x)$ at $x = x_0$, let us integrate the Equation (9) over the interval $[x_1, x_2] = [x_0 - d/2, x_0 + d/2]$ and also consider the limit $d \to 0$, then we obtain the following value:

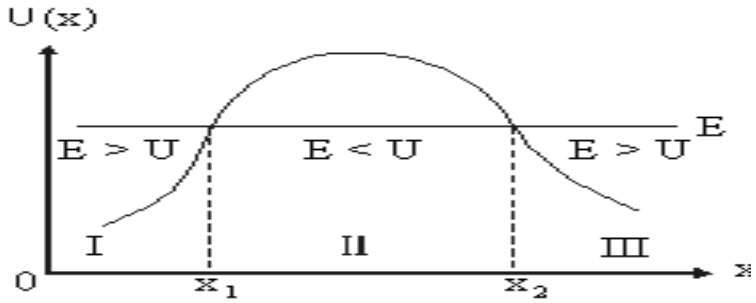
$$F'(x_0 + d/2) - F'(x_0 - d/2) = m_1^2 S\,F(x_0) \qquad (10)$$

Equation (10) shows that the derivation of $F(x)$ is not continuous at the $x = x_0$ point, whereas the wave functions $F(x)$ should be continuous at the same point.

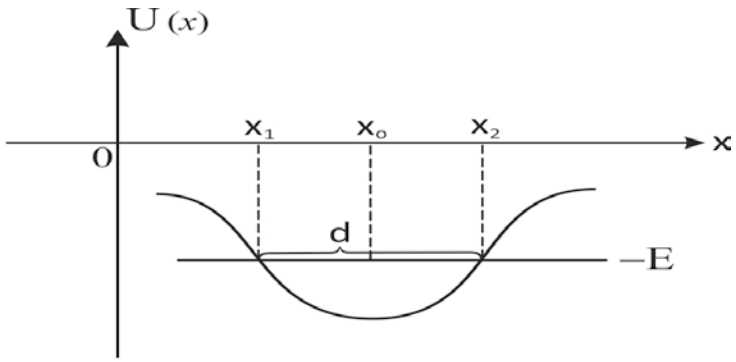
To solve the differential equation given in Equation (9), we can perform the transformation of Fourier of the equation, and then we obtain the following function:



(a)



(b)



(c)

Figure 1: Regions relevant to a particle of energy E moving in a one dimensional potential field, U(x).(a) In the domains I and III, $E < U(x)$, (unbound state); In the domain II, $E > U(x)$, (bound state). (b) In the domains I and III, $E > U(x)$,In the domain II, $E < U(x)$, (unbound state). The roots of the equation $E = U(x)$ are turning points of the corresponding classical motion. (c) Regions for $U(x) < 0$ and $E < 0$.

$$F(x) = A\, e^{-k\,|(x-x_0)|}\,,\quad \left[A = \frac{a^2}{k}\sqrt{\frac{\pi}{2}}\;,\; a^2 = -\frac{2\,m}{\hbar^2\sqrt{2\,\pi}}\,S\,F(x_0)\right] \tag{11}$$

From Equation (11), we get the following functions:

$$F(x) = A\, e^{k(x-x_0)} \text{for} x < x_0 \quad \text{and} \quad F(x) = A\, e^{-k(x-x_0)} \quad \text{for} \quad x > x_0 \tag{12}$$

Substituting the functions given in Equation(12) into Equation (10) and taking the limit$d \to 0$, the following values are obtained:

$$k = \frac{m}{\hbar^2}\,S \text{ or} E = \pm\frac{m}{2\,\hbar^2}\,S^{\,2} \tag{13}$$

The same values given in Equation(13) can also be obtained from Equation(11).To find the integral constant A, the function F(x) can be normalized to 1:

$$\int_{-\infty}^{x_0} A\,A^*\,e^{2k(x-x_0)}dx + \int_{x_0}^{+\infty} A\,A^*\,e^{-2k(x-x_0)}dx = 1.$$

From this equation, we obtain the coefficient of normalization as:

$$|A| = \sqrt{k} = \sqrt{m\,S}\,/\hbar \tag{14}$$

From Equation(12), by the linear combinations of these functions, we have also the following functions:

$$F(x) = A\, e^{k(x-x_0)} + B\, e^{-k(x-x_0)} \tag{15a}$$

$$F(x) = \frac{1}{2}A\left[e^{k(x-x_0)} + e^{-k(x-x_0)}\right] = A\cosh[k(x-x_0)] \tag{15b}$$

$$F(x) = \frac{1}{2}A\left[e^{k(x-x_0)} - e^{-k(x-x_0)}\right] = A\sinh[k(x-x_0)] \tag{15c}$$

Notes

b) The second Step

Let us assume the wave function $\psi(x)$ to be $\psi(x) = F(x)\, e^{i\, G(x)}$,(we assume that $G(x)$ is a real function). If we substitute this function into Equation(4), we get:

$$F''(x) - F(x)\, G'^{2}(x) - k^2 F(x) - m_1^2\, U(x)F(x) + i\,[2\, F'(x)G'(x) + F(x)G''(x)] = 0 \qquad (16)$$

From the real and imaginary parts of Equation(16), we can have the following two equations:

Notes

$$F''(x) - F(x)G'^{2}(x) - k^2 F(x) - m_1^2\, U(x)F(x) = 0 \qquad (17)$$

$$2\, F'(x)G'(x) + F(x)G''(x) = 0 \qquad (18)$$

From Equation(17), the following equations are obtained:

For $F(x) = A\, e^{k(x-x_0)}\,; \quad F(x)\left[m_1^2 U(x) + G'^{2}(x)\right] = 0$ (19a)

For $F(x) = A\, e^{-k(x-x_0)}; \quad F(x)\left[m_1^2 U(x) + G'^{2}(x)\right] = 0$ (19b)

For $F(x) = A\, e^{k(x-x_0)} + B\, e^{-k(x-x_0)}\,; \; F(x)\left[m_1^2 U(x) + G'^{2}(x)\right] = 0$ (19c)

For $F(x) = A\cosh[k(x-x_0)]\,; \; F(x)\left[m_1^2 U(x) + G'^{2}(x)\right] = 0$ (19d)

For $F(x) = A\sinh[k(x-x_0)]\,; \; F(x)\left[m_1^2 U(x) + G'^{2}(x)\right] = 0$ (19e)

From Equations(19a)-(19e),the following two equations are obtained:

$$m_1^2 U(x) + G'^{2}(x) = 0 \qquad (20a)$$

$$F(x) = 0 \qquad (20b)$$

From Equation(20a), the function $G(x)$is obtained as follows:

$$G(x) = \pm\, m_1 \int \sqrt{-U(x)}\; dx \; = \pm\, i\, m_1 \int \sqrt{U(x)}\; dx = \pm i\, Q(x) \qquad (21a)$$

$$Q(x) = m_1 \int \sqrt{U(x)}\; dx \qquad (21b)$$

Thus, the wave function $\psi(x)$ has been written as follows:

$$\psi(x) = F(x)e^{\pm i\, G(x)} \quad \text{or} \quad \psi(x) = F(x - x_0)e^{\pm i\, G(x-x_0)} \qquad (22)$$

The functions given in Equation(22)can also be written as follows:

$$\psi(x) = F(x)\left[A\, e^{i\, G(x)} + B\, e^{-i\, G(x)}\right] \text{ or} \qquad (23a)$$

$$\psi(x) = F(x - x_0)[A\, e^{i\, G(x-x_0)} + B\, e^{-i\, G(x-x_0)}] \qquad (23b)$$

In the functions given in Eqs(23a) and (23b):

a) For $E > U(x)$; $k = m_1\sqrt{-E}$, $G(x) = m_1 \int \sqrt{-U(x)}\, dx$,

b) For $E < U(x)$; $k = m_1\sqrt{E}$, $G(x) = m_1 \int \sqrt{U(x)}\, dx$.

As shown in Figure1a, the total energy is equal to potential energy at the points $x_1 = x_0 - d/2$ and $x_2 = x_0 + d/2$. So, kinetic energy is zero at these points. Now, let us examine the behavior of the function in the interval $[x_0 - d/2\,,\; x_0 + d/2]$.

Now, let us consider Equation(20b), that is: $\mathbf{F(x) = 0}$. Let us assume that the roots of this equation are $x_1 = x_0 - d/2$ and $x_2 = x_0 + d/2$. So, we can write the following equations:

$$F(x_1) = F(x_0 - d/2) = 0 \;;\quad F(x_2) = F(x_0 + d/2) = 0 \tag{24}$$

From Equation(24), the following expressions can be obtained:

a) For $F(x) = A\, e^{k(x-x_0)} + B\, e^{-k(x-x_0)};\; k = m_1\sqrt{-E} = i\, m_1\sqrt{E} = i\, K, [K = m_1\sqrt{E} > 0]$

$$a_{11}A + a_{12}B = 0;\quad a_{21}A + a_{22}B = 0;$$

$$a_{11} = e^{-i\, d\, K/2}\;;\; a_{12} = e^{i\, d\, K/2};\; a_{21} = e^{i\, d\, K/2};\; a_{22} = e^{-i\, d\, K/2}$$

Since A and B have to nonzero values, the determinant of coefficients in this system of equations must be zero. Thus, the following equation can be written as follows:

$$\det\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = -2\, i \sin(d\, K) = 0. \tag{25}$$

Here let us take $d\, K = q$. From Equation (25), we have the following values:
$\sin(d\, K) = \sin(q) = 0 \;\rightarrow\; q = n\,\pi\,,\; [n = 1, 2, 3, 4, \ldots \text{integer}]$.
So, we obtain the quantization condition of energy as follows:

$$K\, d = \sqrt{\frac{2\, m}{\hbar^2}\,|E|}\; d = q,\quad [q = n\,\pi\,,\; (n = 1, 2, 3, \ldots \text{ integer numbers})] \tag{26}$$

Here the coefficient B is obtained as $B = -A$. Thus the function $F(x)$ is written as follows:

$$F(x) = A\left[e^{i\, K\,(x-x_0)} - \; e^{-i\, K\,(x-x_0)}\right] = 2\, i\, A \sin[K(x - x_0)] = B\, \sin[K(x - x_0)].$$

The coefficient B in this function is found by normalizing the function in the interval $[x_1, x_2]$, and one is found as follows: $|B| = \sqrt{2/d}$. Thus the functions $F(x)$ and $\psi(x)$are written as follows:

$$F(x) = \sqrt{2/d}\;\; \sin\,[K(x - x_0)]\;;\; \psi(x) = \sqrt{2/d}\;\; \sin\,[K(x - x_0)]\;\; e^{iG\,(x-x_0)} \tag{27}$$

b) For $F(x) = A\cosh[k(x - x_0)]; k = i\, K$

$$F(x_1) = F(x_0 - d/2) = 0\;; F(x_2) = F(x_0 + \; d/2) = 0$$

$$F(x_1) = F(x_2) = A\cosh(d\, k/2) = A\cos(d\, K/2) = 0$$

$$d\;\; K/2 = q/2 = (2\, n - 1)\,\pi/2 \;\rightarrow q = (2\, n - 1)\pi, \qquad [n = 1,2,3, \ldots \text{integer}]$$

So, we obtain the quantization condition of energy as follows (symmetric case):

$$K\, d = \sqrt{\frac{2\, m}{\hbar^2}\,|E|}\; d = q,\; [q = (2n - 1)\,\pi\,, (n = 1, 2, 3, \ldots \text{integer numbers})] \tag{28}$$

The coefficient A in this function is found by normalizing the function in the interval $[x_1, x_2]$. That is$|A| = \sqrt{2/d}$. Thus, the functions $F(x)$ and $\psi(x)$are written as follows:

$$F(x) = \sqrt{2/d}\;\cos[K\,(x - x_0)];\; \psi(x) = \sqrt{2/d}\;\cos[K(x - x_0)]\; e^{i\, G(x-x_0)} \tag{29}$$

Notes

c) For $F(x) = A\sinh[k(x - x_0)]; k = i\,K$;

$$F(x_1) = F(x_0 - d/2) = 0 \;\; ; \;\; F(x_2) = F(x_0 + d/2) = 0$$

$$F(x_1) = -A\ \sinh(d\,k/2) = -i\,A\sin(d\,K/2) = 0$$

$$F(x_2) = A\ \sinh(d\,k/2) = i\,A\sin(d\,K/2) = 0$$

$$d\ K/2 = q/2 = n\,\pi \ \rightarrow\ q = 2\,n\,\pi\,, \qquad [n = 1, 2, 3, \ldots \text{integer numbers}]$$

Notes

So, we obtain the quantization condition of energy as follows (antisymmetric case):

$$K\,d = \sqrt{\frac{2\,m}{\hbar^2}\,|E|}\ d = q,\ [q = 2\,n\,\pi\,,\ (n = 1, 2, 3, \ldots \text{ integer numbers})] \qquad (30)$$

The coefficient A in this function is found by normalizing the function in the range $[x_1, x_2]$ and one is found as follows: $|A| = \sqrt{2/d}$ .Thus, the functions $F(x)$ and $\psi(x)$are written as follows:

$$F(x) = \sqrt{2/d}\ \sin[K\,(x - x_0)];\ \psi(x) = \sqrt{2/d}\ \ \sin[K\,(x - x_0)]\ e^{i\,G(x - x_0)} \qquad (31)$$

It is possible to combine Equations(28) and (30) in one equation as follows (general case):

$$K\,d = \sqrt{\frac{2\,m}{\hbar^2}\,|E|}\ d = q, \quad [q = n\,\pi\,,\ (n = 1, 2, 3, \ldots \text{ integer numbers})] \qquad (26)$$

Now let us write the kinetic energy of the particle as follows:

$$T = \frac{p^2}{2\,m} = E - U(x)$$

By integrating this equation from x_1 to $x_2$and using Equation(8), the following equation is obtained:

$$\int_{x_1}^{x_2} T\,dx = \int_{x_1}^{x_2} \frac{p^2}{2\,m}\,dx = \int_{x_1}^{x_2} [E - U(x)]dx = \int_{x_1}^{x_2} E\,dx - \int_{x_1}^{x_2} U(x)\,dx = S_k\,.$$

From this the following equation is written:

$$S_k = E\,(x_2 - x_1) - S = E\,d - S \qquad (32)$$

From the Figure1, we can observe that:

a) For the case $E > U(x)$, the kinetic energy is positive and$[E\,(x_2 - x_1) - S] > 0$(bound states).

b) For the case $E < U(x)$, the kinetic energy is imaginary and$[E\,(x_2 - x_1) - S] < 0$ (unbound states).

c) For the case $E = U(x)$, the kinetic energy is zero and $[E\,(x_2 - x_1) - S] = 0$ (minimum energy state or ground state in bound states).

In addition, for the bound states, in the interval$[x_1\,, x_2]$, the kinetic energy is positive, outside this interval, the kinetic energy is imaginary. The minimum point of the potential corresponds to ground state. In ground state, the kinetic energy is zero, namely $T = 0$ and $S_k = 0$. Thus, at the minimum point of the potential, we can write that:

$$E_0(x_2 - x_1) - S = 0 \text{or } S = E_0(x_2 - x_1) = E_0 d.$$

By substituting this value of S into the equation (13), we get the ground state energy expression as follows:

$$E_0 = -\frac{m}{2\hbar^2} S^2 = -\frac{m}{2\hbar^2} E_0^2 d^2 \;\rightarrow\; E_0 = -\frac{2\hbar^2}{m d^2} \tag{33}$$

Here, E_0 represents the ground state energy. The negative sign indicates that the state is bound and it can be omitted for the positive energies in the calculations.

III. Boundary Conditions

Let us divide the potential field into three domains as shown inFigure1 and represent the functions $\psi_1(x)$, $\psi_2(x)$ and $\psi_3(x)$ in each domain. The wave functions and their derivatives should be continuous. Because of these conditions, the above functions must satisfy the following conditions:

$$\psi_1(x_1) = \psi_2(x_1) \;;\; \psi_1'(x_1) = \psi_2'(x_1);\; \psi_2(x_2) = \psi_3(x_2) \;;\; \psi_2'(x_2) = \psi_3'(x_2)$$

$$\lim_{x\to-\infty} \psi_1(x) \to 0 \quad \text{and} \quad \lim_{x\to+\infty} \psi_3(x) \to 0 \tag{34}$$

The normalization of the bound state function requires that the functions vanish at infinity. With these boundary and normalization conditions of the wave functions, we can find the integral constants, A , B andthe energy E.As it will be also seen above, in the bound states, we do not need the solutions of the SE. It is sufficient to know only the classical turning points, x_1 and x_2 ,of the potential function.

Quantization of the energy values can also be found by means of boundary conditions. Let us find them now. In bound states, let us apply the conditions given in Equation(34) to the following functions:

$$A\, e^{k(x-x_0)} + B\, e^{-k(x-x_0)}; A\cosh[k(x-x_0)] \;;\; B\sinh[k(x-x_0)].$$

a) For the function $Ae^{k(x-x_0)} + Be^{-k(x-x_0)}$

According to Figure1a, in the domain I, $E < U(x)$, in the domain II, $E > U(x)$, in the domain III, $E < U(x)$. According to Equations (23a) and (23b), the corresponding wave functions are written as follows:

$$\psi_1(x) = A_1 e^{ik(x-x_0)}\, e^{-Q(x-x_0)} \tag{35a}$$

$$\psi_2(x) = [A_2 e^{k(x-x_0)} + B_2 e^{-k(x-x_0)}]\, e^{iQ(x-x_0)} \tag{35b}$$

$$\psi_3(x) = A_3 e^{-ik(x-x_0)}\, e^{-Q(x-x_0)} \tag{35c}$$

Here, $Q(x-x_0) = m_1 \int \sqrt{-U(x-x_0)}\, dx$, $k = m_1\sqrt{-E} = i\, m_1\sqrt{E}$.
Boundary conditions:

$$\psi_1(x_1) = \psi_2(x_1), \qquad \psi_2(x_2) = \psi_3(x_2), \;\; \psi_1'(x_1) = \psi_2'(x_1),$$

$$\psi_2'(x_2) = \psi_3'(x_2) \lim_{x\to-\infty} \psi_1(x) \to 0 \quad \text{and} \quad \lim_{x\to+\infty} \psi_3(x) \to 0$$

From these conditions, four linear equations are obtained as follows:

$$\begin{bmatrix} a_{11} a_{12} a_{13} a_{14} \\ a_{21} a_{22} a_{23} a_{24} \\ a_{31} a_{32} a_{33} a_{34} \\ a_{41} a_{42} a_{43} a_{44} \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ B_2 \\ A_3 \end{bmatrix} = 0 \qquad (36a)$$

For this system of equations to have a solution different from zero, the determinant of coefficients should vanish, namely;

$$\det \begin{vmatrix} a_{11} a_{12} a_{13} a_{14} \\ a_{21} a_{22} a_{23} a_{24} \\ a_{31} a_{32} a_{33} a_{34} \\ a_{41} a_{42} a_{43} a_{44} \end{vmatrix} = 0 \qquad (36b)$$

If it is taken as follows

$$x_1 = x_0 - d/2, \qquad x_2 = x_0 + d/2\ , \qquad Q'(-d/2) = Q'(d/2) = k,\ \ k = i\,K, \qquad d\,K = q$$

From Equations(36a) and (36b),following equation is obtained:

$$e^{[-i\,q - (1-i)Q(-d/2) + (1+i)Q(d/2)}\left[-1 + e^{2\,i\,q}\right] = 0 \qquad (37)$$

For the equality in Equation (37) to be realized, it has to be $q = n\,\pi$, $(n = 1, 2, 3, \ldots)$. Thus, we obtain the quantization condition of energy as follows:

$$K\,d = \sqrt{\frac{2\,m}{\hbar^2}\,|E|}\ d = q,\ \ [q = n\,\pi,\ (n = 1, 2, 3, \ldots \text{ integer numbers})] \qquad (38)$$

b) For the function $cosh[k\,(x - x_0)]$

According to theFigure1a, in the domain I, $E < U(x)$; in the domain II, $E > U(x)$; in the domain III, $E < U(x)$. According to the equations given in Equations(23a) and (23b), the corresponding wave functions are written as follows:

$$\psi_1(x) = A_1 \cosh[i\,k\,(x - x_0)]\ e^{i\,i\,G(x - x_0)};\ \ \psi_2(x) = A_2 \cosh[\,k\,(x - x_0)]\ e^{i\,G(x - x_0)}$$

$$\psi_3(x) = A_3 \cosh[-i\,k\,(x - x_0)]\ e^{i\,i\,G(x - x_0)};\ \ x_1 = x_0 - d/2 \ \text{ and } x_2 = x_0 + d/2$$

According to the conditions given in Equation(34)it can be written that:

$$\psi_1(x_1) = \psi_2(x_1) \mathbf{or} \psi_1(x_1) - \psi_2(x_1) = 0 \qquad (39a)$$

$$\psi_2(x_2) = \psi_3(x_2) \mathbf{or} \psi_2(x_2) - \psi_3(x_2) = 0 \qquad (39b)$$

From (39a) and (39b), two linear equations are obtained as follows:

$$a_{11} A_1 + a_{12} A_3 = 0;\ \ a_{21} A_1 + a_{22} A_3 = 0 \qquad (39c)$$

$$a_{11} = e^{-G(-d/2)} \cos(d\,k/2)\ ,\ a_{12} = 0\ ; a_{21} = 0\ ,\ a_{22} = -e^{G(d/2)} \cos(d\,k/2)$$

For this system of equations to have a solution different from zero, the determinant of coefficients should vanish, namely:

$$\det \begin{vmatrix} a_{11} a_{12} \\ a_{21} a_{22} \end{vmatrix} = 0 \ \rightarrow\ -\frac{1}{2} e^{-G(-d/2) + G(d/2)} [1 + \cos(d\,k) = 0 \qquad (40)$$

In Equation (40), $-\frac{1}{2} e^{-G(-d/2) + G(d/2)} \neq 0,\ k = m_1\sqrt{-E} = i\,m_1\sqrt{E} = i\,K, (E > 0,\ K = m_1\sqrt{E})$. So, $1 + \cos(d\,k) = 1 + \cos(id\,K) = 1 + \cos(d\,K) = 0$. From this last

equation, we have that: $d\,K = q = n\,\pi$, $(n = 1, 3, 5, 7, \ldots \text{odd integers})$. This is also written as follows:

$$d\,K = q = (2\,n - 1)\pi, \quad (n = 1, 2, 3, \ldots \text{integers}) \tag{41}$$

The solution of the system of equations in (39c) gives: $A_1 = 0$ and $A_3 = 0$. The coefficient $A_2 = A$ is found by the normalization of the function, $\psi_2(x) = A_2 \cosh[k\,(x - x_0)]\; e^{i\,G(x-x_0)}$, namely:

$$\int_{x_0-d/2}^{x_0+d/2} A\cosh[k\,(x - x_0)]\, e^{i\,G(x-x_0)}\, A^*\cosh[k\,(x - x_0)]\, e^{-i\,G(x-x_0)}\, dx =$$

$$= \frac{A\,A^*[d\,K + \sin(d\,K)]}{2\,K} = \frac{A\,A^*\,d}{2} = \frac{d\,|A|^2}{2} = 1 \rightarrow \quad |A| = \sqrt{2/d} = \sqrt{2\,K/q}$$

So, the normalized wave functions in the bound state are as follows:

$$\psi(x) = A\cos[K\,(x - x_0)]\; e^{i\,G(x-x_0)} \text{or} \psi(x) = A\cos[K\,x]\; e^{i\,G(x)} \tag{42}$$

c) For the function $\sinh[k\,(x - x_0)]$

According to the Figure1a, in the domain I, $E < U(x)$, in the domain II, $E > U(x)$, in the domain III, $E < U(x)$. According to Equations(23a) and (23b), the corresponding wave functions are written as follows:

$$\psi_1(x) = A_1 \sinh[i\,k\,(x - x_0)]\; e^{i\,i\,G(x-x_0)}\,; \psi_2(x) = A_2 \sinh[k\,(x - x_0)]\; e^{i\,G(x-x_0)}$$

$$\psi_3(x) = A_3 \sinh[-i\,k\,(x - x_0)]\; e^{i\,i\,G(x-x_0)};\;\; x_1 = x_0 - d/2 \;\text{ and }\; x_2 = x_0 + d/2$$

According to the conditions given in Equation(34) we have:

$$\psi_1(x_1) = \psi_2(x_1) \textbf{ or } \psi_1(x_1) - \psi_2(x_1) = 0 \tag{43a}$$

$$\psi_2(x_2) = \psi_3(x_2) \textbf{ or } \psi_2(x_2) - \psi_3(x_2) = 0 \tag{43b}$$

From Equations(43a) and (43b), the following two linear equations are obtained:

$$a_{11}A_1 + a_{12}A_3 = 0;\;\; a_{21}A_1 + a_{22}A_3 = 0 \tag{44}$$

$$a_{11} = -i\,e^{-G(-d/2)}\sin(d\,k/2)\;;\;\; a_{12} = 0\;;\;\; a_{21} = 0\;;\;\; a_{22} = i\,e^{G(d/2)}\sin(d\,k/2)$$

For this system of equations to have a solution different from zero, the determinant of coefficients should vanish, namely:

$$\det\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = 0 \quad \rightarrow \quad e^{-G(-d/2)+G(d/2)}\sin^2(d\,k/2) = 0 \tag{45}$$

In Equation (45), $e^{-G(-d/2)+G(d/2)} \neq 0$, $k = m_1\sqrt{-E} = i\,m_1\sqrt{E} = i\,K$, $\left(E > 0, K = m_1\sqrt{E}\right)$. So, $\sin^2(d\,k/2) = \sin^2(i\,d\,K/2) = \sin^2(d\,K/2) = 0$. From this last equation, we have the following value:

$$d\,K = q = 2\,n\,\pi, \quad (n = 1, 2, 3, \ldots \text{integers}) \tag{46}$$

Notes

The solution of the system of equations in Equation(44) gives as $A_1 = 0$ and $A_3 = 0$. The coefficient $A_2 = A$ is found by the normalization of the function $\psi_2(x) = A_2 \sinh[k(x - x_0)]\ e^{i G(x-x_0)}$, namely:

$$\int_{x_0-d/2}^{x_0+d/2} A \sinh[k(x - x_0)]\, e^{i G(x-x_0)}\, A^* \sinh[k(x - x_0)]\, e^{-i G(x-x_0)}\, dx =$$

$$= \frac{A A^*[-d K + \sin(d K)]}{2 K} = -\frac{A A^* d}{2} = 1 \rightarrow \quad |A| = \sqrt{2/d} = \sqrt{2 K/q}$$

So, the normalized wave functions in the bound state are as follows:

$$\psi(x) = A \sin[K(x - x_0)]\ e^{i G(x-x_0)} \text{ or } \psi(x) = A \sin[K x]\ e^{i G(x)} \tag{47}$$

Equations(41) and (46)can be combined as follows:

$$d K = q = n \pi, \ (n = 1, 2, 3, 4, \ldots \text{ integers}) \tag{48}$$

So, in the bound states, the normalized wave functions are as follows:

$$\psi(x) = \sqrt{2/d}\ \cos[K(x - x_0)] e^{i G(x-x_0)} \text{ and } \psi(x) = \sqrt{2/d}\ \sin[K(x - x_0)] e^{i G(x-x_0)} \tag{49a}$$

$$\text{Or,} \qquad \psi(x) = \sqrt{2/d}\ \cos[K x)] e^{i G(x)} \text{ and } \psi(x) = \sqrt{2/d}\ \sin[K x)] e^{i G(x)} \tag{49b}$$

The energy value is as follows: $E_q = \frac{\hbar^2}{2 m} \frac{q^2}{d^2} = m_h \frac{q^2}{d^2}$; $(m_h = \frac{\hbar^2}{2 m})$ (49c)

Now, in bound states, let us see the relations between the potential areas (see Figure 2):

a) According to the partial integration $\int u\, dv = u\, v - \int v\, du$can be written as follows:

$$S = S_p = \int_{x_1}^{x_2} U(x) dx = [x\, U(x)]_{x_1}^{x_2} - \int_{x_1}^{x_2} x\, U'(x) dx = x_2\, U(x_2) - x_1\, U(x_1) - S_t;$$

$$S_t = \int_{x_1}^{x_2} x\, U'(x) dx \ ; U(x_1) = U(x_2) = E_q \ ; \ d = x_2 - x_1.$$

Thus, the following can be written:

$$S_p = E\, d - S_t \quad \text{or} \quad E\, d = S_p + S_t \tag{50a}$$

b) Total energy = kinetic energy + potential energy; $E = T + U(x)$. From here, with the following integration:

$$\int_{x_1}^{x_2} E\, dx = \int_{x_1}^{x_2} T\, dx + \int_{x_1}^{x_2} U(x)\, dx \rightarrow \quad E\, d = S_k + S_p \tag{50b}$$

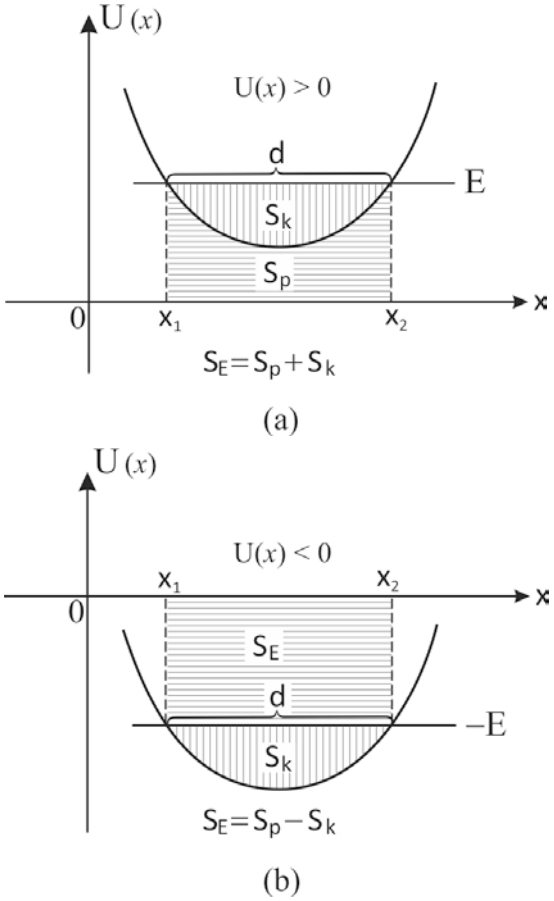


Figure 2: Potential area in the bound state: **(a)** $U(x) > 0$ *and* $E > 0$; **(b)** $U(x) < 0$ *and* $E < 0$

If Equations(50a) and (50b) are compared, it is seen that $S_k = S_t = \int_{x_1}^{x_2} x\, U'(x)dx$.

c) According to Equation(8): $E = -\frac{m}{2\hbar^2}S^2 = -\frac{m}{2\hbar^2}S_p^2 \rightarrow S_p = \sqrt{\frac{2\hbar^2}{m}|E|}$

$$K\,d = q \rightarrow \sqrt{\frac{2m}{\hbar^2}|E|}\,d = q \rightarrow |E| = \frac{\hbar^2}{2m}\frac{q^2}{d^2} = m_h\frac{q^2}{d^2} \rightarrow S_p = 2\,m_h\frac{q}{d} \qquad (50c)$$

d) From Equations(50a) and (50b), we obtain the following equation:

$$S_k = m_h\frac{q}{d}(q-2) \qquad (50d)$$

Thus, from Equations (50a)-(50d), let us rewrite these potential areas as follows:

$$S_p = \int_{x_1}^{x_2} U(x)dx = 2\,m_h\frac{q}{d};\ \text{(Potential energy field)} \qquad (51a)$$

$$S_k = \int_{x_1}^{x_2} x\,U'(x)dx = m_h\frac{q}{d}(q-2);\ \text{(Kinetic energy field)} \qquad (51b)$$

$$S_E = S_p + S_k = m_h\frac{q^2}{d};\qquad \text{(Total energy field)} \qquad (51c)$$

According to Equations (51) for $q = 2$, $S_k = 0$, the ground state occurs; for $q = n\pi$, $(n = 1, 2, 3, \ldots)$, the excited states occur.

Thus Equations(51a)-(51c)indicate that potential areas are quantized.

IV. Summary

It is possible to summarize the results above as follows.We can write the general solutions of the SE in one dimension as follows:

$$\psi(x) = A\, e^{k\,x} e^{\pm i\, G(x)} \text{ or } \psi(x) = A\, e^{k\,(x-x_0)} e^{\pm i\, G((x-x_0)} \tag{52a}$$

$$\psi(x) = A\, e^{-k\,x} e^{\pm i\, G(x)} \text{ or } \psi(x) = A\, e^{-k\,(x-x_0)} e^{\pm i\, G((x-x_0)} \tag{52b}$$

$$\psi(x) = \left[A\, e^{k\,x} + B\, e^{-k\,x}\right] e^{\pm i\, G(x)} \text{ or } \psi(x) = \left[A\, e^{k\,(x-x_0)} + B\, e^{-k(x-x_0)}\right] e^{\pm i\, G(x-x_0)} \tag{52c}$$

$$\psi(x) = A\, \cosh(k\,x)\, e^{\pm i\, G(x)} \text{ or } \psi(x) = A\, \cosh[k(x-x_0)]\, e^{\pm i\, G(x-x_0)} \tag{52d}$$

$$\psi(x) = A\, \sinh(k\,x)\, e^{\pm i\, G(x)} \text{ or } \psi(x) = A\, \sinh[k(x-x_0)]\, e^{\pm i\, G(x-x_0)} \tag{52e}$$

$$\psi(x) = A\, e^{k\,x \pm i\, G(x)} + B\, e^{-k\,x \mp i\, G(x)} \text{ or}$$

$$\psi(x) = A\, e^{k\,(x-x_0) \mp i\, G(x-x_0)} + B\, e^{-k(x-x_0) \mp i\, G(x-x_0)} \tag{52f}$$

In these functions, we have the following values:

a) For $E > U(x)$; $k = m_1\sqrt{-E}$, $G(x) = m_1 \int \sqrt{-U(x)}\, dx$ (53a)

b) For $E < U(x)$; $k = m_1\sqrt{E}$, $G(x) = m_1 \int \sqrt{U(x)}\, dx$ (53b)

m mass or reduced mass of particle, h Planck constant, $\hbar = h/(2\,\pi)$, $m_1 = \sqrt{2\,m}/\hbar$. x_1 and x_2 $(x_2 > x_1)$ are, depending on E, the roots of the equation $E = U(x)$, that is the abscises of the classic turning points,and $x_0 = (x_1 + x_2)/2$; $d = x_2 - x_1$.

This solution is similar to the WKB approach but is not certainly the same. There is approximation in the WKB method, but there is no approach in the method we have given here. Our procedure gives exact results. Those who are familiar with the WKB approach can easily see the differences between the two.

In bound states, the normalized wave functions are as follows [G is taken as real function):

$$\psi(x) = A\, \cos[\,K\,x]\; e^{\pm i\, G(x)} \text{ or } \psi(x) = A\, \cos[\,K\,(x-x_0)]\; e^{\pm i\, G(x-x_0)} \tag{54a}$$

$$\psi(x) = B\, \sin[\,K\,x]\; e^{\pm i\, G(x)} \text{ or } \psi(x) = B\, \sin[\,K\,(x-x_0)]\; e^{\pm i\, G(x-x_0)} \tag{54b}$$

$$A = B = \sqrt{2/d} = \sqrt{2K/q}; K = m_1\sqrt{|E|} = \sqrt{\frac{2\,m}{\hbar^2}}\sqrt{|E|}\;;\; G(x) = m_1 \int \sqrt{|U(x)|}\, dx$$

x_1 and x_2 are the roots of the equation:$|E| = |U(x)|$ or $|E| = |U(x-x_0)|$.From these, we have the following equations:

$$x_0 = (x_1 + x_2)/2 \;\; ; \;\; d = x_2 - x_1; x_1 = x_0 - d/2 \;\; ; \;\; x_2 = x_0 + d/2 \;;\; E = U(x) \;;$$

$$|E| = |U(x_1)| = |U(x_2)| \text{or} |E| = |U(x_0 - d/2)| = |U(x_0 + d/2)|;$$

$$2\,|E| = |U(x_0 - d/2)| + |U(x_0 + d/2)| \tag{54c}$$

$$K\,d = q \;\rightarrow\; \sqrt{\frac{2\,m}{\hbar^2}|E|}\;d = q \;\rightarrow\; |E| = \frac{\hbar^2}{2\,m}\frac{q^2}{d^2} = m_h\,\frac{q^2}{d^2}; [m_h = \frac{\hbar^2}{2\,m}] \tag{55}$$

For $q = 2$ ground state occurs;for $q = n\,\pi\,, (n = 1, 2, 3, \ldots)$ excited states occur. The energy values are also given by the following formulas:

$$E = -\frac{m}{2\,\hbar^2}S^2 = -\frac{m}{2\,\hbar^2}S_p^2\;;\; S_p = \sqrt{\frac{2\,\hbar^2}{m}|E|};\; S = S_p(x_0, d) = 2\,m_h\,\frac{q}{d} \tag{56a}$$

$$S_k(x_0, d) = m_h\,\frac{q}{d}(q-2) \tag{56b}$$

We can give the practical procedure to find the energy values as follows:

As seen in Equation(55), the total energy values depend on d; so the d value should be calculated to find the energy values. It can be calculated by one of the equations given in Equation(54c), but to find the values of d and energy E, the practical procedure can be given as follows:

First, solving the equation $|U(x)| = m_h\,q^2/y\,,\ (y = d^2)$, the following values are found as follows: $x_1\,,\ x_2\,,\ d(y) = x_2 - x_1,\ d_2(y) = d(y) * d(y)$. Then, the equation $y = d_2(y)$is solved,and the y value is found. So, the energy value is obtained as follows(especially, this rule provides convenience in numerical solutions):

$$|E| = m_h\,\frac{q^2}{y} = m_h\,\frac{q^2}{d^2} = \frac{\hbar^2}{2\,m}\frac{q^2}{d^2} \tag{57}$$

For $q = 2$, the ground state occurs; for $q = n\,\pi\,, (n = 1, 2, 3, \ldots)$the excited states occur.

V. Examples of One Dimensional Potentials

a) Potential: $U(x) = a\,|x|^p\,,\ (a > 0\,,\ p > 0)$

i. *Energy*

According to the practical procedure above:

$$E = U(x) = a\,|x|^p = m_h\frac{q^2}{y} \rightarrow \quad x_1 = -\left[\frac{m_h}{a}\frac{q^2}{y}\right]^{1/p};\, x_2 = \left[\frac{m_h}{a}\frac{q^2}{y}\right]^{1/p}$$

$$d = x_2 - x_1 = 2\left[\frac{m_h}{a}\frac{q^2}{y}\right]^{1/p};\; d_2(y) = d * d = 4\left[\frac{m_h}{a}\frac{q^2}{y}\right]^{2/p};\; y = d_2(y)$$

$$y = \left[\frac{a\;2^{-p}}{m_h\,q^2}\right]^{-2/(p+2)} \quad ; \quad E_q = m_h\frac{q^2}{y} = m_h\,q^2\left[\frac{a\;2^{-p}}{m_h\,q^2}\right]^{2/(p+2)} \tag{5.1.1}$$

For $q = 2$, the ground state occurs; for $q = n\,\pi\,, (n = 1, 2, 3, \ldots)$, the excited states occur.

In the formula given in (5.1.1), if $p = 2$ and $a = \frac{1}{2}\,m\,\omega^2$, it is found that $E_q = \frac{q}{4}\,\hbar\,\omega$. This is the energy of the simple harmonic oscillator. We have $E_0 = \frac{1}{2}\,\hbar\,\omega$ ground state energy for $q = 2\,; E_q = \frac{n\,\pi}{2}\,\hbar\,\omega,\ (n = 1, 2, 3, \ldots)$excited state energy for $q = n\,\pi$. The well-known energy of the simple harmonic oscillator is $E_n = \left(n + \frac{1}{2}\right)\hbar\,\omega,\ (n = 0, 1, 2, \ldots)$. The ground state energy $E_0 = \frac{1}{2}\,\hbar\,\omega$ is the same but the excited energy $E_q = E_n = \frac{n\,\pi}{4}\,\hbar\,\omega$ is different. This difference is observed in the experimentally measured energy spectra of nuclear nuclei, but this phenomenon cannot

be explained in harmonic oscillatory models. This event can be explained here. I think that the latter is more accurate because there is no approximation in ours solutions.

For the same potential, the ground state energy obtained from super symmetric quantum mechanics (SQ) is as follows [4]:

$$E_0 = \left[\frac{0.8862\ \Gamma\left(\frac{3}{2}+\frac{1}{p}\right)}{\Gamma\left(1+\frac{1}{p}\right)}\frac{\hbar^2}{2\,m}a^{\frac{2}{p}}\right]^{p/(p+2)} \tag{5.1.2}$$

From Equation (5.1.2), for $p = 2$ and $a = \frac{1}{2}\,m\,\omega^2$, we find approximate value as follows: $E_0 = 0.999985\,\frac{1}{2}\hbar\,\omega \approx \frac{1}{2}\hbar\,\omega$. As seen that new solution gives complete results. In this potential for $p = 1$ (V-Form potential), $E_0 \approx 0.794\left[\frac{\hbar^2 a^2}{m}\right]^{1/3}$ is obtained from the formula given in Equation(5.1.1); obtained $E_0 \approx 0.763\left[\frac{\hbar^2 a^2}{m}\right]^{1/3}$ from SQ; obtained $E_0 \approx 0.813\left[\frac{\hbar^2 a^2}{m}\right]^{1/3}$ from the variation method;and obtained $E_0 \approx 0.885\left[\frac{\hbar^2 a^2}{m}\right]^{1/3}$ from WKB method. These three values are approximately the same; however the new solution is complete.

ii. *Wave Functions*

$$G(x) = m_1\int\sqrt{|U(x)|}\,dx = \sqrt{\frac{2\,m}{\hbar^2}}\int\sqrt{U(x)}dx = Q(x) = \sqrt{\frac{2\,m}{\hbar^2}}\sqrt{a}\frac{2\,|x|^{(p+2)/2}}{p+2}$$

$$\psi(x) = A\cos[Kx]e^{i\,G(x)} = \sqrt{2\,K/q}\cos[Kx]e^{i\,Q(x)} = \sqrt{2/d}\cos[Kx]e^{iQ(x)} \tag{5.1.3a}$$

$$\psi(x) = B\sin[Kx]e^{iG(x)} = \sqrt{2\,K/q}\sin[Kx]e^{i\,Q(x)} = \sqrt{2/d}\ \sin[Kx]e^{iQ(x)} \tag{5.1.3b}$$

In the case of simple harmonic oscillator, $G(x) = Q(x) = \sqrt{\frac{2\,m}{\hbar^2}}\sqrt{a}\frac{2\,|x|^{(p+2)/2}}{p+2} = \frac{m\,\omega}{2\,\hbar}x^2$.
The well-known wave function of the harmonic oscillator is as follows:

$$\psi_n(\rho) = A_n e^{-\rho^2/2}H_n(\rho);[\rho = \sqrt{\frac{m\,\omega}{\hbar}}\,x] \tag{5.1.4}$$

Here, $H_n(\rho)$ is Hermit polynomials. If Equations (5.1.3a) and (5.1.3b) are expanded in series, polynomials are obtained. So, the well-known function given in Equation(5.1.4) of harmonic oscillator is an approximate function.

b) Infinitely high square potential well or finite square potential well

We consider a particle of mass m captured in a box limited by $0 \le x \le a$. The corresponding potential is given: $U(x) = 0$ for $0 < x < a$; $U(x) = \infty$ for $x < 0$ *and* $x > a$.

i. *Energy*

The turning points of this potential are given by the following equation: $U(x) = E$. From this equation, we can find the classical turning points of the potential function as follows: $x_1 = 0$ and $x_2 = a$; $x_0 = (x_1 + x_2)/2 = a/2$, $d = x_2 - x_1 = a$. By substituting this value of d into the equation, $d\,K = q$, and then solving for $|E|$, we can have the

Ref

4. Cooper, F.; Khare, A., Sukhatme, U., Supersymmetry in Quantum Mechanics, 2001, World Scientific.

energy value as:$E_q = \frac{\hbar^2}{2\,m}\frac{q^2}{a^2} = m_h\frac{q^2}{a^2}$; for $q = 2$ the ground state occurs; for $q = n\,\pi$, $(n = 1, 2, 3, \ldots)$ the excited states occur.

The well-known energy infinitely high potential well is $E_n = \frac{\hbar^2}{2\,m}\frac{(n\,\pi)^2}{a^2}$. The well-known energy finite potential well is found the following equations:

(a) For the states of even parity: $\sqrt{\frac{|E|}{U_0 - |E|}} = \tan\left\{\frac{a}{\hbar}[2\,m(U_0 - |E|)]^{1/2}\right\}$

(b) For the states of odd parity: $\sqrt{\frac{|E|}{U_0 - |E|}} = -\text{cotan}\left\{\frac{a}{\hbar}[2\,m(U_0 - |E|)]^{1/2}\right\}$

It is seen that two energy values are the same for infinitely high potential well, but they do not are the same for finite potential well.

ii. *Wave functions*

Here, $U(x) = 0$.So,$G(x) = m_1\int\sqrt{|U(x)|}\,dx = 0$

$$\psi(x) = A\cos[K\,x]e^{i\,G(x)} = \sqrt{2/a}\cos[K\,x] = \sqrt{2\,K/q}\cos[K\,x]$$

$$\psi(x) = B\sin[K\,x]e^{i\,G(x)} = \sqrt{2/a}\sin[K\,x] = \sqrt{2\,K/q}\sin[K\,x]$$

$$\psi(x) = A\cos\left[K(x - \frac{a}{2})\right] = \sqrt{2/a}\cos\left[K(x - \frac{a}{2})\right] = \sqrt{2\,K/q}\cos\left[K(x - \frac{a}{2})\right]$$

$$\psi(x) = B\sin\left[K(x - \frac{a}{2})\right] = \sqrt{2/a}\sin\left[K(x - \frac{a}{2})\right] = \sqrt{2\,K/q}\sin\left[K(x - \frac{a}{2})\right]$$

c) Trigonometric potential well

We consider the potential energy of the particle, U(x)so that $U(x) = U_0\,\text{cotg}^2(\pi x/a)$, $[U_0 > 0\,,\ a > 0$ and $0 < x < a\,]$.

i. *Energy*

The roots of the equation: $E_q = U(x) = m_h\frac{q^2}{y} \rightarrow U_0\,\text{cotg}^2[\pi\,x/a] = m_h\frac{q^2}{y}$;

$$x_1 = -\frac{1}{\pi}\,\text{arc cotg}\left[\sqrt{\frac{m_h}{U_0}\frac{q^2}{y}}\right];x_2 = \frac{1}{\pi}\,\text{arc cotg}\left[\sqrt{\frac{m_h}{U_0}\frac{q^2}{y}}\right];d = x_2 - x_1\ ;\ y = d * d$$

$$y = \frac{4}{\pi^2}\,\text{arc cotg}^2\left[\sqrt{\frac{m_h}{U_0}\frac{q^2}{y}}\right];E_q = m_h\frac{q^2}{d^2} = m_h\frac{q^2}{y}\,. \qquad (5.3.1)$$

Equation(5.3.1)is not solved analytically. So, it may be solved by the numerical method for the exact values. We have for $q = 2$, the ground state; for $q = n\,\pi$, $(n = 1, 2, 3, \ldots)$ the excited states.

ii. *Wave Functions*

$$G(x) = Q(x) = m_1\int\sqrt{|U(x)|}\,dx = m_1\int\sqrt{U(x)}\,dx =$$

$$= m_1\int\sqrt{U_0\,\text{cotg}^2(\pi x/a)}\,dx = \sqrt{\frac{2\,m\,a^2\,U_0}{\hbar^2\pi^2}}\ln\left[\sin(\frac{\pi x}{a})\right]$$

$$\psi(x) = A\cos[K\,x)]e^{i\,G(x)} = \sqrt{2\,K/q}\cos[K\,x]e^{i\,Q(x)} = \sqrt{2/d}\ \cos[K\,x]e^{i\,Q(x)}$$

$$\psi(x) = B\sin[K\,x)]e^{i\,G(x)} = \sqrt{2\,K/q}\sin[K\,x]e^{i\,Q(x)} = \sqrt{2/d}\ \sin[K\,x]e^{i\,Q(x)}$$

d) Infinitely high parabolic potential well

We consider the potential energy of the particle, $U(x) = U_0\left(\frac{a}{x} - \frac{x}{a}\right)^2$, $[U_0 > 0\,, a > 0,\ x > 0]$.

i. *Energy*

The positive roots of the equation of $E = U(x) = U_0\left(\frac{a}{x} - \frac{x}{a}\right)^2 = m_h\frac{q^2}{y}$ are as follows:

$$x_1 = \sqrt{\frac{a^2\left[m_h q^2 + 2\,y\,U_0 - q\sqrt{m_h}\sqrt{m_h q^2 + 4\,y\,U_0}\right]}{2\,y\,U_0}};\quad x_2 = \sqrt{\frac{a^2\left[m_h q^2 + 2\,y\,U_0 + q\sqrt{m_h}\sqrt{m_h q^2 + 4\,y\,U_0}\right]}{2\,y\,U_0}}$$

$$d_2 = d^2 = (x_2 - x_1)^2$$

$$= \frac{a}{2}\left[\sqrt{\frac{\left[m_h q^2 + 2\,y\,U_0 + q\sqrt{m_h}\sqrt{m_h q^2 + 4\,y\,U_0}\right]}{y\,U_0}}\right.$$

$$\left. - \sqrt{\frac{\left[m_h q^2 + 2\,y\,U_0 - q\sqrt{m_h}\sqrt{m_h q^2 + 4\,y\,U_0}\right]}{y\,U_0}}\right]^2$$

The root of the equation of $d_2 = y$ is as follows:

$$y = \sqrt{a^2\frac{m_h\,q^2}{U_0}} \text{and} E_q = m_h\frac{q^2}{d^2} = m_h\frac{q^2}{y} = \sqrt{\frac{m_h U_0}{a^2}}\ q \rightarrow \quad E_q = \sqrt{\frac{\hbar^2 U_0}{2\,m\,a^2}}\ q$$

We have ground state for $q = 2$;the excited states for $q = n\pi\,,\ (n = 1, 2, 3, \ldots)$[2]. For $m = 1$ and $\hbar = 1$, this energy value is $E_n = \frac{\pi}{2}\,n\sqrt{\frac{2\,U_0}{a^2}}$. For this potential, the energy values obtained from Supersymmetric WKBand standard WKB, respectively, are as follows:

$$E_n = \sqrt{\frac{2\,U_0}{a^2}}\left[2\,n + \sqrt{1 + 8\,a^2 U_0}\right] - 2\,U_0 \text{and} E_n = \sqrt{\frac{2\,U_0}{a^2}}\left[2\,n + 1 + \sqrt{2a^2 U_0}\right] - 2\,U_0$$

ii. *Wave functions*

$$G(x) = m_1\int\sqrt{|U(x)|}\,dx = \ m_1\int\sqrt{U(x)}\,dx = m_1\int\sqrt{U_0\left(\frac{a}{x} - \frac{x}{a}\right)^2}\ dx =$$

$$= m_1\int\sqrt{U_0}\left(\frac{a}{x} - \frac{x}{a}\right)\,dx = \ Q(x)\ ;\quad Q(x) = \sqrt{\frac{2\,m\ U_0}{\hbar^2}}\left[a\ \ln(x) - \frac{x^2}{2\,a}\right]$$

$$\psi(x) = A\cos[K\,x]e^{\pm i\,Q(x)};\ \psi(x) = B\sin[K\,x]e^{\pm i\,Q(x)}$$

$$|A| = |B| = \sqrt{2/d} = \sqrt{2\,K/q}$$

e) Potential $U(x) = ax^2 + b/x^2$

We consider the potential energy of the particle as $U(x) = a x^2 + b / x^2$, where a and b are positive constants.

i. *Energy*

The roots of the equation of $U(x) = a x^2 + b/x^2 = m_h \frac{q^2}{y} = E_q$ are as follows:

$$x_1 = -\sqrt{\frac{E_q+\delta}{2a}},\ x_2 = \sqrt{\frac{E_q-\delta}{2a}},\ x_3 = -\sqrt{\frac{E_q-\delta}{2a}},\ x_4 = \sqrt{\frac{E_q+\delta}{2a}};[\delta = \sqrt{E_q^2 - 4ab}]$$

From these grandeurs, we get as follows:

$$d_{31} = x_3 - x_1 = -\sqrt{\frac{E_q+\delta}{2a}} + \sqrt{\frac{E_q-\delta}{2a}};\ d_{31}^2 = E_q/a - 2\sqrt{b/a};$$

$$d_{42} = x_4 - x_2 = \sqrt{\frac{E_q+\delta}{2a}} - \sqrt{\frac{E_q-\delta}{2a}}\ ;\ d_{42}^2 = E_q/a - 2\sqrt{b/a}$$

From these equations, we can easily obtain $d_{31} = -d_{42} = d$, $d^2 = E_q/a - 2\sqrt{b/a}$

From the solution of the equation of $E_q = m_h \frac{q^2}{d^2}$, we get the positive energy value as follows:

$$E_q = \sqrt{a\,b} + \sqrt{a\,b + a\,m_h q^2} = \sqrt{a\,b} + \sqrt{a\,b + a\,\frac{\hbar^2}{2m} q^2} \qquad (5.5.1)$$

For $q = 2$ ground state occurs; for $q = n\pi$, $n = 1, 2, 3, \dots)$ excited states occur.
For $m = 1$ and $\hbar = 1$, this energy becomes:

$$E_q = \sqrt{a\,b} + \sqrt{a\,b + \frac{a}{2}\pi^2 n^2}\ , (n = 1, 2, 3, \dots). \qquad (5.5.2a)$$

The energies obtained from Super symmetric WKB and Standard WKB[2] respectively are as follows:

$$E_n = \sqrt{2a}\left[2n + 1 + \sqrt{\frac{1}{4} + 2b}\right], (n = 0,1,2,3, \dots)$$

$$E_n = \sqrt{2a}\left[2n + 1 + \sqrt{2b}\right], \quad (n = 0, 1, 2, 3, \dots). \qquad (5.5.2c)$$

It can be assumed that the values given in Equations (5.5.1) and (5.5.2a) are more accurate because there is no approximation.

ii. *Wave Functions*

$$G(x) = m_1 \int \sqrt{|U(x)|}\, dx = m_1 \int \sqrt{U(x)}\, dx = m_1 \int \sqrt{a x^2 + \frac{b}{x^2}}\, dx =$$

$$= m_1 \frac{1}{2}\left\{\sqrt{b + a x^4} + \sqrt{b}\left[\ln(x^2) - \ln(b + \sqrt{b}\sqrt{b + a x^4})\right]\right\} = Q(x)$$

$$Q(x) = \sqrt{\frac{m}{2\hbar^2}}\left\{\sqrt{b + a x^4} + \sqrt{b}\left[\ln(x^2) - \ln(b + \sqrt{b}\sqrt{b + a x^4})\right]\right\}$$

Ref
2. Erbil, H. H.,IREPHY Vol.1, 2007, N.4, 197-213.

$$\psi(x) = A\cos[K\,x]e^{i\,Q(x)} \text{ and } \psi(x) = B\sin[K\,x]e^{i\,Q(x)};$$

$$|A| = |B| = \sqrt{2/d} = \sqrt{2\,K/q}$$

VI. The Radial Schrödinger Equation for Spherical Symmetric Potentials

Notes

The time-independent Schrödinger equation (SE) in three dimensions is given as follows,

$$\Delta\Psi(\vec{r}) + \frac{2\,m}{\hbar^2}[E - V(\vec{r})]\,\Psi(\vec{r}) = 0 \tag{58}$$

Here, E and V are the total and potential energies, respectively, m is the mass or reduced mass of particle. Spherical polar coordinates $x = r\sin(\theta)\cos(\phi)$, $y = r\sin(\theta)\sin(\phi)$, $z = r\cos(\theta)$are appropriate for the symmetry of the problem. The SE given in Equation(58), expressed in these coordinates, is as follows:

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right]\Psi(r,\theta,\phi) + \frac{1}{r^2}\hat{\mathcal{L}}^2(\theta,\phi)\Psi(r,\theta,\phi) + \frac{2\,m}{\hbar^2}[E - V(r,\theta,\phi)]\Psi(r,\theta,\phi) = 0 \tag{59a}$$

$$\hat{\mathcal{L}}^2(\theta,\phi) = \frac{\partial^2}{\partial\theta^2} + \cot g(\theta)\frac{\partial}{\partial\theta} + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2} \tag{59b}$$

The potential energy of a particle which moves in a central, spherically symmetric field of force depends only upon the distance r between the particle and the force center. Thus, the potential energy should be $V(r,\theta,\phi) = V(r)$. Solution of Equations (59a) and (59b) can be found by the method of separation of variables. To apply this method, the solution is assumed to be in the following form:

$$\Psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi) \text{ or } \Psi(r,\theta,\phi) = R(r)\,|j\,m> \tag{60}$$

In Equation(60), R(r) is independent of the angles and $Y(\theta,\phi)$ or |jm> is independent of r. Substituting Equation(60) into Equation(59a) and rearranging it, the following two equations are obtained:

$$\frac{\partial^2 R(r)}{\partial r^2} + \frac{2}{r}\frac{\partial R(r)}{\partial r} + \left\{\frac{2\,m}{\hbar^2}[E - V(r)] - \frac{C}{r^2}\right\}R(r) = 0 \tag{61}$$

$$\hat{\mathcal{L}}^2(\theta,\phi)\,Y(\theta,\phi) + C\,Y(\theta,\phi) = 0 \tag{62}$$

where C is constant. Equation(62) is independent of the total energy E and of the potential energy V(r), andtherefore, the angular dependence of the wave functions is determined by the property of spherical symmetry, and admissible solutions of Equation(62) are valid for every spherically symmetric system regardless of the special form of the potential function. The solutions of Equation(62) can be found in any quantum mechanics and mathematical physics textbooks and the solutions are known as spherical harmonic functions, $Y_{\ell\mu}(\theta,\phi)$, where $C = \ell(\ell+1), (\ell = 0,1,2,3,\dots)$ arepositive integer numbers and $\mu = -\ell, -\ell+1, -\ell+2, \dots 0, 1, 2, \dots, \ell$. Equation(61) is the radial SE. Substituting $C = \ell(\ell+1)$ and $F(r) = r\,R(r)$values into Equation(61), the radial wave equation is obtained as follows:

$$\frac{\partial^2 F(r)}{\partial r^2} + \frac{2\,m}{\hbar^2}[E - U(r)]F(r) = 0 \tag{63}$$

Here, $U(r) = V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}$ is the effective potential energy. Equation (63)is one dimensional differential equation and is the same as Equation(2). In Equation(2), the free variable is x, while in Equation (63) the free variable is r. So, the solution procedure of one dimensional differential equation has been given above in Equations (52a)-(57). Now let us give some examples.

a) Coulomb type central potential well

The potential energy of hydrogen- like atom is$V(r) = -Ze^2/r$.Ifthe centrifugal potential function is added to this potential $V(r)$, we have the following effective potential function:

$$U(r) = -\frac{a}{r} + \frac{b}{r^2}, \left[a = Ze^2 \text{ and } b = \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right].$$

i. *Energy*

The classical turning points of this effective potential are given by the following equation: $-\frac{a}{r} + \frac{b}{r^2} = -|E| = -m_h\frac{q^2}{y}$. From this equation, we can find the classical turning points of this effective potential function and $d_2$as follows:

$$r_1 = \frac{a\,y - \sqrt{a^2y^2 - 4\,b\,m_h\,y\,q^2}}{2\,m_h q^2}\;;\; r_2 = \frac{a\,y + \sqrt{a^2y^2 - 4\,b\,m_h\,y\,q^2}}{2\,m_h q^2};\; d_2 = (r_2 - r_1)^2 = \frac{y\,[y\,a^2 - 4\,b\,m_h q^2]}{m_h^2 q^4}$$

The root of the equation of $d_2 = y$is $y = \frac{m_h q^2[m_h q^2 + 4\,b]}{a^2}$, and $|E_q| = m_h\frac{q^2}{d^2} = m_h\frac{q^2}{y}$

$$E_q = -\frac{2\,m\,e^4 Z^2}{\hbar^2[4\,\ell + 4\,\ell^2 + q^2]} = -\frac{m\,e^4}{2\,\hbar^2}\frac{Z^2}{[\,\ell(\ell+1) + q^2/4]} = -E_0\frac{Z^2}{[\,\ell(\ell+1) + q^2/4]},\ \left[E_0 = \frac{m\,e^4}{2\,\hbar^2}\right]. \quad (6.1.1)$$

We have the ground state for $q = 2$; the excited states for $q = n\,\pi$, $(n = 1, 2, 3, \ldots)$. For the hydrogen atom; $Z = 1$ atom number, m electron mass, e electron charge and in the ground state is$\ell = 0$. From Equation(6.1.1), $E_0 = -13.6$ eV is obtained. This is the well-known ground state energy of the hydrogen atom. The well-known excited state energy of hydrogen-like atoms is given as follows:$E_n = -E_0\frac{Z^2}{n^2}$, $(n = 1, 2, 3, \ldots)$. There is no obviously $\ell = 0$ quantum number in this formula, but in Equation (6.1.1)this number of quantum is clearly visible [5].

ii. *Wave Functions*

$$G(r) = m_1\int\sqrt{|U(r)|}\,dr = \sqrt{\frac{2\,m}{\hbar^2}}\int\sqrt{-U(r)}\,dr = \sqrt{\frac{2\,m}{\hbar^2}}\int\sqrt{\frac{a}{r} - \frac{b}{r^2}}\,dr = Q(r)$$

$$Q(r) = 2\sqrt{\frac{2\,m}{\hbar^2}}\left[\sqrt{a\,r - b} - \sqrt{b}\,\arctan\left(\sqrt{\frac{a\,r - b}{b}}\right)\right]$$

$$F(r) = A\cos[K\,r]e^{i\,Q(r)} \text{and} F(r) = \sqrt{\frac{2}{d}}\cos[K\,r]e^{i\,Q(r)} = \sqrt{\frac{2\,K}{q}}\cos[K\,r]e^{i\,Q(r)}$$

Ref
5. Erbil, H. H., IREPHY Vol.2, 2008, 1, 1-10.

$$F(r) = B\sin\left[\frac{q}{d}\,r\right]e^{i\,Q(r)} \text{and} F(r) = \sqrt{\frac{2}{d}}\sin\left[\frac{q}{d}\,r\right]e^{i\,Q(r)} = \sqrt{\frac{2\,K}{q}}\sin\left[\frac{q}{d}\,r\right]e^{i\,Q(r)}$$

$$\Psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi) = \frac{F(r)}{r}\,Y(\theta,\phi) = \frac{F(r)}{r}\,|jm> \qquad (6.1.2)$$

In Equation(6.1.2),m is not mass, it is magnetic quantum number. The known wave function of the hydrogen atom is an exponential function including Laguerre polynomials. Our results are more accurate because there is no approach.

Notes

b) Spherical symmetric square well(infinitely high or finite)

Consider a particle of mass m captured in a box limited by $0 \le r \le a$ .The corresponding central potential can be given by $V(r) = 0$ for $0 \le r \le a$; $V(r) = \infty$ for $r < 0$ *and* $r > a$. With this potential, the effective potential is as follows:

$$U(r) = \frac{b}{r^2}\ ;\ \left[\,b = \frac{\hbar^2}{2\,m}\ell(\ell+1) = m_h\ell(\ell+1)\,,\ m_h = \frac{\hbar^2}{2\,m}\right]$$

i. *Energy*

With this effective potential, the equation $U(r) = \frac{b}{r^2} = \frac{m_h\,q^2}{y}$ can be written. From this equation, the classical turning points and some grandeur are found as follows [5]:

$$r_1 = \frac{1}{q}\sqrt{\frac{b\,y}{m_h}}\ ;\ r_2 = a\,,\ ;\ d_2 = (r_2 - r_1)^2 = \left[a - \frac{1}{q}\sqrt{\frac{b\,y}{m_h}}\right]^2.$$

From the solution of the equation of $d_2 = y$; we can obtain $y = \frac{m_h a^2 q^2}{\left[\sqrt{b} \pm \sqrt{m_h}\,q\right]^2}$ and the energy value as follows:

$$E_q = \frac{\left[\sqrt{b} \pm \sqrt{m_h}\,q\right]^2}{a^2} = \frac{\hbar^2}{2\,m\,a^2}\left[\sqrt{\ell(\ell+1)} \pm q\right]^2 \qquad (6.2.1)$$

For $q = 2$ground state occurs; for $q = n\,\pi\,,\ (n = 1, 2, 3, \ldots)$, excited states occur. The known allowed energies are given as follows [3]:

$$E_{n\ell} = \frac{\hbar^2}{2\,m\,a^2}\beta_{n\ell}^2 \qquad (6.2.2)$$

Here, $\beta_{n\ell}$, the n^{th} zero of the ℓ^{th} spherical Bessel functions. Equation(6.2.1) can be written as follows:

$$E_q = E_{n\ell} = \frac{\hbar^2}{2\,m\,a^2}\left[\sqrt{\ell(\ell+1)} \pm n\,\pi\right]^2. \qquad (6.2.3)$$

Some values of $\beta_{n\ell}$ and energies calculated according to Equations(6.2.2) and (6.2.3)[with sign + in Equation(6.2.3)] are given in the Table1.

Table 1: Some Energy Values of the Infinitely High Spherical Symmetric Square Well (Unit $\hbar^2/(2\,m\,a^2)$)

$n\ell$	$\beta_{n\ell}$	$E_{n\ell}$ From (6.2.2)	$E_{n\ell}$ From (6.2.3)
1 s	3.142	9.872	9.870
1 p	4.493	20.187	20.755
1 d	5.763	33.212	31.260
2 s	6.283	39.476	39.478
2 p	7.725	59.676	59.250
2 d	9.095	82.719	76.260

ii. *Wave Functions*

$$G(r) = m_1 \int \sqrt{|U(r)|}\, dr = \sqrt{\frac{2\,m}{\hbar^2}} \int \sqrt{|U(r)|}\, dr = m_1 \int \sqrt{\frac{b}{r^2}}\, dr = \sqrt{\frac{2\,m}{\hbar^2}} \int \sqrt{\frac{b}{r^2}}\, dr$$

$$G(r) = m_1 \int \sqrt{\frac{b}{r^2}}\, dr = \sqrt{\frac{2\,m}{\hbar^2}}\sqrt{b}\,\ln(r) = \sqrt{\ell(\ell+1)}\,\ln(r) = Q(r)$$

$$F(r) = A\cos[K\,r]e^{i\,G(r)} = A\cos[K\,r]e^{i\,Q(r)}$$

$$F(r) = B\sin[K\,r]e^{i\,G(r)} = \sin[Kr)]e^{i\,Q(r)}$$

$$F(r) = A\cos\left[\frac{q}{d}\,r\right]e^{i\,G(r)} = A\cos\left[\frac{q}{d}\,r\right]e^{i\,Q(r)}$$

$$F(r) = B\sin\left[\frac{q}{d}\,r\right]e^{i\,G(r)} = B\sin\left[\frac{q}{d}\,r\right]e^{i\,Q(r)}\ ; \qquad |A| = |B| = \sqrt{2/d} = \sqrt{2\,K/q}$$

$$\Psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi) = \frac{F(r)}{r}\,Y(\theta,\phi) \tag{6.2.4}$$

c) Three dimensional isotropic harmonic oscillator potential

The potential energy of three dimensional isotropic harmonic oscillators is given as follows: $V(r) = \frac{1}{2}\,m\,\omega^2 r^2$. With this potential, the effective potential $U(r)$ is as follows:

$$U(r) = \frac{1}{2}\,m\,\omega^2 r^2 + \frac{\hbar^2\ell(\ell+1)}{2\,m}\frac{1}{r^2} = a\,r^2 + \frac{b}{r^2};\ \left[a = \frac{1}{2}\,m\,\omega^2 \text{ and } b = \frac{\hbar^2\ell(\ell+1)}{2\,m}\right]$$

i. *Energy*

From this effective potential, the positive roots of the equation $E_q = m_h\frac{q^2}{y} = U(r)$ are:

$$r_1 = \sqrt{\frac{E_q-\delta}{2\,a}}\ ;\ r_2 = \sqrt{\frac{E_q+\delta}{2\,a}};\ \left[E_q = m_h\frac{q^2}{y}\ ;\ \delta = \sqrt{E_q^2 - 4\,a\,b}\ \right]$$

With these roots, $d = r_2 - r_1 = \sqrt{\frac{E_q+\delta}{2\,a}} - \sqrt{\frac{E_q-\delta}{2\,a}}\ ;\ d_2 = y = d*d = d^2$

By substituting this value of d_2 into the equation, $y = m_h\frac{q^2}{y}$, and then solving for E_q, we can obtain the appropriate energy as follows:

$$E_q = \frac{1}{2}\hbar\omega[\sqrt{\ell(\ell+1)} + \sqrt{\ell(\ell+1)+q^2}\,] \tag{6.3.1}$$

Notes

For $q = 2$ ground state occur;for $q = n\pi$, $(n = 1, 2, 3, \ldots)$ excited states occurs. The known energy values are given as follows [6]:

$$E_{n\ell} = (2n + \ell + 3/2)\,\hbar\omega \ , \ (n = 0, 1, 2, 3, \ldots.) \qquad (6.3.2)$$

Some values of the energies calculated according to Equations(6.3.1) and (6.3.2)are given in theTable2.

Notes

Table 2: Some energy values of the isotropic harmonic oscillator (unit $\hbar\omega$)

$n\,\ell$	$E_{n\ell}$ [according to (6.3.2)]	$E_{n\ell}$ [according to (6.3.1)]
1 s	3.500	1.571
1 p	4.500	2.430
1 d	5.500	3.217
2 s	5.500	3.142
2 p	6.500	3.927
2 d	7.500	4.597

ii. *Wave Functions*

$$G(r) = m_1 \int \sqrt{|U(r)|}\,dr = \sqrt{\frac{2m}{\hbar^2}} \int \sqrt{U(r)}\,dr = \sqrt{\frac{2m}{\hbar^2}} \int \sqrt{a r^2 + \frac{b}{r^2}}\,dr =$$

$$= Q(r) = m_1 \frac{1}{2}\left\{\sqrt{a r^4 + b} - \sqrt{b}\ln\left[2\,\frac{\sqrt{b} + \sqrt{a r^4 + b}}{r^2}\right]\right\}$$

$$F(r) = A\cos[K r]e^{i G(r)} = A\cos[K r]e^{i Q(r)} = A\cos\left[\frac{q}{d} r\right]e^{i Q(r)}$$

$$F(r) = B\sin[K r]e^{i G(r)} = B\sin[K r]e^{i Q(r)} = B\sin\left[\frac{q}{d} r\right]e^{i Q(r)}$$

$$|A| = |B| = \sqrt{2/d} = \sqrt{2K/q}\ ; \ \Psi(r, \theta, \phi) = R(r)\,Y(\theta, \phi) = \frac{F(r)}{r}\,Y(\theta, \phi)$$

The known radial wave functions are [6]: $R_{n\ell}(\rho) = A\,\rho^{\ell+1}e^{-\frac{1}{2}\rho^2}\mathcal{L}_n^{\ell+1/2}(\rho^2)$.

Here, $\rho = \sqrt{m\omega/\hbar}\,r$ and $\mathcal{L}$ is the Laguerre polynomial.

d) Three-dimensional isotropic harmonic oscillator with spin-orbit coupling,(Shellmodel in nuclear physics)

The nuclear shell model describes no interacting particles, moving in the common potential well, which is formed by all particles of the nucleus. The dimensional isotropic harmonic oscillator potential with spin-orbit coupling is originally used as the nuclear average field for shell model calculation of the spherical nuclei. The simple potential energy of a three dimensional isotropic harmonic oscillator is given by:

$$V_0(r) = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2) = \frac{1}{2}\,m\omega^2 r^2.$$

The spin–orbit interaction potential must be added to this simple potential. The spin–orbit interaction potential is given by:

$$V_{\ell sj}(r) = -\frac{\hbar^2}{2m^2c^2}\frac{1}{r}\frac{dV_0(r)}{dr}\vec{\ell}.\vec{s}\ ; \ \left\{\vec{\ell}.\vec{s} = \frac{1}{2}[j(j+1) - \ell(\ell+1) - s(s+1)]\right\}$$

Here ℓ, s and j are the orbital, spin and total angular momentum quantum numbers of a particle, respectively. It is possible to find the derivation of this expression in any quantum mechanics text book. If $V_{\ell sj}(r)$is calculated, the following value is found:

$V_{\ell sj}(r) = -\frac{\hbar^2\omega^2}{4\,m\,c^2}[j(j+1) - \ell(\ell+1) - s(s+1)] = -C_{\ell sj}$. If $s = 1/2$ (for fermions) is accepted, $V_{\ell sj}(r) = -\frac{\hbar^2\omega^2}{4\,m\,c^2}\left[j(j+1) - \ell(\ell+1) - \frac{3}{4}\right] = -C_{\ell sj}$ is obtained. Thus, the harmonic oscillator simple and effective potentials with spin-orbit coupling become as follows:

$$V(r) = V_0(r) + V_{\ell sj}(r)\,;\ U(r) = a\,r^2 - C_{\ell sj} + b/r^2;\left[a = \frac{1}{2}\,m\,\omega^2\,,\ b = \frac{\hbar^2}{2\,m}\,\ell(\ell+1)\right]$$

i. *Energy*

From this effective potential, the positive roots of the equation $E_q = m_h\frac{q^2}{y} = U(r)$ are as follows:

$$r_1 = \sqrt{\frac{(E_q + C_{\ell sj}) - \delta}{2\,a}}\,; r_2 = \sqrt{\frac{(E_q + C_{\ell sj}) + \delta}{2\,a}}\,;\ [\delta = \sqrt{(E_q + C_{\ell sj})^2 - 4ab}\,]\,.$$

With these roots: $d = r_2 - r_1 = \sqrt{\frac{E_q + \delta}{2\,a}} - \sqrt{\frac{E_q - \delta}{2\,a}}\,;\ d_2 = y = d * d = d^2$.

By substituting this value of d_2 into the equation$y = m_h\frac{q^2}{y}$, and then solving it for E_q, we can obtain the appropriate energy as follows:

$$E_q = \frac{1}{2}\,\hbar\,\omega\left[\sqrt{\ell(\ell+1)} - C_j + \sqrt{(\sqrt{\ell(\ell+1)} - C_j)^2 + q^2}\right],\left[C_j = C_{\ell sj}/(\hbar\,\omega)\right] \qquad (6.4.1)$$

For $q = 2$ ground state occurs; for $q = n\pi$, $(n = 1, 2, 3, \ldots)$ excited states occurs. The known energy values (with first order perturbation) are as follows [3, 6]:

$$E_{n\ell} = (2n + \ell + 3/2)\hbar\,\omega - \frac{C_0}{4\,\hbar\,\omega}[j(j+1) - \ell(\ell+1) - s(s+1)]\hbar\omega \qquad (6.4.2)$$

Here, $n = 0, 1, 2,..$, integer numbers and C_0 is a positive parameter. In Table3, some energy values calculated according to Equations(6.4.1) and (6.4.2) are given, with the values:

$$C_0 = 0.015\,\hbar\,\omega\,,\ s = 1/2 \text{ and } C_j = \frac{C_0}{4\,\hbar\,\omega}[j(j+1) - \ell(\ell+1) - 3/4]\hbar\omega$$

Table 3: Some energy values of the isotropic harmonic oscillator with spin-orbit coupling

States	According to (6.4.2) (unit $\hbar\omega$)	According to (6.4.1) (unit$\hbar\omega$)
$1d_{5/2}$	3.493	3.211
$1f_{5/2}$	4.515	4.083
$1f_{7/2}$	4.489	4.061
$1g_{7/2}$	5.519	4.986
$1g_{9/2}$	5.485	4.955

ii. *Wave Functions*

$$G(r) = m_1 \int \sqrt{|U(r)|}\, dr = \sqrt{\frac{2\,m}{\hbar^2}} \int \sqrt{U(r)}\; dr = Q(r)$$

$$Q(r) = \sqrt{\frac{2\,m}{\hbar^2}} \left\{ \frac{1}{2} \sqrt{a\,r^4 - C_{\ell sj}\,r^2 + b} \right.$$
$$- \frac{C_{\ell sj}}{4\sqrt{a}} \ln \left[2\sqrt{a\,r^4 - C_{\ell sj}\,r^2 + b} + \frac{2\,a\,r^2 - C_{\ell sj}}{\sqrt{a}} \right]$$
$$\left. - \frac{\sqrt{b}}{2} \ln \left[2\sqrt{b(a\,r^4 - C_{\ell sj}\,r^2 + b)} - C_{\ell sj}\,r^2 + 2\,b \right] + \sqrt{b} \ln(r) \right\}$$

$$F(r) = A \cos[K\,r] e^{i\,G(r)} = A \cos[K\,r] e^{i\,Q(r)} = A \cos\left[\frac{q}{d}\,r\right] e^{i\,Q(r)}$$

$$F(r) = B \sin[K\,r] e^{i\,G(r)} = B \sin[K\,r] e^{i\,Q(r)} = B \sin\left[\frac{q}{d}\,r\right] e^{i\,Q(r)}$$

$$|A| = |B| = \sqrt{2/d} = \sqrt{2\,K/q} \quad ; \Psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi) = \frac{F(r)}{r}\,Y(\theta,\phi)$$

The known radial wave functions are [6]: $R_{n\ell}(\rho) = A\,\rho^{\ell+1} e^{-\frac{1}{2}\rho^2} \mathcal{L}_n^{\ell+1/2}(\rho^2)$.

Here $\rho = \sqrt{m\,\omega/\hbar}\; r$ and $\mathcal{L}$ is the Laguerre polynomial.

e) Three axial deformed harmonic oscillator potential anisotropic harmonic oscillator potential (Nilsson model in the nuclear physics)

i. *Effective potential*

The nucleus in the shell model is assumed to have a spherical shape. Therefore, particles move in a spherically symmetric potential. There are, however, convincing arguments that nuclei with the neutron and proton numbers sufficiently far from the magic numbers have no spherical symmetry ellipsoidal shapes. In this case, it is said to deformed shell model. In deformed shell model calculations, it is used the three dimensional anisotropic harmonic oscillator potential which is given as follows:

$$V_0(x,y,z) = \frac{1}{2}\mu(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \qquad (6.5.1)$$

Here μ is mass or reduced mass. In the case of deformed nuclei, it is generally restricted to axially symmetric nuclei and it taken the z-axis as symmetry axis. So, it is accepted $\omega_x = \omega_y \neq \omega_z = \omega_\perp$ in the anisotropic harmonic oscillator potential. The motion of a particle in an axially symmetric potential, with additional symmetry plane, perpendicular to symmetry axis was described by Nilsson. The no-spherical nuclei have the shape of an ellipsoid of revolution. It is, however, possible that some transitional nuclei have shapes of a three axial ellipsoid. It is also possible that the shapes of excited states differ from the ground state shapes and that some exited states have three axial ellipsoidal forms. In the three axial cases, $\omega_x \neq \omega_y \neq \omega_z$. The no-axial shape is characterized by two parameters ε and γ. For $\varepsilon > 0$, $\gamma = 0^0$ situation corresponds to the axially symmetric prolate ellipsoid, $\gamma = 60^0$ corresponds to the oblate ellipsoid. When $\gamma \neq 0^0$ and $\gamma \neq 60^0$, the ellipsoid has no axial symmetry, and the projection quantum

number of the total angular momentum on any axis is not one conserved quantity. The angular frequencies ω_x, ω_y, ω_z are connected with the deformation parameters ε and γ by the following expressions:

$$\omega_x = \omega_0(\varepsilon,\gamma)[1-\frac{2}{3}\,\varepsilon\cos\left(\gamma+\frac{2\pi}{3}\right)] \quad (6.5.2a)$$

$$\omega_y = \omega_0(\varepsilon,\gamma)[1-\frac{2}{3}\,\varepsilon\cos\left(\gamma-\frac{2\pi}{3}\right)] \quad (6.5.2b)$$

$$\omega_z = \omega_0(\varepsilon,\gamma)[1-\frac{2}{3}\,\varepsilon\cos(\gamma)] \quad (6.5.2c)$$

If it is required a constant volume as deformation changes, it needs:

$$\omega_x\omega_y\omega_z = \omega_{00}^3 \quad (6.5.3a)$$

From Equation (6.5.3a) we get the following value:

$$\omega_0(\varepsilon,\gamma) = 3\,\omega_{00}[27-9\,\varepsilon^2-2\,\varepsilon^3\cos(3\,\gamma)\,]^{-1/3} \quad (6.5.3b)$$

Let us express the potential given in Equation (6.5.1) the following spherical coordinates:

$$x = r\sin(\theta)\cos(\phi)\,,\ y = r\sin(\theta)\sin(\phi)\,,\ z = r\cos(\theta) \quad (6.5.4)$$

If the potential given in Equation(6.5.1)is calculated by considering Equations(6.5.2a) and (6.5.4), the following is obtained:

$$V_0(r,\varepsilon,\gamma) = \frac{1}{2}\mu\,\omega_{00}^2 r^2[A(\varepsilon,\gamma)\cos^2(\theta) + B(\varepsilon,\gamma)\sin^2(\theta)\cos^2(\phi) + C(\varepsilon,\gamma)\sin^2(\theta)\sin^2(\phi)]$$

$$A(\varepsilon,\gamma) = \frac{[3-2\,\varepsilon\cos(\gamma)]^2}{[27-9\,\varepsilon^2-2\,\varepsilon^3\cos(3\,\gamma)]^{2/3}}\ ;\ B(\varepsilon,\gamma) = \frac{[3+2\,\varepsilon\cos(\frac{\pi}{6}+\gamma)]^2}{[27-9\,\varepsilon^2-2\,\varepsilon^3\cos(3\,\gamma)]^{2/3}}\ ;$$

$$C(\varepsilon,\gamma) = \frac{[3+2\,\varepsilon\cos(\frac{\pi}{6}-\gamma)]^2}{[27-9\,\varepsilon^2-2\,\varepsilon^3\cos(3\,\gamma)]^{2/3}} \quad (6.5.5)$$

Let us express the function given in Equation (6.5.5) in the terms of spherical harmonic functions, $Y_q^2(\theta,\phi) = Y_q^2\,,\ (q = 0,-2,+2)$, as follows:

$$\cos^2(\theta) = \frac{1}{3}+\frac{2}{3}\sqrt{\frac{4\pi}{5}}Y_0^2$$

$$\sin^2(\theta)\cos^2(\phi) = \frac{1}{15}[5-2\sqrt{5\,\pi}Y_0^2+\sqrt{30\,\pi}(Y_2^2+Y_{-2}^2)]$$

$$\sin^2(\theta)\sin^2(\phi) = \frac{1}{15}[5-2\sqrt{5\,\pi}Y_0^2-\sqrt{30\,\pi}(Y_2^2+Y_{-2}^2)]$$

$$V_0(r,\varepsilon,\gamma) = \tfrac{1}{2}\,\mu\,\omega^2(\varepsilon,\gamma)r^2 = \tfrac{1}{2}\mu\,\omega_{00}^2\,\beta^2(\varepsilon,\gamma)r^2 \quad (6.5.6)$$

$$\omega^2(\varepsilon,\gamma) = \omega_{00}^2\,\beta^2(\varepsilon,\gamma)$$

$$\beta^2(\varepsilon,\gamma) = \tfrac{2}{9}[2\,A(\varepsilon,\gamma)\text{-}3(B(\varepsilon,\gamma)+C(\varepsilon,\gamma))]\sqrt{\tfrac{\pi}{5}}Y_0^2 + [B(\varepsilon,\gamma)-C(\varepsilon,\gamma)]\sqrt{\tfrac{2\pi}{15}}(Y_2^2+Y_{-2}^2)]$$

The spin-orbit interaction potential is given as follows:

$$V_{\ell sj}(\varepsilon,\gamma,r) = -\frac{\hbar^2}{2\,\mu^2 c^2}\frac{1}{r}\frac{dV_0(r,\varepsilon,\gamma)}{dr} < \vec{\ell}\,.\,\vec{s} >;\ \{< \vec{\ell}\,.\,\vec{s} > = \frac{1}{2}[j(j+1) - \ell(\ell+1) - s(s+1)]\}$$

If $V_{\ell sj}(\varepsilon,\gamma,r)$is calculated, the following value is found:

$$V_{\ell sj}(\varepsilon,\gamma,r) = C_{00}\,\beta^2(\varepsilon,\gamma)\,\hbar\,\omega_{00}\ ;\ \ C_{00} = -\frac{\hbar\,\omega_{00}}{4\,\mu\,c^2}\,[j(j+1) - \ell(\ell+1) - s(s+1)]$$

Notes

Thus, the anisotropic harmonic oscillator potential with spin-orbit coupling becomes as follows:

$$V(r,\varepsilon,\gamma) = [\tfrac{1}{2}\,\mu\,\omega_{00}^2 r^2 + C_{00}\hbar\,\omega_{00}]\,\beta^2(\varepsilon,\gamma) \qquad (6.5.7)$$

With this potential, the effective potential $U(r,\varepsilon,\gamma)$ is obtained as follows:

$$U(r,\varepsilon,\gamma) = \left[\tfrac{1}{2}\,\mu\,\omega_{00}^2 r^2 + C_{00}\hbar\,\omega_{00}\right]\,\beta^2(\varepsilon,\gamma) + \frac{\hbar^2}{2\,\mu\,r^2}\ell(\ell+1) \qquad (6.5.8)$$

Here, $\omega_{00}$is the isotropic oscillator angular frequency. The Coulomb potential must be added to the potential given in Equation (6.5.8) when the proton levels are calculated. The Coulomb potential in the spherical case, neglecting the effect of the surface, is as follows:

$$V_c(r) = \frac{(Z-1)\,e^2}{r}\begin{Bmatrix} \frac{3\,r}{2\,R_0} - \frac{1}{2}\left(\frac{r}{R_0}\right)^2 & , \quad \text{for} \quad r \le R_0 \\ 1 & , \quad \text{for} \quad r > R_0 \end{Bmatrix}$$

Here, R_0 is the radius of the spherical nucleus and Z is the charge number. Thus, in the nucleus, $r \le R_0$, we have as follows:

$$V_c(r) = b_c + a_c r^2\,,\ \ [a_c = -\frac{(Z-1)e^2}{2\,R_0^3}\,,\ \ b_c = \frac{3\,(Z-1)e^2}{2\,R_0}\,] \qquad (6.5.9)$$

In the quadratic deformed case, the Coulomb potential is obtained as follows:

$$V_c(r) = \frac{3\,(Z-1)\,e^2}{2\,R_0}\left\{-8.9723 - 3.3241\,\varepsilon + 8.14235\,\sqrt{1.5+\varepsilon} + a_c r^2\,,\ \ \text{for} \quad r \le R_0\right\}$$

$$V_c(r) = \frac{(Z-1)\,e^2}{R_0}\left\{\frac{R_0}{r} - 4.76142 - 1.58717\,\varepsilon + 3.88768\,\sqrt{1.5+\varepsilon}\ \ ,\ \ \text{for} \quad r > R_0\right\}$$

Because in the nucleus $r \le R_0$, in the case quadratic, the Coulomb potential can be rewritten as follows:

$$V_c(r) = b_c(\varepsilon) + a_c r^2 \qquad (6.5.10)$$

$$a_c = -\frac{(Z-1)e^2}{2\,R_0^3}\,, \qquad b_c(\varepsilon) = \frac{3\,(Z-1)e^2}{2\,R_0}\,(-8.9723 - 3.3241\,\varepsilon + 8.14235\,\sqrt{1.5+\varepsilon}\,)$$

It is seen that for $\varepsilon = 0$, Equation (6.5.10) is equal to Equation (6.5.9).

On the other hand, the total wave function is $\psi(r,\theta,\phi) = R(r)|\ell jm> = \frac{F(r)}{r}|\ell jm>$ and the radial SE is written as follows:

$$\frac{d^2F(r)}{dr^2}|\ell jm> + \frac{2\mu}{\hbar^2}[E - U(r,\varepsilon,\gamma)]F(r)|\ell jm> = 0$$

$$\frac{d^2F(r)}{dr^2}|\ell jm> + \frac{2\mu}{\hbar^2}F(r)[E - U(r,\varepsilon,\gamma)]|\ell jm> = 0 \qquad (6.5.11)$$

In Equation (6.5.11), $[E - U(r,\varepsilon,\gamma)]|\ell jm>$ is calculated as follow:

$$[E - U(r,\varepsilon,\gamma)]|\ell jm> = E|\ell jm> - U(r,\varepsilon,\gamma)|\ell jm>$$

$$U(r,\varepsilon,\gamma)|\ell jm> = \left[\left[\frac{1}{2}\mu\omega_{00}^2 r^2 + C_{00}\hbar\omega_{00}\right]\beta^2(\varepsilon,\gamma)\right]|\ell jm> + \frac{\hbar^2}{2\mu r^2}\ell(\ell+1)]|\ell jm>$$

$$\beta^2(\varepsilon,\gamma)]|\ell jm> = \{\frac{2}{9}[2A(\varepsilon,\gamma) - 3(B(\varepsilon,\gamma) + C(\varepsilon,\gamma))]\sqrt{\frac{\pi}{5}}Y_0^2 + [B(\varepsilon,\gamma) - C(\varepsilon,\gamma)]\sqrt{\frac{2\pi}{15}}(Y_2^2 +$$

$$Y_{-2}^2)\}|\ell jm> = \frac{2}{9}[2A(\varepsilon,\gamma) - 3(B(\varepsilon,\gamma) + C(\varepsilon,\gamma))]\sqrt{\frac{\pi}{5}}Y_0^2|\ell jm> + [B(\varepsilon,\gamma) - C(\varepsilon,\gamma)]\sqrt{\frac{2\pi}{15}}[Y_2^2 +$$

$$Y_{-2}^2]|\ell jm> \qquad (6.5.12)$$

If we calculate $Y_0^2|\ell jm> = a_{20}|\ell jm>$ *and* $[Y_2^2 + Y_{-2}^2]|\ell jm> = a_{22}|\ell jm>$ in Equation (6.5.12), by the Wigner-Eckart, we have found the following values: $a_{22} = 0$ and $a_{20}(\ell, j, m) = \sqrt{\frac{\pi}{2\ell+1}}\frac{j+j^2-3m^2}{2j(j+1)} = a_{20}$. Thus, $\beta^2(\varepsilon,\gamma,a_{20})$ are written as follows:

$$\beta^2(\varepsilon,\gamma,a_{20}) = \frac{2}{9}[2A(\varepsilon,\gamma) - 3(B(\varepsilon,\gamma) + C(\varepsilon,\gamma))]\sqrt{\frac{\pi}{5}}a_{20} \qquad (6.5.13)$$

So, we have found the effective potential for anisotropic harmonic oscillator as follows;

$$U(r;\varepsilon,\gamma,a_{20}) = \frac{1}{2}\mu\omega_{00}^2\beta^2(\varepsilon,\gamma,a_{20})r^2 + C_{00}\hbar\omega_{00}\beta^2(\varepsilon,\gamma,a_{20}) + \frac{\hbar^2}{2\mu r^2}\ell(\ell+1) \qquad (6.5.14)$$

In the case of electric charged particle, the Coulomb potential should be also added to this effective potential.

ii. *Energy*

Let us write the effective potential given in Equation (6.5.14) as follows:

$$U(r;\varepsilon,\gamma,a_{20}) = U(r) = a r^2 + \frac{b}{r^2} + \delta \qquad (6.5.15a)$$

$$a = \frac{1}{2}\mu\omega_{00}^2\beta^2(\varepsilon,\gamma,a_{20}),\ b = \frac{\hbar^2}{2\mu}\ell(\ell+1),\ \delta = C_{00}\hbar\omega_{00}\beta^2(\varepsilon,\gamma,a_{20}) \qquad (6.5.15b)$$

The positive roots of the Equation $U(r) = E = E_q$ are obtained as follows:

$$r_1 = \sqrt{\frac{E-\delta-\sqrt{(E-\delta)^2-4ab}}{2a}}\ ;\ r_2 = \sqrt{\frac{E-\delta+\sqrt{(E-\delta)^2-4ab}}{2a}} \qquad (6.5.16)$$

From Equations (6.5.16) one is obtained the following values:

$$d(E) = r_2 - r_1 = \sqrt{\frac{E-\delta+\sqrt{(E-\delta)^2-4ab}}{2a}} - \sqrt{\frac{E-\delta-\sqrt{(E-\delta)^2-4ab}}{2a}}$$

$$r_0(E) = \frac{1}{2}\left[\sqrt{\frac{E-\delta+\sqrt{(E-\delta)^2-4\,a\,b}}{2\,a}} + \sqrt{\frac{E-\delta-\sqrt{(E-\delta)^2-4\,a\,b}}{2\,a}}\right]$$

Solving the equation $E_q = m_h \frac{q^2}{d^2}$, we find the following energy values:

Notes

$$E(n,\ell,j,m) = E_q = \tfrac{1}{2}(2\sqrt{a\,b}+\delta+\sqrt{4a(b+m_h q^2)+4\sqrt{a\,b}\,\delta+\delta^2}),[m_h = \hbar^2/(2\,\mu)] \qquad (6.5.17)$$

For $q = 2$ ground state occurs; for $q = n\,\pi$, $(n = 1, 2, 3, \ldots)$ excited states occurs.

In Table 4, some energy values calculated according to Equations (6.5.17), with the value: $C_{00} = -0.005\,[j(j+1) - \ell(\ell+1) - 3/4]$

Table 4: Some energy values of the three-axial harmonic oscillator with spin-orbit coupling and a few deformation parameters, calculated according to Equation (6.5.17), (Unit $\hbar\omega_0$)

States $\lvert n(\ell)\ j\ m >$	$E(n,\ell,j,m)$ $\varepsilon = 0$, $\gamma = 0^0$	$E(n,\ell,j,m)$ $\varepsilon = 0.35$, $\gamma = 0^0$	$E(n,\ell,j,m)$ $\varepsilon = 0.35$, $\gamma = 30^0$
1 f 7/2 5/2	4.05725	4.26292	4.24841
1 f 5/2 5/2	4.08772	4.72319	4.66325
1 g 9/2 5/2	4.95055	4.96802	4.97658
1 g 7/2 5/2	4.99146	5.23363	5.21707
2 d 5/2 5/2	4.58982	5.39758	5.32077
1 h 11/2 5/2	5.87240	5.77594	5.79967
1 h 9/2 5/2	5.92375	5.95938	5.96804
2 f 7/2 5/2	5.30836	5.57777	5.55877
2 f 5/2 5/2	5.33431	6.16217	6.08410
1 i 13/2 5/2	6.81291	6.64084	0.67543

iii. *Wave functions*

$$G(r) = m_1 \int \sqrt{|U(r)|}\,dr = \sqrt{\frac{2\,\mu}{\hbar^2}} \int \sqrt{a\,r^2 + \frac{b}{r^2} + \delta}\,dr = Q(r)$$

$$Q(r) = \frac{1}{4}\sqrt{\frac{2\,\mu}{\hbar^2}}\,\{2 * \sqrt{b + a\,r^4 + r^2\,\delta} + \frac{\delta\,\mathrm{Log}\left[2\,a\,r^2 + \delta + 2\sqrt{a}\,\sqrt{b + a\,r^4 + r^2\delta}\right]}{\sqrt{a}} +$$

$$2\sqrt{b}\left(\mathrm{Log}[r^2] - \mathrm{Log}\left[2b + r^2\delta + 2\sqrt{b}\sqrt{b + ar^4 + r^2\delta}\right]\right)\}$$

$$F(r) = A\cos[K\,r]e^{i\,G(r)} = A\cos[K\,r]e^{i\,Q(r)} = A\cos\left[\frac{q}{d}\,r\right]e^{i\,Q(r)}$$

$$F(r) = B\sin[K\,r]e^{i\,G(r)} = B\sin[K\,r]e^{i\,Q(r)} = B\sin\left[\frac{q}{d}\,r\right]e^{i\,Q(r)}$$

$$|A| = |B| = \sqrt{2/d} = \sqrt{2\,K/q}$$

$$\Psi(r,\theta,\phi) = R(r)\,|\ell jm> = \frac{F(r)}{r}\,|\ell jm> \qquad (6.5.18)$$

This problem has been examined in detail with numerical calculations and comparisons in [7].

f) Periodic potential of arbitrary form

Periodic effective potentials are as follows: $U(r) = U(r+P)$. Here P is the period of the potential. As the derivatives appearing in Hamiltonian operator are the same for the new variable $(r+P)$, so we have the following SE:

$$(\hat{H} - E)F(r) = 0 \text{ and } (\hat{H} - E)F(r+P) = 0 \qquad (6.6.1)$$

The two functions $F(r)$ and $F(r+P)$ may, therefore, differ only by a constant factor as β, to be $F(r+P) = \beta\,F(r)$. By applying this new relationship to $F(r+2\,P)$, we obtain as follows: $F(r+2\,P) = \beta\,F(r+P) = \beta^2 F(r)$ and step by step, one sees that it has as follows:

$$F(r+n\,P) = \beta^n F(r) \qquad (6.6.2a)$$

By successive shift to the left, it would result in the same:

$$F(r-n\,P) = \beta^{-n} F(r) \qquad (6.6.2b)$$

Under these conditions we see in given Equations (6.6.2a) and (6.6.2b) if $|\beta| > 1$, then $F(r)$ tends to infinity when $r \to \infty$; and $|\beta| < 1$, then $F(r)$ tends to infinity when $r \to -\infty$. So, for $F(r)$ remains finite for $r = \pm\infty$,it is necessary that $|\beta| = 1$,that is to say that β to be a phase factor (here γ is any real number) as follows:

$$\beta = e^{i\,\gamma} \qquad (6.6.2c)$$

Thus, the energy and the radial SE have respectively to be as follows:

$$U(r) = U(r+n\,P) = E \qquad (6.6.3a)$$

$$F(r \pm n\,P) = e^{\pm i\,n\,\gamma} F(r),\ (n \text{ is integer}) \qquad (6.6.3b)$$

i. *Example*

Potential: $U(r) = U_0 \sin(a\,r)^2$, $[U_0 > 0\ \ and\ \ a > 0\ constants,\ P = \pi/a\,]$.

ii. *Energy*

Solution of Equation $U(r) = U(r+n\,P) = E$gives: $r_1 = -n\,P - \frac{1}{a}\arcsin(\sqrt{E/U_0})$; $r_2 = -n\,P + \frac{1}{a}\arcsin(\sqrt{E/U_0})$. From these equations we have as follows:

$$d = r_2 - r_1 = \frac{2}{a}\arcsin\left(\sqrt{E/U_0}\right) \text{ and } E = E_q = m_h\frac{q^2}{d^2}\ ,\ [m_h = \hbar^2/(2\,m)].$$

This last equation cannot be solved analytically. Solving numerically this equation the energy values are obtained. For $q = 2$ ground state occurs; for $q = n\,\pi$, $(n = 1, 2, 3, \ldots)$ excited states occurs.

iii. Wave functions

$$G(r) = m_1 \int \sqrt{|U(r)|}\,dr = \frac{m_1}{a}\sqrt{U_0}\cos(a\,r) = Q(r), \qquad [m_1 = \sqrt{2\,m}/\hbar\,]$$

$$F(r) = A\cos[K\,r]e^{i\,G(r)} = A\cos[K\,r]e^{i\,Q(r)} = A\cos\left[\frac{q}{d}\,r\right]e^{i\,Q(r)}$$

$$F(r) = B\sin[K\,r]e^{i\,G(r)} = B\sin[K\,r]e^{i\,Q(r)} = B\sin\left[\frac{q}{d}\,r\right]e^{i\,Q(r)}$$

$$|A| = |B| = \sqrt{2/d} = \sqrt{2\,K/q}$$

From $F(r+P) = \beta\,F(r)$ we can write $\beta = F(r+P)/F(r) = 1$.
This problem has been examined in detail in[8] with the examples.

g) Trigonometric and Hyperbolic Pöschl-Teller potential wells

i. *Trigonometric Pöschl-Teller potential well*

The trigonometric Pöschl-Teller potential is given as follows:

$$U(x) = \frac{\hbar^2\alpha^2}{2\,m}\left[\frac{\kappa\,(\kappa-1)}{\sin^2(\alpha\,x)} + \frac{\lambda\,(\lambda-1)}{\cos\,(\alpha\,x)^2}\right] = U_0\left[\frac{A}{y} + \frac{B}{1-y}\right] \qquad (6.7.1)$$

$$U_0 = \frac{\hbar^2\alpha^2}{2\,m}, \qquad A = \kappa\,(\kappa-1),\ B = \lambda\,(\lambda-1), \qquad \kappa > 1, \qquad \lambda > 1, \qquad y = \sin^2(\alpha\,x)$$

a. *Energy*

Roots of the equation $U(y) = E$ are y_1 and y_2. If they are calculated, they are found as follows:

$$y_1 = \frac{E+A\,U_0-B\,U_0-\sqrt{-4\,A\,E\,U_0+[E+(A-B)U_0]^2}}{2\,E}\ ;\ y_2 = \frac{E+A\,U_0-B\,U_0+\sqrt{-4\,A\,E\,U_0+[E+(A-B)U_0]^2}}{2\,E}$$

According to $y = \sin^2(\alpha\,x) \rightarrow x = \frac{1}{\alpha}\arcsin[\sqrt{y}]$, we can write the following values:

$$x_1 = \frac{1}{\alpha}\arcsin\left[\sqrt{y_1}\right], \qquad x_2 = \frac{1}{\alpha}\arcsin\left[\sqrt{y_2}\right], \quad d = x_2 - x_1$$

The exact solution of the equation $m_1\sqrt{E}\,d = q$ gives the exact energy values. But this equation cannot be solved analytically, it can be solved numerically.
This equation can also be solved approximately as follows:

$$\arcsin(X) \approx X \rightarrow\ x_1 \approx \frac{1}{\alpha}\sqrt{y_1}, \qquad x_2 \approx \frac{1}{\alpha}\sqrt{y_2}, \qquad d \approx x_2 - x_1 \approx \frac{1}{\alpha}[\sqrt{y_2} - \sqrt{y_1}]$$

The solution of the $m_1\sqrt{E}\,d = q$, $[m_1 = \sqrt{2\,m}/\hbar]$ gives the approximate energy values as follows:

$$E = U_0\left[A + B + q^2 \pm 2\sqrt{A\,(B+q^2)}\right] = U_0[\sqrt{A} \pm \sqrt{B+q^2}\,]^2 \qquad (6.7.2)$$

For $q = 2$ ground state occurs; for $q = n\,\pi$, $(n = 1, 2, 3, \ldots)$ excited states occurs.

b. *Wave functions*

$$G(x) = m_1\int\sqrt{|U(x)|}\,dx = \sqrt{\frac{2\,m}{\hbar^2}}\int\sqrt{U_0\left[\frac{A}{\sin^2(\alpha\,x)} + \frac{B}{\cos^2(\alpha\,x)}\right]}\,dx = Q(x)$$

$$F(x) = A\cos[K\,x]e^{i\,G(x)} = A\cos[Kx\,]e^{i\,Q(x)} = A\cos\left[\frac{q}{d}\,x\right]e^{i\,Q(x)}$$

8. Erbil, H. H., IREPHY,2012, 6, 439-447.

$$F(x) = B\sin[K\,x]e^{i\,G(x)} = B\sin[K\,x]e^{i\,Q(x)} = B\sin\left[\frac{q}{d}\,x\right]e^{i\,Q(x)}$$

$$|A| = |B| = \sqrt{2/d} = \sqrt{2\,K/q} \qquad (6.7.3)$$

ii. *Hyperbolic Pöschl-Teller potential well*

The hyperbolic Pöschl-Teller potential is given as follows:

$$U(x) = \frac{\hbar^2\alpha^2}{2\,m}\left[\frac{\kappa\,(\kappa-1)}{\sinh^2(\alpha\,x)} + \frac{\lambda\,(\lambda-1)}{\cosh^2(\alpha\,x)}\right] = U_0\left[\frac{A}{y} + \frac{B}{1+y}\right] \qquad (6.7.4)$$

$$U_0 = \frac{\hbar^2\alpha^2}{2\,m}\,, A = \kappa\,(\kappa-1),\;\; B = \lambda\,(\lambda-1), \kappa > 1\,, \lambda > 1\,, y = \sinh^2(\alpha\,x)$$

a. *Energy*

Roots of the equation $U(y) = E$ are y_1 and y_2. Solving this equation, they are found as follows:

$$y_1 = \frac{-E+A\,U_0+B\,U_0-\sqrt{4\,A\,E\,U_0+[E-(A+B)U_0]^2}}{2\,E}; y_2 = \frac{-E+A\,U_0+B\,U_0+\sqrt{4\,A\,E\,U_0+[E-(A+B)U_0]^2}}{2\,E}$$

According to $y = \sinh^2(\alpha\,x) \rightarrow x = \frac{1}{\alpha}\,\text{arcsinh}\,[\sqrt{y}]$, we can write the following values:

$$x_1 = \frac{1}{\alpha}\text{arcsinh}\left[\sqrt{y_1}\right]\,, \qquad x_2 = \frac{1}{\alpha}\text{arcsinh}\left[\sqrt{y_2}\right],\;\; d = x_2 - x_1$$

The exact solution of the equation $m_1\sqrt{E}\,d = q\,,\; [m_1 = \sqrt{2\,m}/\hbar]$ gives the exact energy values. But this equation cannot be solved analytically, it can be solved numerically. This equation can also be solved approximate as follows:

$$\text{arcsinh}(X) \approx X \rightarrow\;\; x_1 \approx \frac{1}{\alpha}\sqrt{y_1}\,, \qquad x_2 \approx \frac{1}{\alpha}\sqrt{y_2}\,, \qquad d \approx x_2 - x_1 \approx \frac{1}{\alpha}[\sqrt{y_2} - \sqrt{y_1}\,]$$

The solution of the $m_1\sqrt{E}\,d = q\,,\; [m_1 = \sqrt{2\,m}/\hbar]$ gives the approximate energy values as follows:

$$E = U_0\left[-A + B - q^2 \pm 2\sqrt{A\,(-B+q^2)}\right] = U_0[\sqrt{-A} \pm \sqrt{B-q^2}\,]^2 \qquad (6.7.5)$$

For $q = 2$ ground state occurs; for $q = n\,\pi\,,\; (n = 1, 2, 3, \ldots)$ excited states occurs.

b. *Wave functions*

$$G(x) = m_1\int\sqrt{|U(x)|}\,dx = \sqrt{\frac{2\,m}{\hbar^2}}\int\sqrt{U_0\left[\frac{A}{\sinh^2(\alpha\,x)} + \frac{B}{\cosh^2(\alpha\,x)}\right]}\,dx = Q(x)$$

$$F(x) = A\cos[K\,x]e^{i\,G(x)} = A\cos[Kx\,]e^{i\,Q(x)} = A\cos\left[\frac{q}{d}\,x\right]e^{i\,Q(x)}$$

$$F(x) = B\sin[K\,x]e^{i\,G(x)} = B\sin[K\,x]e^{i\,Q(x)} = B\sin\left[\frac{q}{d}\,x\right]e^{i\,Q(x)}$$

$$|A| = |B| = \sqrt{2/d} = \sqrt{2\,K/q} \qquad (6.7.6)$$

This problem has been examined in detail in [9].

h) Saxon-Woods type central potential

Saxon-Woods type potential function is given as: $V_1(r) = -\frac{V_0}{1+e^{(r-R_0)/a}}$; $[a,\ V_0\ , R_0\ ]$ are parameters. The spin-orbit interaction potential energy term can be added to this potential. The spin-orbit interaction potential energy term is given as follows:

$$V_{\ell sj}(r) = -\frac{\hbar^2}{4\,\mu^2 c^2}\frac{1}{r}\frac{dV_1(r)}{dr}[j(j+1) - \ell(\ell+1) - s(s+1)],\ [\mu \text{ is reduced mass}].$$

Notes

If this function is calculated, the following potential is found:

$$V_{\ell sj} = -C_{\ell sj}\ \frac{1}{r}\frac{e^{r/a}}{\left[1+e^{\left[\frac{r-R_0}{a}\right]}\right]^2};\ \{C_{\ell sj} = \frac{\hbar^2 c^2 V_0\, e^{-R_0/a}}{4\,\mu^2 c^4\, a}[j(j+1) - \ell(\ell+1) - s(s+1)]\}.$$

The centrifugal energy is given by $V_c(r) = \frac{\hbar^2 \ell(\ell+1)}{2\,\mu}\frac{1}{r^2}$. The Coulomb potential $V_{cp}(r)$ for charged particles must also be gotten if they exist. So, the effective potential can be obviously written as $U(r) = V_1(r) + V_{\ell sj} + V_c(r) + V_{cp}(r)$ orit is obviously as follows:

$$U(r) = -\frac{V_0}{1+e^{\left[\frac{r-R_0}{a}\right]}} - C_{\ell sj}\ \frac{1}{r}\frac{e^{r/a}}{\left[1+e^{\left[\frac{r-R_0}{a}\right]}\right]^2} + \frac{\hbar^2\ell(\ell+1)}{2\,\mu}\frac{1}{r^2} + V_{cp}(r)$$

The classical turning points of this effective potential cannot be found analytically and, therefore, it must be found numerically. The classical turning points are the roots of the equation $U(r) = -|E_q| = -m_h\, q^2/y$. Let these roots be $r_1(y)$ and $r_2(y)$. With these roots, first,$d^2 = [r_2(y) - r_1(y)]^2 = d_2(y)$is found, and after solving the equation $d_2(y) = y$, the following is found y and $E_q = m_h q^2/y$. For $q = 2$ ground state occurs; for $q = n\,\pi$, $(n = 1, 2, 3, \ldots)$ excited states occurs.

i. *Numeric calculations*

Let us calculate the energy values of $Cu(29, 68)$. We have taken the potentials as follows:

$$V_{cp}(r) = (Z-1)e^2\,\frac{3\,R_{co}^2 - r^2}{2\,R_{co}^3}\ ,\ [\text{Coulomb potential in the sphere}].$$

$$V(r) = -\frac{V_0}{1+e^{(r-R_0)/a_0}}\ ,\qquad (\text{Saxon} - \text{Woods potentials})$$

$$\alpha(L,S,J) = 0.5\,[J(J+1) - L(L+1) - S(S+1)]$$

$$V_{LSJ}(r) = -\frac{\hbar^2}{2\,\mu}\frac{1}{r}\,\alpha(L,S,J)\,\frac{V_{s0}}{a_{s0}}\frac{e^{(r-R_{s0})/a_{s0}}}{[1+e^{(r-R_{s0})/a_{s0}}]^2}\ ,\qquad (\text{spin} - \text{orbit potential})$$

For protons: $U(r) = V(r) + V_{LSJ}(r) + V_c(r) + V_{cp}(r)$

For neutrons: $U(r) = V(r) + V_{LSJ}(r) + V_c(r)$.

The parameters in these potentials have been calculated by the method of Volya [10, 11] and their values are: $a_{s0} = a_0 = 0.662;\ R_{co} = R_0 = 5.142885\ ;\ V_0 = 47.655271\ ;$

$V_{so} = 28.422020\,; R_{so} = 4.726557$. The values of dareobtained by solving the following equation:$U(r_0 - d/2) + U(r_0 + d/2) = -2\,\frac{\hbar^2}{2\,\mu}\frac{q^2}{d^2}$ and energy values have been calculated with the following formula: $E_q = -\frac{\hbar^2}{2\,\mu}\frac{q^2}{d^2}$. The results are seen in the Table5.

Table 5: A few energy values of the Cu (29, 68) nucleus with Saxon-Woods potential (unit MeV)

States	E_q(MeV) (neutron)	E_q (MeV) (proton)
1 s 1/2	-45.6256	-33.9536
1 p 3/2	-15.1995	-11.3653
1 p 1/2	-15.1987	-11.3644
1 d 5/2	-6.5021	-4.9028
1 d 3/2	-6.5011	-4.9015
2 s 1/2	-45.6061	-33.9536
1 f 7/2	-3.4830	-2.6484
2 p 3/2	-25.1702	-18.8825

i) Relativistic Dirac equation in a central potential and its solution

Consider a Dirac particle (spin is$1/2$) of mass m captured in a central potential well, $V(r)$. With this potential, Dirac Hamiltonian can be written as follows[12]:

$$H_D = \vec{\alpha}.\vec{p} + \beta\, m + V(r) \tag{6.9.1}$$

Here, we have relativistic units: $\hbar = c = 1\,, \vec{p} = -i\,\vec{\nabla}\,, \vec{\alpha} = (\alpha_x, \alpha_y, \alpha_z)$ and $\beta$are hermitical 4-operators acting on the spin variables alone. Including the position vector$\vec{r}$ and the velocity $\vec{\alpha} = d\vec{r}/dt$. Dirac Hamiltonian given in Equation (6.9.1) is invariant by rotation and reflection, then:

$$[H_D,\ \vec{J}] = 0,\ [H_D, \hat{P}] = 0$$

Here, $\vec{J}$ total angular momentum and $\hat{P}$ parity operators. We are looking for the eigenvalues and eigenfunctions of this Hamiltonian. It is convenient to write the functions of solution as:

$$\Phi = \begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}\ ,\ \chi = \begin{pmatrix}\psi_3\\ \psi_4\end{pmatrix}\ ,\ \Psi = \begin{pmatrix}\Phi\\ \chi\end{pmatrix} \tag{6.9.2}$$

Projecting Ψ on $\beta = +1$ and $\beta = -1$ sub-spaces, there is also as follows:

$$\tfrac{1}{2}(1+\beta)\Psi = \begin{pmatrix}\Phi\\ 0\end{pmatrix}\ ,\ \tfrac{1}{2}(1-\beta)\Psi = \begin{pmatrix}0\\ \chi\end{pmatrix} \tag{6.9.3}$$

Φ and χ are functions of r and of the $\mu-$compenant of the spin on the z-axis. We may as well consider them as function of the radial variable r and angular variables (θ, ϕ, μ). Let us assume that Ψ is a common eigenfunctions of the operators J^2, J_z and P. We denote by (JM) the quantum numbers determining the total angular momentum. We denote the parities by the $\bar{\omega}$ quantum number, namely:

$\bar{\omega} = +1$for the states of parity $(-1)^{j+1/2}$;$\bar{\omega} = -1$ for the states of parity $(-1)^{j-1/2}$.

$$\bar{\omega}^2 = 1 \tag{6.9.4}$$

Then, we may write the following equations:

$$\hat{J}^2\begin{pmatrix}\Phi\\ \chi\end{pmatrix} = J(J+1)\begin{pmatrix}\Phi\\ \chi\end{pmatrix},\ \hat{J}_z\begin{pmatrix}\Phi\\ \chi\end{pmatrix} = M\begin{pmatrix}\Phi\\ \chi\end{pmatrix},\ \hat{P}\begin{pmatrix}\Phi\\ \chi\end{pmatrix} = (-1)^{J+\bar{\omega}/2}\begin{pmatrix}\Phi\\ -\chi\end{pmatrix} \tag{6.9.5}$$

$\mathcal{Y}^M_{LJ}(\theta,\varphi,\mu)$ is the function of total angular momentum (JM) formed by the composition of the spin-$1/2$ and the spherical harmonics of order 1. The parity of this function is $(-1)^L$. According to the composition of angular momentum, L can have two following values:

$$L = \ell = J + \bar{\omega}/2 \ \text{ and } \ L = \ell' = J - \bar{\omega}/2 \tag{6.9.6}$$

Two functions $\mathcal{Y}^M_{\ell J}(\theta,\varphi,\mu)$ and $\mathcal{Y}^M_{\ell' J}(\theta,\varphi,\mu)$ have the opposite parity. $\mathcal{Y}^M_{\ell J}(\theta,\varphi,\mu)$ and $\mathcal{Y}^M_{\ell' J}(\theta,\varphi,\mu)$ have the parity $(-1)^{J+\bar{\omega}/2}$ and $(-1)^{J-\bar{\omega}/2}$ respectively.

Following Equation (6.9.5), Φ and χ are functions of (r,θ,φ,μ) variables and they have parity $(-1)^{J+\bar{\omega}/2}$ and $(-1)^{J-\bar{\omega}/2}$ respectively. These functions Φ and χ have been product of two functions, the one is function of r, and the other is function of total angular momentum function. Consequently, if $\Psi^M_{\bar{\omega}J}$ represents a state of angular momentum (JM) and of parity $(-1)^{J+\bar{\omega}/2}$, it can be written as following form:

$$\Psi^M_{\bar{\omega}J} = \frac{1}{r}\begin{pmatrix} F(r)\mathcal{Y}^M_{\ell J}\\ i\,\Theta(r)\mathcal{Y}^M_{\ell' J}\end{pmatrix} \tag{6.9.7}$$

Therefore we want to solve the following eigenvalue problem:

$$H_D\,\Psi^M_{\bar{\omega}J} = E\,\Psi^M_{\bar{\omega}J} \tag{6.9.8}$$

To solve Equation(6.9.8), it should be separated angular and radial variables in the operator H_D. We introduce the radial momentum p_r and radial velocity α_r as follows:

$$p_r = -i\,\frac{1}{r}\frac{\partial}{\partial r}r,\ \ \alpha_r = \vec{\alpha}.\hat{r} = \rho_1(\vec{\sigma}.\vec{r})/r \tag{6.9.9}$$

Here $\hat{r}$ is unit vector and $\vec{\sigma}$ is Pauli spin matrix vector. Let us consider the following vector equation:

$$(\vec{\sigma}.\vec{A})(\vec{\sigma}.\vec{B}) = (\vec{A}.\vec{B}) + i\,\vec{\sigma}.(\vec{A}x\vec{B}) \tag{6.9.10}$$

Here, $\vec{A}$ and $\vec{B}$ are any two vectors. According to Equation (6.9.10) it can be written as follows:

$$(\vec{\alpha}.\vec{r})(\vec{\alpha}.\vec{p}) = (\vec{\sigma}.\vec{r})(\vec{\sigma}.\vec{p}) = \vec{r}.\vec{p} + i\,\vec{\sigma}.\vec{L} = r\,p_r + i\,(1+\vec{\sigma}.\vec{L}) \tag{6.9.11}$$

Hence, multiplying on the left by α_r/r and using the property $\alpha_r^2 = 1$, we get:

$$\vec{\sigma}.\vec{p} = \alpha_r\left[p_r + \frac{i}{r}\,(1+\vec{\sigma}.\vec{L})\right] \ \text{ and } \ (1+\vec{\sigma}.\vec{L}) = J^2 - L^2 + 1/4 \tag{6.9.12}$$

It can also be shown that:

$$\left(1+\vec{\sigma}.\vec{L}\right)\Psi_{\bar{\omega}J}^{M}=-\frac{\bar{\omega}}{2}(2J+1)\beta\Psi_{\bar{\omega}J}^{M} \tag{6.9.13}$$

Substituting Equation (6.9.12) and Equation (6.9.13) into (6.9.8), the following equation can be obtained:

$$\left[\alpha_r\left(p_r-\frac{i\,\bar{\omega}\,(J+1/2)\,\beta}{r}\right)+m\,\beta+V(r)\right]\Psi_{\bar{\omega}J}^{M}=E\,\Psi_{\bar{\omega}J}^{M} \tag{6.9.14}$$

The following two equations can also be shown:

$$(\vec{\sigma}.\vec{r})\mathcal{Y}_{\ell J}^{M}=-\mathcal{Y}_{\ell' J}^{M}\ \text{and}\ (\vec{\sigma}.\vec{r})\mathcal{Y}_{\ell' J}^{M}=-\mathcal{Y}_{\ell J}^{M} \tag{6.9.15}$$

Substituting the function (6.9.7) in (6.9.14) and using the expression (6.9.9), the following two equations are obtained:

$$\left[-\frac{d}{dr}+\frac{\bar{\omega}\,(J+1/2)}{r}\right]\Theta(r)=[E-m-V(r)]F(r) \tag{6.9.16a}$$

$$\left[\frac{d}{dr}+\frac{\bar{\omega}\,(J+1/2)}{r}\right]F(r)=[E+m-V(r)]\Theta(r) \tag{6.9.16b}$$

This system of radial equations plays the role of the radial equation of the non-relativist theory. The normalization expression of the function $\Psi_{\bar{\omega}J}^{M}$, after integration over angles is given by the following expression:

$$\left(\Psi_{\bar{\omega}J}^{M},\Psi_{\bar{\omega}J}^{M}\right)=\int_0^\infty(|F(r)|^2+|\Theta(r)|^2)\,dr \tag{6.9.17}$$

Putting $\tau=\bar{\omega}\,(J+1/2)$ in Equations(6.9.16a) and (6.9.16b) let us rewrite them in the matrix form as follows:

$$\begin{pmatrix}\frac{dF(r)}{dr}\\ \frac{d\Theta(r)}{dr}\end{pmatrix}=\frac{d}{dr}\begin{pmatrix}F(r)\\ \Theta(r)\end{pmatrix}=A\begin{pmatrix}F\\ \Theta\end{pmatrix} \tag{6.9.18a}$$

$$A=\begin{pmatrix}-\tau/r & [E+m-V(r)]\\ -[E-m-V(r)] & \tau/r\end{pmatrix} \tag{6.9.18b}$$

Differentiating Equations (6.9.18a) and (6.9.18b), we obtain the following equation:

$$\frac{d}{dr}\begin{pmatrix}\frac{dF(r)}{dr}\\ \frac{d\Theta(r)}{dr}\end{pmatrix}=\begin{pmatrix}\frac{d^2F(r)}{dr^2}\\ \frac{d^2\Theta(r)}{dr^2}\end{pmatrix}=\frac{d^2}{dr^2}\begin{pmatrix}F(r)\\ \Theta(r)\end{pmatrix}=B\begin{pmatrix}F\\ \Theta\end{pmatrix}=\varepsilon_i\begin{pmatrix}F\\ \Theta\end{pmatrix} \tag{6.9.19}$$

Here, $B=\frac{dA}{dr}+A^2$ and ε_i is eigenvalue of B matrix and it has been calculated as follows:

$$\varepsilon_i=m^2-E^2+\frac{\tau^2}{r^2}+2\,E\,V(r)-V(r)^2\pm\sqrt{\tau^2/r^4-[V'(r)]^2} \tag{6.9.20}$$

Equation (6.9.20) contains the central potential and the spin-orbit interaction potential, whereas, there is Laplace operator in the relativistic energy operator. When Laplace operator is expressed in spherical coordinates, it occurs the centrifugal potential energy term as $L(L+1)/r^2$. Therefore, it should also be added this potential term to the expression (6.9.20). If we put $\tau^2=(J+1/2)^2$ in Equation (6.9.20), we can rewrite it as follows:

Notes

Notes

$$U_{re}(r) = 2\,E\,V(r) - V(r)^2\,;\;\; U_J = (J+1/2)^2/r^2\,;\;\; U_L = L(L+1)/r^2$$

$$U_{rez}(r) = \sqrt{(J+1/2)^2/r^4 - [V'(r)]^2}$$

$$U_{re\,1}(r) = U_{re}(r) + U_J(r) + U_L(r) - U_{rez}(r)$$

$$U_{re\,2}(r) = U_{re}(r) + U_J(r) + U_L(r) + U_{rez}(r)$$

$$U_{rei}(r) = U_{re}(r) + U_J(r) + U_L(r) \pm U_{rez}(r)$$

$$\varepsilon_i = m^2 - E^2 + U_{rei}(r),\;\; (i = 1,\; 2) \qquad (6.9.21)$$

According to Equation (6.9.19) we can write the following two equations:

$$\frac{d^2F(r)}{dr^2} - \varepsilon_i\,F(r) = 0\;\;;\;\; \frac{d^2\Theta(r)}{dr^2} - \varepsilon_i\Theta(r) = 0 \qquad (6.9.22)$$

We see in Equation (6.9.22) that $F(r) = \Theta(r)$, then it is sufficient to examine only $F(r)$. So, from Equation (6.9.22), we can write the following equation:

$$\frac{d^2F(r)}{dr^2} + [\alpha - U_{rei}]F(r) = 0\,,\;\; (\alpha = E^2 - m^2) \qquad (6.9.23)$$

From the other side, the radial SE which is given in Equation (63)can be written as follows:

$$\frac{d^2F(r)}{dr^2} + [\beta - U_e(r)]F(r) = 0\,,\;\; [\beta = \frac{2\,m}{\hbar^2}E\,,\;\; U_e(r) = \frac{2\,m}{\hbar^2}U(r)] \qquad (6.9.24)$$

If Equation (6.9.24) is compared with the Equation (6.9.23), it is seen that both equations are the same form. So they have the same form solution. Let $U(r) = U_{rei}(r)$. Now let us see the solution of Equation(6.9.23) for the bound state.

i. *Energy*

For $\alpha > U(r)$ bound state; $k = i\sqrt{|\alpha|} = i\,K$, $G(r) = \int\sqrt{-U(r)}\,dr$. r_1 and r_2, $(r_1 < r_2)$are the roots of the following equation:

$$\alpha - U(r) = 0 \;\text{ or }\; (m^2 - E^2) - U(r) = 0 \qquad (6.9.25)$$

The bound state energies are given by the solution of the following equation:

$$K\,d = q,\; [d = r_2 - r_1\,,\;\; K = \sqrt{|\alpha|} = \sqrt{|(E^2 - m^2)|} = \sqrt{m^2 - E^2}, (m > |E|] \qquad (6.9.26)$$

For $q = 2$ ground state occurs; for $q = n\,\pi\,,\;\; (n = 1, 2, 3, \ldots)$ excited states occurs.

ii. *Wave functions*

Now let us find the function $F(r)$ in bound states. In bound states, always $E > U(r)$, that is $\alpha > U(r)$. Therefore:

$$K = \sqrt{|\alpha|} = \sqrt{|E^2 - m^2|} = \sqrt{m^2 - E^2} = K > 0$$

$$G(r) = i\int\sqrt{U(r)}\;dr = i\int\sqrt{-|U(r)|}\;dr = \int\sqrt{|U(r)|}\;dr = Q(r)$$

$$F(r) = A\cos[K\,r]e^{i\,G(r)} = A\cos[K\,r]e^{i\,Q(r)} = A\cos\left[\frac{q}{d}\,r\right]e^{i\,Q(r)}$$

$$F(r) = B\sin[K\,r]e^{i\,G(r)} = B\sin[K\,r]e^{i\,Q(r)} = B\sin\left[\frac{q}{d}\,r\right]e^{i\,Q(r)}$$

$$|A| = |B| = \sqrt{2/d} = \sqrt{2\,K/q}$$

According to Equation (6.9.7), we can write the complete wave function as follows:

$$\Psi^{M}_{\varpi J} = \frac{1}{r}\begin{pmatrix} F(r)\mathcal{Y}^{M}_{\ell J} \\ i\,\Theta(r)\mathcal{Y}^{M}_{\ell' J} \end{pmatrix} = \frac{1}{r}\begin{pmatrix} F(r)\mathcal{Y}^{M}_{\ell J} \\ i\,F(r)\mathcal{Y}^{M}_{\ell' J} \end{pmatrix} = \frac{F(r)}{r}\begin{pmatrix} \mathcal{Y}^{M}_{\ell J} \\ i\,\mathcal{Y}^{M}_{\ell' J} \end{pmatrix} \tag{6.9.27}$$

This function is eigen-function of Dirac Hamiltonian in the bound states.

iii. *Application to an atom of hydrogen-like*

The following central potential can be taken for an atom of hydrogen-like:

$$V(r) = -\frac{Z\,e^2}{r}$$

Here Z is atomic number and e electron charge. With this potential, we consider two case solutions:

a. *Relativistic case (Dirac equation)*

- *Energy*

$$U(r) = U_{rei}(r) = -\frac{2\,E\,Z\,e^2}{r} + \frac{b_i}{r^2}\,, \qquad (i = 1,2)$$

$$b_1 = (j+1/2)^2 + L(L+1) - Z^2e^4 - \sqrt{\tau^2 - Z^2e^4}$$

$$b_2 = (j+1/2)^2 + L(L+1) - Z^2e^4 + \sqrt{\tau^2 - Z^2e^4}$$

$$\tau = j + 1/2\,, \quad b_i = b_1 \text{ or } b_2$$

The roots of the equation $[\alpha - U_{rei}(r)] = 0$ or $[(E^2 - m^2) - U_{rei}(r)] = 0$ are as follows:

$$r_1 = \frac{E\,Z\,e^2 - \sqrt{E^2Z^2e^4 - b_i(m^2 - E^2)}}{(m^2 - E^2)}\,, \quad r_2 = \frac{E\,Z\,e^2 + \sqrt{E^2Z^2e^4 - b_i(m^2 - E^2)}}{(m^2 - E^2)}$$

$$d = r_2 - r_1 = \frac{2\sqrt{E^2Z^2e^4 - b_i(m^2 - E^2)}}{(m^2 - E^2)}\,, \qquad K = \sqrt{|\alpha|} = \sqrt{(m^2 - E^2)}\,, (m > E)$$

The roots of the equation $K\,d = q$ are as follows:

$$E = E^{(i)}_q = \pm m\sqrt{\frac{4\,b_i + q^2}{4\,b_i + q^2 + 4\,Z^2e^4}}\,, \ (i = 1,2) \tag{6.9.28}$$

For $q = 2$ ground state occurs; for $q = n\,\pi$, $(n = 1,2,3,\ldots)$ excited states occurs. Let us take the $(+)$ sign in Equation (6.9.28). So we have the following energies:

$$E^{new}_{reb\,1} = m\sqrt{\frac{4\,b_i + q^2}{4\,b_1 + q^2 + 4\,Z^2e^4}}\ ; \quad E^{new}_{reb\,2} = m\sqrt{\frac{4\,b_i + q^2}{4\,b_2 + q^2 + 4\,Z^2e^4}} \tag{6.9.29}$$

- *Wave functions*

$$U(r) = U_{rei}(r) = -\frac{2\,E_i\,Z\,e^2}{r} + \frac{b_i}{r^2} = -\frac{a_i}{r} + \frac{b_i}{r^2}\,, \qquad (i = 1,2)$$

Notes

$$a_i = 2\,E_i\,Z\,e^2\,, \qquad (E_i = E_{erbi}^{new})$$

$$|U_{rei}(r)| = \frac{a_i}{r} - \frac{b_i}{r^2}\,, \qquad (i = 1,2)$$

$$G_i(r) = \int \sqrt{|U_{rei}(r)|}\,dr = \int \sqrt{\frac{a_i}{r} - \frac{b_i}{r^2}}\,dr = Q_i(r)$$

$$Q_i(r) = 2\left\{\sqrt{a_i r - b_i} - \sqrt{b_i}\,\arctan\left[\sqrt{a_i r - b_i)/b_i}\right]\right\}$$

$$K_i = \sqrt{|E_i^2 - m^2|} = \sqrt{m^2 - E_i^2} = K_i > 0\,, \qquad (m > E_i)$$

$$F_i(r) = A_i\cos[K_i\,r]e^{i\,G_i(r)} = A_i\cos[K_i\,r]e^{i\,Q_i(r)} = A_i\cos\left[\frac{q_i}{d_i}\,r\right]e^{i\,Q_i(r)}$$

$$F_i(r) = B_i\sin[K_i\,r]e^{i\,G_i(r)} = B_i\sin[K_i\,r]e^{i\,Q_i(r)} = B_i\sin\left[\frac{q_i}{d_i}\,r\right]e^{i\,Q_i(r)}$$

$$|A_i| = |B_i| = \sqrt{2/d_i} = \sqrt{2\,K_i/q_i}$$

$$\Psi_{\bar{\omega}J}^{M} = \frac{1}{r}\begin{pmatrix} F(r)\mathcal{Y}_{\ell J}^{M} \\ i\,\Theta(r)\mathcal{Y}_{\ell' J}^{M}\end{pmatrix} = \frac{1}{r}\begin{pmatrix} F(r)\mathcal{Y}_{\ell J}^{M} \\ i\,F(r)\mathcal{Y}_{\ell' J}^{M}\end{pmatrix} = \frac{F_i(r)}{r}\begin{pmatrix} \mathcal{Y}_{\ell J}^{M} \\ i\,\mathcal{Y}_{\ell' J}^{M}\end{pmatrix} \qquad (6.9.30)$$

b. *No-relativistic case [Schrödinger equation (SE)]*

- *Energy*

$$\tau = J + 1/2 \;\;;\;\; U_{rez}(r) = \frac{\sqrt{\tau^2 - Z^2e^4}}{r^2}\;;$$

$$U_{scbi}(r) = -\frac{Z\,e^2}{r} + \frac{1}{2\,m}\left[U_J(r) + U_L(r) \pm U_{rez}(r)\right] = -\frac{Z\,e^2}{r} + \frac{b_i}{r^2}\,, \qquad (i = 1,2)$$

$$b_1 = \frac{1}{2\,m}\left[\tau^2 + L(L+1) - Z^2e^4 - \sqrt{\tau^2 - Z^2e^4}\right]$$

$$b_2 = \frac{1}{2\,m}\left[\tau^2 + L(L+1) - Z^2e^4 + \sqrt{\tau^2 - Z^2e^4}\right]$$

$$\alpha = 2\,m\,E_{scbi} = 2\,m\,E \;\;;\;\; U_{sc}(r) = 2\,m\,U_{scbi}(r)$$

The roots of the equation $-|\alpha| - U_{sc}(r) = 0$ are as follows:

$$r_1 = \frac{Z\,e^2 - \sqrt{Z^2e^4 - 4\,b_i|E|}}{2\,|E|} \;\;;\;\; r_1 = \frac{Z\,e^2 + \sqrt{Z^2e^4 - 4\,b_i|E|}}{2\,|E|}$$

$$d = r_2 - r_1 = \frac{\sqrt{Z^2e^4 - 4\,b_i|E|}}{|E|} \;\;;\;\; K = \sqrt{|\alpha|} = \sqrt{2\,m\,|E|}$$

The roots of the equation $K\,d = q$ are as follows:

$$|E| = E_{scbi}^{new} = \frac{2\,m\,Z^2e^4}{8\,m\,b_i + q^2}\,, \;\; (i = 1,2) \qquad (6.9.31a)$$

So, the following energy values are obtained:

$$|E| = E_{scb\,1}^{new} = \frac{2\,m\,Z^2e^4}{8\,m\,b_1+q^2}\ ;\ |E| = E_{scb\,2}^{new} = \frac{2\,m\,Z^2e^4}{8\,m\,b_2+q^2} \tag{6.9.31b}$$

If we take $b_1 = b_2 = \frac{L(L+1)}{2\,m}$ in Equation (6.9.31a) we obtain the following energy:

$$|E| = E_q^{new} = \frac{m\,e^4}{2\,\hbar^2}\frac{Z^2}{L(L+1)+q^2/4} \tag{6.9.31c}$$

For $q = 2$ ground state occurs; for $q = n\,\pi$, $(n = 1, 2, 3, \dots)$ excited states occurs.

- *Wave functions*

The wave functions in the no-relativistic case (case of Schrödinger) as follows:

$$U_i(r) = U_{scbi}(r) = -\frac{Z\,e^2}{r} + \frac{b_i}{r^2} = -\frac{a}{r} + \frac{b_i}{r^2}\ ,\qquad [a = Z\,e^2\ ;\ i = 1,2]$$

$$G_i(r) = \int \sqrt{|U_i(r)|}\,dr = Q_i(r)\ ;\ K_i = \sqrt{2\,m\,|E_i|}$$

$$Q_i(r) = \int \sqrt{\frac{a}{r} - \frac{b_i}{r^2}}\,dr = 2\left\{\sqrt{a\,r - b_i} - \sqrt{b_i}\,\arctan\left[\sqrt{a\,r - b_i}/\sqrt{b_i}\right]\right\}$$

$$F_i(r) = A_i\cos[K_i\,r]e^{\pm i\,G_i(r)} = A_i\cos[K_i\,r]e^{\pm i\,Q_i(r)} = A_i\cos\left[\frac{q_i}{d_i}\,r\right]e^{\pm i\,Q_i(r)}$$

$$F_i(r) = B_i\sin[K_i\,r]e^{\pm i\,G_i(r)} = B_i\sin[K_i\,r]e^{\pm i\,Q_i(r)} = B_i\sin\left[\frac{q_i}{d_i}\,r\right]e^{\pm i\,Q_i(r)}$$

$$|A_i| = |B_i| = \sqrt{2/d_i} = \sqrt{2\,K_i/q_i}$$

$$\Psi_J^M = \frac{1}{r}\begin{pmatrix} F_i(r)\mathcal{Y}_{\ell J}^M \\ i\,F_i(r)\mathcal{Y}_{\ell' J}^M \end{pmatrix} = \frac{F_i(r)}{r}|LJM> \tag{6.9.32}$$

Here, $|LJM>$ is the wave function of total angular momentum.

c. *Classical solutions of Dirac and Schrödinger equations for this potential*

We consider the following potential:

$$U_i(r) = U_{rei}(r) = -\frac{a_i}{r} + \frac{b_i}{r^2}\ ,\ [i = 1,2] \tag{6.9.33}$$

With this potential, let us rewrite the following radial differential equation:

$$\frac{d^2F(r)}{dr^2} + [\alpha - U_i(r)]F(r) = 0 \tag{6.9.34}$$

In Equation (6.9.34); if we take: $\alpha = (E^2 - m^2)$, $a_i = 2\,E_i\,Z\,e^2$and $b_i = \left[\tau^2 + L(L+1) - Z^2e^4 \pm \sqrt{\tau^2 - Z^2e^4}\right]$we obtain Dirac equation (DE). If we take: $\alpha = 2\,m\,E_i$; $a_i = 2\,m\,Z\,e^2$and$b_i = \left[\tau^2 + L(L+1) - Z^2e^4 \pm \sqrt{\tau^2 - Z^2e^4}\right]$, $(\hbar = 1)$ we obtain Schrödinger equation (SE).

The classical solution of the differential Equation(6.9.34) is as follows:

$$F(r) = c_1 M_{k,\mu}(\beta) + c_2 W_{k,\mu}(\beta)$$

$$M_{k,\mu}(\beta) = e^{-\beta/2}\beta^{(\mu+1/2)}F_1^1(\mu - k + 1/2, 1 + 2\,\mu, \beta)$$

$$W_{k,\mu}(\beta) = e^{-\beta/2}\beta^{(\mu+1/2)}F_1^2(\mu - k + 1/2, 1 + 2\,\mu, \beta)$$

$$k = \frac{a_i}{\sqrt{\alpha}}, \quad \mu = \frac{1}{2}\sqrt{1 + 4\,b_i}, \quad \beta = 2\sqrt{\alpha}\,r$$

Notes

Here F_1^1 and F_1^2 are confluent and hypergeometric series, respectively. According to thefeatures of these series, if $\mu - k + 1/2 = -(n-1)$, $(n = 1, 2, 3, \dots)$, the function of F_1^1 is polynomial. Solving this equation, the values of energy are found as follows:

- *Relativistic case (Dirac energy)*

$$P_1 = 2\,(-1+n)^2n^2 + e^4Z^2[1 + 2(-1+n)n]$$

$$P_{2b_i} = [-4\,(-1+n)n + 2\,e^4Z^2]b_i + 2\,b_i^2 + e^4Z^2(-1+2\,n)\sqrt{1+4\,b_i}$$

$$P_3 = [(-1+n)^2 + e^4Z^2][n^2 + e^4Z^2]$$

$$P_{4bi} = 2\,(n - n^2 + e^4Z^2)b_i + b_i^2$$

$$E_{rebi}^{cls} = m\sqrt{\frac{P_1 + P_{2bi}}{2\,(P_3 + P_{4bi})}}\,, \quad (b_i = b_1 \text{ and } b_2) \qquad (6.9.35)$$

- *No-relativistic case (Schrödinger energy)*

$$E_{scbi}^{cls} = \frac{m\,e^4Z^2[-1-2\,b_i - \sqrt{1+4\,b_i} + 2\,n\,(1 - n + \sqrt{1+4\,b_i})]}{4(n - n^2 + b_i)^2}\,, \quad (b_i = b_1 \text{ and } b_2) \qquad (6.9.36)$$

The well-known energy value for this potential (in the relativistic case-Dirac energy) is as follows:

$$E_{nJ}^{cls} = m\left\{1 + \frac{Z^2e^4}{\left[n - J - 1/2 + \sqrt{(J+1/2)^2 - Z^2e^4}\right]^2}\right\}^{-1/2}, \qquad (c = 1, \hbar = 1, n = 1, 2, 3, \dots) \quad (6.9.37)$$

The well-known energy value for this potential (in the no-relativistic case-Schrödinger energy) is as follows:

$$\left|E_n^{cls}\right| = \frac{m\,e^4}{2\,\hbar^2}\frac{Z^2}{n^2}\,, \quad (n = 1, 2, 3, \dots) \qquad (6.9.38)$$

We give some energy values calculated by the new formulas (6.9.29), (6.9.31b), (6.9.31c), (6.9.38) in Table 6, and by the classical solution formulas (6.9.35), (6.9.36), (6.9.37), (6.9.38) in Table 7. The values of new solutions have been compared with the ones of classical solutions. In these numerical calculations, we have taken only the potentials with $b_1$parameters, because of $(\lim_{r\to 0} U(r) \to +\infty)$ in the s-states for $b_2$parameters, so such potential is not accessible in bound states. Electron mass$0.511003\ MeV/c^2$;electron charge$e^2 = 1/137.0360$; proton mass$938.280\ MeV/c^2$; $\hbar\,c = 197.329\,MeV.fm$ or $\hbar = 1;\ Z = 1,$ m reduced mass.

It seems in Table 6: in second colon; the same n-states have the same energy values, there are degeneracy; in third colon; the same n and l-states have the same energy values. There is less degeneracy in these states. In fourth and fifth colons, every

state has the different energy value, there is no degeneracy. That is that the degeneracy is completely eliminated with spin-orbit interaction and centrifugal potential energy. But both of which have almost the same energy values. Then the solutions of SE and Dirac equations give almost the same energy values for the same potential energy. So, there is no need to solve the Dirac equation to find the energy values of the quantum systems, it is sufficient to solve the SE with a well-defined potential.

Table 6: Energy values of the some electron states by new formulas

States n L_J	$\lvert E_n^{cls}\rvert$(eV)	$\lvert E_q^{new}\rvert$ (eV)	$\lvert E_{scb1}^{new}\rvert$(eV)	$\lvert m - E_{reb1}^{new}\rvert$(eV)
1 $s_{1/2}$	13.5926	13.5926	13.5988	13.5982
2 $s_{1/2}$	3.39815	5.50887	5.51128	5.51119
2 $p_{1/2}$	3.39815	3.04262	3.04393	3.04391
2 $p_{3/2}$	3.39815	3.04262	2.10262	2.10261
3 $s_{1/2}$	1.51029	1.37722	1.37781	1.37780
3 $p_{1/2}$	1.51029	1.14516	1.14565	1.14565
3 $p_{3/2}$	1.51029	1.14516	0.98045	0.98045
3 $d_{3/2}$	1.51029	0.85652	0.76098	0.76098
3 $d_{5/2}$	1.51029	0.85652	0.62180	0.62180

It seems in Table 6: in second and third colons; the same n-sates have almost the same energy values; in third colon; the same n and l-stateshave the same energy values, there is degeneracy. In fourth and fifth colons, every state has the different energy value, there is no degeneracy. That is that the degeneracy is completely eliminated with spin-orbit interaction and centrifugal potential energy. But both of which have almost the same energy values.

Then the solutions of SE and Dirac equations give almost the same energy values for the same potential energy. So, there is no need to solve Dirac equation to find the energy values of the quantum system, it is sufficient to solve the SE with a well-defined potential. The energy values of the second and third colons are different from the energy values of fourth and fifth colon, except for s-states, because of the potential does not include the centrifugal potential energy term in the second and third colons.

Table 7: Energy values of the some electron states by classical formulas

States n L_J	$\lvert E_n^{cls}\rvert$ (eV)	$\lvert m - E_{nJ}^{cls}\rvert$ (eV)	$\lvert E_{scb1}^{cls}\rvert$ (eV)	$\lvert m - E_{reb1}^{cls}\rvert$ (eV)
1 $s_{1/2}$	13.5926	13.5986	13.5991	13.5986
2 $s_{1/2}$	3.39815	3.39966	3.39966	3.39966
2 $p_{1/2}$	3.39815	3.39966	1.51094	1.51093
2 $p_{3/2}$	3.39815	3.39961	1.07204	1.07204
3 $s_{1/2}$	1.51029	1.51095	1.51096	1.51095
3 $p_{1/2}$	1.51029	1.51095	0.84990	0.84990
3 $p_{3/2}$	1.51029	1.51094	0.65353	0.65353
3 $d_{3/2}$	1.51029	1.51094	0.47116	0.47116
3 $d_{5/2}$	1.51029	1.51093	0.37773	0.37773

Notes

It seems that our new results are very compatible, because there is any approximation in our solutions whereas there some approximation in classical solutions. Both Dirac and SE give almost the same values of energy for potential in classical or new method. So, whether the new method or classical method, it is not need to solve Dirac equation, it is sufficient to solve only the SE to find the energy values for a well-defined potential.

Notes

VII. Transmission Coefficient for an Arbitrary form Potential Barrier

a) Determination of the wave functions

From the solutions of Equations (52), let us consider the following functions:

$$F(r) = A\, e^{k\, r \pm iG(r)} + B\, e^{-k\, r \mp iG(r)} \tag{64}$$

Here, (a) For the case where$E > U(r)$, $k = i\, m_1\sqrt{E}$, $G(r) = i\, m_1 \int \sqrt{U(r)}\ dr$.

(b) For the case where $E < U(r)$, $k = m_1\sqrt{E}$, $G(r) = m_1 \int \sqrt{U(r)}\ dr$.

Let us divide the potential into three domains, as seen in Figure3. In region I,$E > U_1$; in region II,$E < U_2$; and in region III, $E > U_3$. Now, consider that a particle with total energy E comes from the left to the right as in Figure3 and hits the barrier at the pointr_1. According to the function given in (64), the wave functions can be obtained for these three regions as follows:

$$\begin{aligned} F_1(r) &= A_1 e^{i\, K\, r \pm Q_1(r)} + B_1 e^{-i\, K\, r \mp Q_1(r)} \\ F_2(r) &= A_2 e^{K\, r \mp i\, Q_2(r)} + B_2 e^{-K\, r \pm i\, Q_2(r)} \\ F_3(r) &= A_3 e^{i\, K\, r \pm Q_3(r)} \end{aligned} \tag{65}$$

$$K = m_1\sqrt{E}, \qquad Q_p(r) = m_1 \int \sqrt{U_p(r)}\ dr, \qquad (p = 1, 2, 3)$$

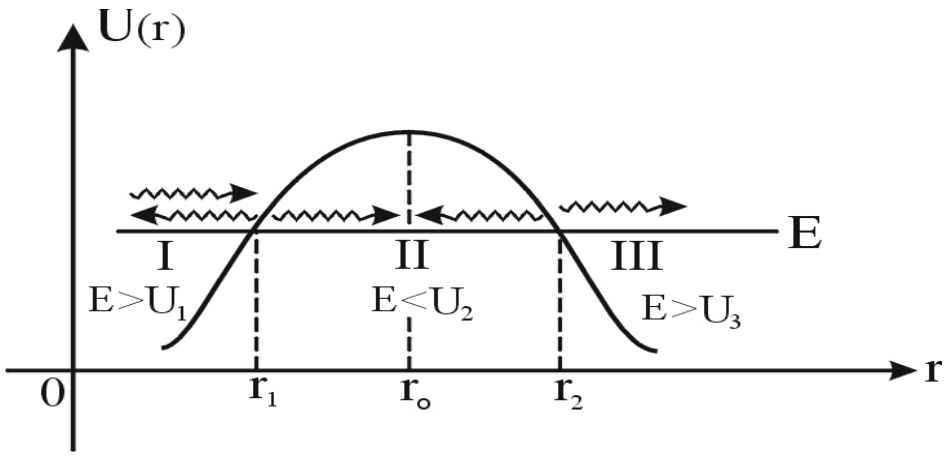


Figure 3: The unbounded state (potential barrier) and tunneling

In the calculations of the above functions, the fact that the waves travel both from left to right and right to left in the region I and only from left to right in the region III have been taken into account. Since there is no wave coming from right to left in the region III, so the coefficient B_3 must be zero.

b) Calculation of the transmission coefficient T

To calculate the transmission coefficient T, the coefficients A_i and B_i in the functions given in Equation(65)must be found. In order to find these coefficients, the following boundary conditions are used:

$$F_1(r_1) = F_2(r_1);\quad F_1'(r_1) = F_2'(r_1);\quad F_2(r_2) = F_3(r_2);\quad F_2'(r_2) = F_3'(r_2)$$

$$E = U_1(r_1) = U_2(r_1);\ E = U_2(r_2) = U_3(r_2);\ m_1\sqrt{E} = m_1\sqrt{U_p(r_1)} = m_1\sqrt{U_p(r_2)} = K$$

$$m_1\sqrt{E} = m_1\sqrt{U_p(r_1)} = m_1\sqrt{U_p(r_2)} = K$$

$$Q_p(r) = m_1 \int \sqrt{U_p(r)}\ dr \ \rightarrow\ Q_p'(r) = m_1\sqrt{U_p(r)}\ ;\ Q_p'(r_1) = Q_p'(r_2) = K$$

In the functions given in Equation(65), there are five unknown coefficients. Four of them can be found in term of A_1. All of the coefficients have been calculated in this study, but here, only the coefficient A_3 is sufficient. According to the signs of the exponential terms in Equation(65), two expressions for A_3 can be found as follows:
For the lower part of signs:

$$A_3 = \frac{2\exp[(1+i)K r_1 + (1-i)K r_2 - Q_1(r_1) + i\,Q_2(r_1) + i\,Q_2(r_2) + Q_3(r_2)]}{\exp[2\,K r_1 + 2\,i\,Q_2(r_1)] + \exp[2\,K r_2 + 2\,i\,Q_2(r_2)]}A_1$$

For the upper part of signs:

$$A_3 = \frac{2\exp[(1+i)K r_1 + (1-i)K r_2 + Q_1(r_1) + i\,Q_2(r_1) + i\,Q_2(r_2) - Q_3(r_2)]}{\exp[2\,K r_1 + 2\,i\,Q_2(r_2)] + \exp[2\,K r_2 + 2\,i\,Q_2(r_1)]}A_1$$

The transmission coefficient is defined as follows:

$$T = \frac{A_3 A_3^*}{A_1 A_1^*} = \frac{|A_3|^2}{|A_1|^2} = \frac{2}{\cosh[2\,K\,d] + \cos[2\,P]} \tag{66}$$

$$P = Q_2(r_2) - Q_2(r_1) = \sqrt{\frac{2m}{\hbar^2}}\int_{r_1}^{r_2}\sqrt{U_2(r)}\,dr$$

$$Q_2(r) = m_1\int\sqrt{U_2(r)}\ dr = \sqrt{\frac{2m}{\hbar^2}}\int\sqrt{U_2(r)}\ dr$$

From the literature [13], the transmission coefficient T (or the barrier penetration probability) which is calculated by the WKB is known as follows:

$$T = e^{-2g}\ ,\ \left[g = \sqrt{\frac{2m}{\hbar^2}}\int_{r_1}^{r_2}\sqrt{U_2(r) - E}\,dr\right] \tag{67}$$

In Equations(66) and (67), r_1 and r_2 are abscises of the points that the particle hits and leaves the potential barrier, respectively and they are found solving the equation $E = U_2(r)$.

Notes

c) Application to cold emission

i. *Calculation of transmission coefficient*

Cold emission of electrons from a metal surface is the basis of an important device known as scanning tunneling microscope (STM). An STM consists of a very sharp conducting probe which is scanned over the surface of a metal (or any other solid conducting medium). A large voltage difference is applied between the probe and the surface. The surface electric fieldstrength immediately below the probe tip is proportional to the applied potential difference, and inversely proportional to the spacing between the tip and the surface. Electrons tunneling between the surface and the probe tip cause a weak electric current. The magnitude of this current is proportional to the tunneling probability T. It follows that the current is an extremely sensitive function of the surface electric fieldstrength, and, hence, of the spacing between the tip and the surface (assuming that the potential difference is held constant). An STM can thus be used to construct a very accurate contour map of the surface under investigation. In fact, STMs are capable of achieving sufficient resolution to image individual atoms.

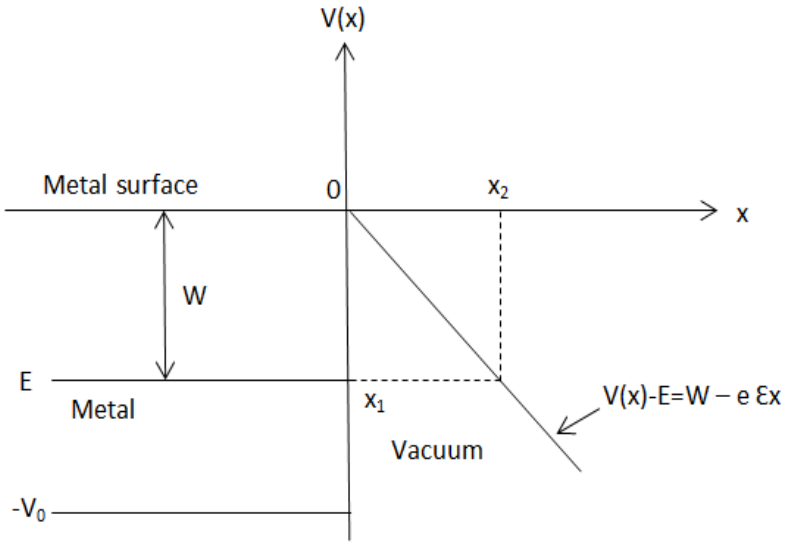


Figure 4: The potential barrier for an electron in a metal surface subject to an external electric field

Suppose that a cold metal surface is subject to a large uniform external electric field of strength $\in$, which is directed such that it accelerates electrons *away* from the surface. The electrons just below the surface of a metal can be regarded as being in a potential well of depth W, where W is called the *work function* of the surface. Adopting a simple one dimensional treatment of the problem let the metal lie at $x < 0$, and the surface at $x = 0$. The applied electric field is shielded from the interior of the metal. Hence, the energy E, for example, of an electron just below the surface is unaffected by the field. In the absence of the electric field, the potential barrier just above the surface is simply $U(x) - E = W$. The electric field modifies this to $U(x) - E = W - e \in x$.The potential barrier is sketched in Figure4. It can be seen, in Figure 4 that an electron just below the surface of the metal is confined by a triangular potential barrier which extends from$x = x_1$ to x_2, where $x_1 = 0$ and $x_2 = W/(e \in)$. In Equation (66), if it is put that:

$$d = x_2 - x_1 = W/(e\ \in)\ ;\ m_1 = \sqrt{\frac{2\,m}{\hbar^2}}$$

$$K = \sqrt{\frac{2\,m}{\hbar^2}E} = m_1\sqrt{E} = m_1\sqrt{-|E|} = i\,m_1\sqrt{W}$$

$$Q_2(x) = m_1\int\sqrt{-e\ \in x} = i\,\frac{2\sqrt{2\,m\,e\ \in}}{3\,\hbar}x^{3/2} = i\sqrt{\frac{8\,m\,e\ \in}{9\,\hbar^2}}x^{3/2}$$

With these values, the following transmission coefficient is obtained:

$$T = T_{new} = \frac{2}{\cosh[2\,K\,d]+\cos[2\,Q_2(x_2)]} = \frac{2}{\cos\left[\frac{2\sqrt{2\,m}}{\hbar\,e\,\in}W^{3/2}\right]+\cosh\left[\frac{4\sqrt{2\,m}}{3\,\hbar\,e\,\in}W^{3/2}\right]} \quad (68)$$

Here, in calculation of Equation(68), the following equation is used:

$$\cosh(i\,y) = \cos(y)\ \text{and}\ \cos(i\,y) = \cosh(y)$$

Using the WKB approximation, the probability of such an electron tunneling through the barrier and consequently being emitted from the surface is calculated as follows:

$$T = T_{wkb} = \exp\left[-2m_1\int_{x_1}^{x_2}\sqrt{U(x)-E}\right]dx = \exp\left[-2m_1\int_{x_1}^{x_2}\sqrt{W-e\ \in x}\right]dx$$

$$T = T_{wkb} = \exp\left[-\frac{4\sqrt{2\,m}}{3\,\hbar\,e\,\in}W^{3/2}\right] \quad (69)$$

The above result given in Equation(69) is known as the *Fowler-Northeim* formula. This formula is the result of WKB approximation. The formula given in Equation(68) is exact formula because there is no approximation. It is seen that there are a lot of difference between them.

ii. *Numerical calculations and comparison of Equations(68) and (69)*

The barrier penetration probabilities or the transmission coefficients T have been calculated from Equations (68) and (69). In the calculations, the electron mass, $m\,c^2 = 0.511003\ MeV$; the electroncharge, $e = 1.19999\ (MeV.fm)^{1/2}$ have been taken. The obtained values for the different metals are seen in Table 8. InTable 8, it can be seen that the new method is more appropriate than the classical WKB method. In the calculations of the current-voltage characteristics of a diode in semi conductor physics, it is expected to have better results. In calculations one has been taken $\hbar\,c = 197.329\ MeV.fm$

Notes

Table 8: Comparison of the transmission coefficients values calculated with classical and new method

Metals	Work function W (eV)	Transmission coefficient T_{new} from equation (68)			Transmission coefficient T_{wkb} from equation (69)		
		Electric field ∈ (V/cm)			Electric field ∈ (V/cm)		
		$5x10^6$	$5x10^7$	$1x10^7$	$5x10^6$	$5x10^7$	$1x10^7$
Na	2.46	$5.12448x10^{-23}$	0.0206	$1.43171x10^{-11}$	$1.28112x10^{-23}$	0.0051	$3.57928x10^{-12}$
Al	4.08	$5.07471x10^{-49}$	0.000052	$1.42474x10^{-24}$	$1.26868x10^{-49}$	0.000013	$3.56185x10^{-25}$
Cu	4.70	$1.40147x10^{-60}$	$3.60174x10^{-6}$	$2.36768x10^{-30}$	$3.50368x10^{-61}$	$9.00435x10^{-7}$	$5.91919x10^{-31}$
Zn	4.31	$3.25862x10^{-53}$	0.000020	$1.14169x10^{-26}$	$8.14656x10^{-54}$	$4.91018x10^{-6}$	$2.85422x10^{-27}$
Ag	4.73	$3.68836x10^{-61}$	$3.15165x10^{-6}$	$1.21464x10^{-30}$	$9.22090x10^{-62}$	$7.87911x10^{-7}$	$3.03659x10^{-31}$
Pt	6.35	$4.59212x10^{-95}$	$1.28249x10^{-9}$	$1.35530x10^{-47}$	$1.14803x10^{-95}$	$3.20624x10^{-10}$	$3.38826x10^{-48}$
Pb	4.14	$4.19617x10^{-50}$	0.000040	$4.09691x10^{-25}$	$1.04904x10^{-50}$	0.000010	$1.02423x10^{-25}$
Fe	4.50	$9.20656x10^{-57}$	$8.67486x10^{-6}$	$1.91902x10^{-28}$	$2.30164x10^{-57}$	$2.16872x10^{-6}$	$4.79754x10^{-29}$

d) Application to alpha decay in atom nuclei and calculation of half-life

i. *Calculation of half-life formula*

An α-particle is the nucleus of a helium atom. It consists of two protons and two neutrons. In the process of α-decay of nuclei, an α-particle is assumed to move in a spherical region determined by the daughter nucleus. The central feature of this one-body model is that the α-particle is preformed inside the parent nucleus. The theory does not prove that α-particle is preformed but it proves that it behaves as if it is [14]. Figure5 shows a plot, suitable for the purposes of the theory, of the potential energy between the α-particle and the residual nucleus for various distances between their centers. The horizontal line $E = E_\alpha$ is the disintegration energy. There are three regions of interest. In the spherical region $r < r_1$ we are inside the nucleus and speak of a potential well with of depth of $-U_0$, where U_0 is taken as a positive number. Classically, the α-particle can move in this region with a kinetic energy $E_\alpha + U_0$ but cannot escape from it. The region $r_1 < r < r_2$ forms a potential barrier because here the potential energy is more than the total available energy E_α. The region $r > r_2$ is a classically permitted region outside the barrier. From the classical point of view, an α-particle in the spherical potential well would reverse its motion every time it tried to pass beyond $r = r_1$ of tunneling through such a barrier. A consistent model for this process assumes that α-particle is bounded to the nucleus by a spherical potential well $V_1(r)$ or a spherical effective potential well $U_1(r)$ and that the α-particle is repelled from the residual nucleus by the central Coulomb potential barrier $V_2(r)$ or the effective central Coulomb potential barrier $U_2(r)$. The original radioactive nucleus has the charge Ze and the α-particle has the charge $2e$. So the Coulomb potential barrier is asfollows:

$$V_2(r) = \frac{2(Z-2)e^2}{r} = \frac{c}{r},\ [c = 2(Z-2)e^2].$$

Thus, the corresponding effective potential function is obtained as,

$$U_2(r) = \frac{c}{r} + \frac{b}{r^2}, \qquad [b = \frac{\hbar^2}{2m}\ell(\ell+1).$$

This effective potential is depicted in Figure5. There are three domains in this effective potential.

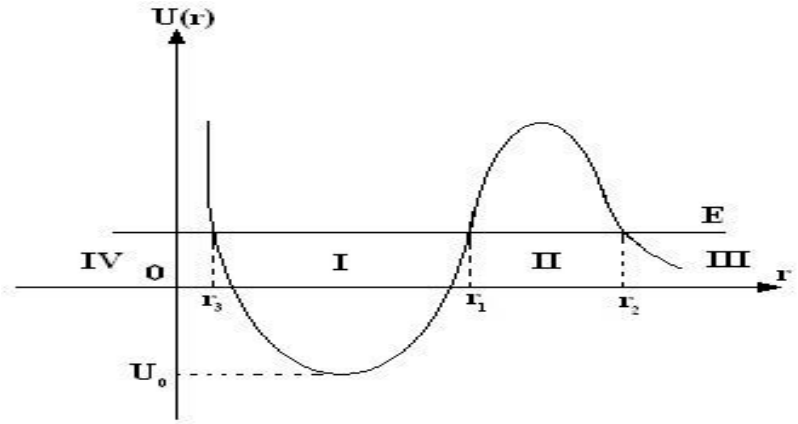


Figure 5: Effective potential function for the α-decay process of the nuclei

According to the one-body theory, the disintegration constant λ of an alpha emitter is given by: $\lambda = f\,T$, [T transmission coefficient]. Here f is the frequency with which the α-particle presents itself at the barrier and T is the probability of transmission through the barrier. The quantity f is roughly of the order of $\frac{v}{2\,(r_1 - r_3)}$, where v is relative speed of the alpha particle inside the nucleus. $t_{1/2} = 0.693/\lambda$ is used for the calculations of nuclear half-life. The relative speed of the alpha particle can be found from its kinetic energy that is equal to the difference between the disintegration energy of the alpha particle, E_α, and the ground state energy of the nucleus, E_0, namely;

$$K.E. = \frac{1}{2} m\, v^2 = [E_\alpha - (-|E_0|)] = E_\alpha + |E_0| \tag{70}$$

From Equation (70), the following is obtained:

$$v = \sqrt{\frac{2\,(E_\alpha + |E_0|)}{m}} \quad \text{and} \quad \frac{1}{v} = \sqrt{\frac{m}{2\,(E_\alpha + |E_0|)}}$$

If the values of $1/v$ and $\lambda = f\,T$ are substituted into $t_{1/2} = 0.693/\lambda$, then the followingformula is obtained:

$$t_{1/2} = \frac{0.693}{\lambda} = \frac{0.693}{f\,T} = 0.693\,\frac{2\,(r_1 - r_3)}{T}\frac{1}{v} = 0.693\,\frac{2\,(r_1 - r_3)}{T}\sqrt{\frac{m}{2\,(E_\alpha + |E_0|)}}.$$

To simplify the numerical calculations, this formula can be rewritten in following form:

$$t_{1/2} = 0.693\,\frac{2\,(r_1 - r_3)}{c}\sqrt{\frac{m\,c^2}{2\,(E_\alpha + |E_0|)}}\frac{1}{T} \tag{71}$$

Here, $m = \frac{m_n m_\alpha}{m_n + m_\alpha}$ is the reduced mass. (m_n and m_α are the mass of the nucleus and α-particle).

Notes

Notes

ii. *Determination of the potential functions*

In our numerical calculations, we have taken the harmonic oscillator type central potential as seen in Figure6. The central potential parts $V_1(r), V_2(r), V_3(r)$ and the central effective potential parts $U_1(r), U_2(r), U_3(r)$ are as follows:

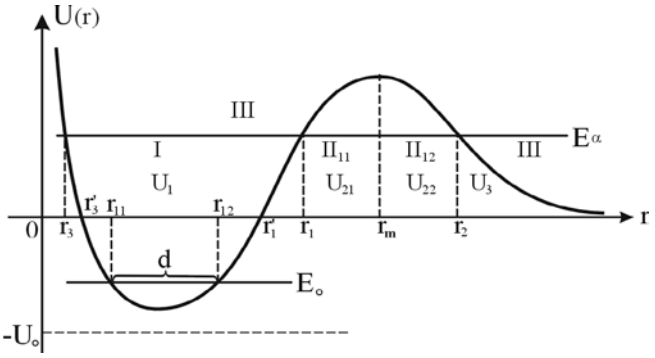


Figure 6: Central harmonic oscillator type effective potential

$$V_1(r) = -U_0 + a\,r^2\,;\; U_1(r) = -U_0 + a\,r^2 + \frac{b}{r^2}\;;\quad [r_3 \le r \le r_1]\quad [\text{I region}]$$

$$V_{21}(r) = a\,r^2\,;\; U_{21}(r) = a\,r^2 + \frac{b}{2}\;;\; [r_1 \le r \le r_m] \qquad (II_1 \text{ region})$$

$$V_{22}(r) = \frac{c}{r}\;;\; U_{22}(r) = \frac{c}{r} + \frac{b}{r^2}\;;\quad [r_m \le r \le r_2] \qquad (II_2 \text{ region})$$

$$V_3(r) = \frac{c}{r}\;;\quad U_3(r) = \frac{c}{r} + \frac{b}{r^2}\;;\qquad [r_2 \le r \le \infty] \qquad (\text{III region})$$

Here, $R = R_0\left[(A-4)^{1/3} + 4^{1/3}\right]$ is the total rayon of the nucleus and alpha particle. From the solution of the equation $E_\alpha = U_1(r) = -U_0 + a\,r^2 + \frac{b}{r^2}$, we can obtain as follows:

$$r_1 = \sqrt{\frac{(E_\alpha + U_0) + \sqrt{(E_\alpha + U_0)^2 - 4\,a\,b}}{2\,a}}\;;\; r_3 = \sqrt{\frac{(E_\alpha + U_0) - \sqrt{(E_\alpha + U_0)^2 - 4\,a\,b}}{2\,a}}$$

From the solution of the equation $E_\alpha = U_{22}(r) = \frac{c}{r} + \frac{b}{r^2}$; we can obtain as follows:

$$r_2 = \frac{c + \sqrt{c^2 + 4\,b\,E_\alpha}}{2\,E_\alpha}\,.$$

From the solution of the equation $E_0 = U_1(r) = -U_0 + a\,r^2 + \frac{b}{r^2}$, we can obtain as:

$$r_{11} = \sqrt{\frac{(E_0 + U_0) - \sqrt{(E_0 + U_0)^2 - 4\,a\,b}}{2\,a}}\;;\; r_{12} = \sqrt{\frac{(E_0 + U_0) + \sqrt{(E_0 + U_0)^2 - 4\,a\,b}}{2\,a}}\;;$$

$$d_0 = r_{12} - r_{11}\;;\quad d = r_2 - r_1.$$

From the solution of the equation $E_0 = -\frac{2\,\hbar^2}{m\,d_0^2}$, we obtain the ground state energy as follows:

$$E_0 = \sqrt{a\,b} - \frac{1}{2}\left[U_0 + \sqrt{4\,a\,b - \frac{8\,a\,\hbar^2}{m} - 4\sqrt{a\,b}\,U_0 + U_0^2}\right]$$

With these grandeurs the coefficients of transmission are written as follow:

$$T_{wkb} = e^{-2\,P_{wkb}}\ ;\ P_{wkb} = \sqrt{\frac{2\,m}{\hbar^2}}\left(\int_{r_1}^{r_m}\sqrt{U_{21}(r)-E_\alpha}\,dr + \int_{r_m}^{r_2}\sqrt{U_{22}(r)-E_\alpha}\,dr\right) \quad (72)$$

$$T_{new} = \frac{2}{\cosh\,[2\,K\,d]+\cos\,[2\,\{Q_2(r_2)-Q_2(r_1)\}]} = \frac{2}{\cosh\,[2\,K\,d]+\cos\,[2\,P_{new}\,]} \quad (73)$$

$$P_{new} = \sqrt{\frac{2\,m}{\hbar^2}}\left(\int_{r_1}^{r_m}\sqrt{U_{21}(r)}\,dr + \int_{r_m}^{r_2}\sqrt{U_{22}(r)}\,dr\right) \quad (74)$$

$$t_{1/2}^{wkb} = 0.693\,\frac{2\,(r_1-r_3)}{c}\sqrt{\frac{m\,c^2}{2\,(E_\alpha-E_0)}}\frac{1}{T_{wkb}} \quad (75)$$

$$t_{1/2}^{new} = 0.693\,\frac{2\,(r_1-r_3)}{c}\sqrt{\frac{m\,c^2}{2\,(E_\alpha-E_0)}}\frac{1}{T_{new}} \quad (76)$$

The parameters a and r_m in potentials can be calculated. To calculate the parameter a, the following equation is used the equation: $U_1(r) = -U_0 + a\,r^2 + \frac{b}{r^2} = 0$. The roots of this equation are found as follow:

$$r_1' = \sqrt{\frac{U_0+\sqrt{U_0^2-4\,a\,b}}{2\,a}}\ ; \qquad r_3' = \sqrt{\frac{U_0-\sqrt{U_0^2-4\,a\,b}}{2\,a}}$$

As it can be seen in Figure6, the r_1' can be taken as sum of the radii of the nucleus and the alpha particle. That is, since the radius of the alpha particle is $R_\alpha = R_0\,4^{1/3}$ and the radius of the nucleus $R_N = R_0(A-4)^{1/3}$, the total radius is as follows:

$$R_c = R_\alpha + R_N = R_0\left[\,4^{1/3} + (A-4)^{1/3}\right]$$

Thus it can be taken as follows: $(r_1')^2 = R_c^2 = [U_0 + \sqrt{U_0^2 - 4\,a\,b}]/(2\,a)$. From this equation, the value of a is obtained as follows:

$$a = \frac{U_0}{R_c^2} - \frac{b}{R_c^4} = \frac{U_0\,R_c^2 - b}{R_c^4}.$$

To calculate the parameter r_m, the equation $U_1(r) = U_{22}(r)$ is used and the resolution of this equation gives:

$$r_m = \frac{2\,\sqrt[3]{3}\,a\,U_0 + \sqrt[3]{2}\,X}{6^{2/3}\,a\,X};\ X = \left[9\,a^2 c + \sqrt{3\,a^3(27\,a\,c^2 - 4\,U_0^3)}\right]^{2/3}$$

Therefore, the potential depends only on R_0 and U_0 parameters, which simplifies the numerical calculations.

iii. *Numerical calculations*

To calculate the transmission coefficient T, (or barrier penetration probability), Equations (72) and (73) have been used, and the half-life values, Equations (75) and (76) have been used. The experimental half-life values of the nuclei were taken from [15]. Calculations were made for twenty nuclei and the results are visible in Tables 9. In this table, the half-life values calculated from the new formula and WKB formula are compared with the experimental results. For R_0 parameter 1.22value has been taken.

Ref

15. Mughabghab, S. F.; Divadeenam, M.; Holden, N. E., Neutron Cross Sections 1/A, 1981, Academic Press.

Notes

Firstly, U_0 values were changed the interval $5-50$ MeV by step 0.001 until $t_{1/2}^{new}/t_{1/2}^{exp}$ value is between 0.999 and 1.001, and one U_{00} value was found. Secondly, U_0 values were changed between $(U_{00}-1)$ and $(U_{00}+1)$ by step 0.00001 until the values of $t_{1/2}^{new}/t_{1/2}^{exp}$ is equal to 1 or close to 1, and thus the best U_0 value was found. We have taken calculated values a and r_m parameters given Equations given above for every value of the U_0 parameters. The half-life values calculated from the new formula and WKB formula are compared with the experimental results. As seen in the table that $t_{1/2}^{new}$ values have better results than $t_{1/2}^{wkb}$ values. One can be seen that the new formula is more appropriate than classical formula (WKB). Table9 shows that the new formula gives very good results with the experiment.

In this table; first column is nucleus; second column is the experimental energy value of the alpha particle; third and fourth columns ($I_i^{\pi_i}$ and $I_f^{\pi_f}$) are the initial and final state spins (parity) of the nucleus, respectively. Fifth column (ℓ_α) is the orbital angular momentum of the alpha particle; sixth column is the experimental value of the half-life of the nucleus; the seventh column is the most value of the parameter U_0; eighth and ninth columns are the WKB and new values of the half-life of the nucleus, respectively; tenth and eleventh columns are the ratios of half-lives. In these tables: y year; d day; h hour; m minute; s second.

Table 9: Comparisonofthe experimental half-life values and the results calculated using the new and WKB formulas with the harmonic oscillator type well potential for the parameter $R_0 = 1.22$ fm.

$^{A}_{Z}X$	E_α(MeV)	$I_i^{\pi_i}$	$I_f^{\pi_f}$	ℓ_α	$t_{1/2}^{exp}$	U_0 (MeV)	$t_{1/2}^{wkb}$	$t_{1/2}^{new}$	$t_{1/2}^{wkb}/t_{1/2}^{exp}$	$t_{1/2}^{new}/t_{1/2}^{exp}$
$^{208}_{84}$Po	5.2155	0^+	0^+	0	2.898 y	16.1149	0.00163 y	2.898 y	0.00056	1
$^{210}_{84}$Po	5.4075	0^+	0^+	0	138.376 d	16.8183	0.05718 d	138.376 d	0.00041	1
$^{210}_{86}$Rn	6.1585	0^+	0^+	0	2.40 h	9.65884	0.00002 h	2.40 h	$7.8447*10^{-6}$	1
$^{212}_{86}$Rn	6.3850	0^+	0^+	0	23.9 m	10.6042	0.00022 m	23.9001 m	$9.26232*10^{-6}$	1
$^{218}_{86}$Rn	7.2630	0^+	0^+	0	0.035 s	6.73448	$3.06062*10^{-8}$ s	0.0350003 s	$8.74664*10^{-7}$	1.00001
$^{222}_{86}$Rn	5.5903	0^+	0^+	0	3.8235 d	6.4726	$6.39451*10^{-6}$ d	3.82352 d	$1.67242*10^{-6}$	1.00001
$^{222}_{88}$Ra	6.6810	0^+	0^+	0	38.00 s	6.70216	0.00003 s	38.0003 s	$6.72179*10^{-7}$	1.00001
$^{226}_{88}$Ra	4.8706	0^+	0^+	0	1600 y	8.20157	0.04662 y	1600 y	0.00003	1
$^{228}_{90}$Th	5.5201	0^+	0^+	0	1.9116 y	6.8677	$3.81955*10^{-6}$ y	1.91161 y	$1.99809*10^{-6}$	1.00001
$^{230}_{90}$Th	4.7700	0^+	0^+	0	75380 y	8.97807	5.33862 y	75380.3 y	0.00008	1
$^{232}_{90}$Th	4.0828	0^+	0^+	0	$1.405*10^{10}$ y	50.9229	$3.48334*10^{10}$ y	$1.405*10^{10}$ y	2.47924	1
$^{234}_{92}$U	4.8585	0^+	0^+	0	$2.455*10^{5}$ y	9.52352	19.4874 y	245501 y	0.00008	1
$^{236}_{92}$U	4.5720	0^+	0^+	0	$2.342*10^{7}$ y	11.8220	20371 y	$2.342*10^{7}$ y	0.00087	1
$^{238}_{94}$Pu	5.5932	0^+	0^+	0	87.7 y	7.92354	0.00029 y	87.7003 y	$3.29958*10^{-6}$	1
$^{240}_{94}$Pu	5.2558	0^+	0^+	0	6563 y	8.31556	0.06286 y	6563 y	$9.57858*10^{-6}$	1
$^{242}_{94}$Pu	4.9844	0^+	0^+	0	$3.733*10^{5}$ y	9.6180	19.9753 y	373301 y	0.00005	1
$^{246}_{96}$Cm	5.4748	0^+	0^+	0	4730 y	9.13514	0.04485 y	4730 y	$9.48227*10^{-6}$	1
$^{248}_{96}$Cm	5.1617	0^+	0^+	0	$3.40*10^{5}$ y	10.0730	13.9342 y	$3.40*10^{5}$ y	0.00004	1
$^{252}_{98}$Cf	6.2169	0^+	0^+	0	2.645 y	7.72806	$1.83639*10^{-6}$ y	2.645 y	$6.94287*10^{-7}$	1
$^{209}_{84}$Po	4.9792	$1/2^-$	$5/2^-$	2	102 y	25.4692	0.85586 y	102 y	0.00839	1
$^{211}_{84}$Po	7.5945	$9/2^+$	$1/2^-$	5	0.516 s	22.0306	0.00006 s	0.516001 s	0.00011	1
$^{212}_{85}$At	7.8289	1^-	5^+	5	0.314 s	23.7771	0.00003 s	0.314 s	0.00011	1

$^{229}_{90}$Th	5.1676	$5/2^+$	$1/2^+$	2	7340 y	30.8213	84.5910 y	7340 y	0.01152	1
$^{233}_{92}$U	4.9086	$5/2^+$	$5/2^+$	2	1.592*10^5 y	10.0846	16.2122 y	1.592*10^5 y	0.00010	1
$^{237}_{93}$Np	4.9591	$5/2^+$	$3/2^-$	1	2.144*10^6 y	36.7733	90440.2 y	2.144*10^6 y	0.04218	1
$^{239}_{94}$Pu	5.2445	$1/2^+$	$7/2^-$	3	24110 y	11.0755	1.65331 y	24110 y	0.00007	1
$^{241}_{95}$Am	5.6378	$5/2^-$	$5/2^+$	1	432.2 y	10.3320	0.00658 y	432.2 y	0.00002	1
$^{243}_{95}$Am	5.4381	$5/2^-$	$5/2^+$	1	7370 y	11.9873	0.44434 y	7370 y	0.00006	1
$^{247}_{97}$Bk	5.8890	$3/2^-$	$5/2^-$	2	1380 y	19.4567	0.41219 y	1380 y	0.00030	1
$^{251}_{98}$Cf	6.1758	$1/2^+$	$9/2^-$	5	898 y	29.3742	1.69578 y	898.001 y	0.00189	1

Here, the general transmission coefficient formula for a potential barrier with an arbitrary form has been easily calculated without making any approximation. In this calculation, a new formula that we developed for the solution of the radial SE has been used. The transmission coefficient obtained from the new method is given by the formula in Equation(73). In this formula, it could be difficult to calculate the integral $\int \sqrt{U_2(r)}\, dr$. If these calculations cannot be made analytically, they should then be performed by numerical methods.

In the application of the general transmission coefficient formula to the α-decay, threedimensional harmonic oscillator potential well has been used. The results have been given in the tables together with the experimental values. The tables also contain the "ratio" column for comparison. It can be seen in Table 9 that the ratios for taken all nuclei are equal or close to 1 (one). The deviations from 1 are within the experimental error. Hence, it is said that the results obtained from the new method are more realistic. In the WKB method, the wave functionsare sinusoidal outside the potential barrier. But they are not sinusoidal inside of the potential barrier and they are exponential functions. That is that the wave functions are sinusoidal while entering into the potential barrier, but are not sinusoidal in the potential barrier and they are become sinusoidal again after sorting from the barrier. So, the entering wave into the potential barrier is sinusoidal, is not sinusoidal in potential barrier, and after the potential barrier it becomes again sinusoidal. How appropriate is this event? Where as in new method, the wave functions are sinusoidal everywhere (before the potential barrier, inside the potential barrier and after the potential barrier), but they have different phases inside and outside of the potential barrier. Thus, the wave function has different phases inside and outside the potential barrier, but it advances everywhere as sinusoidal functions. It can also be said that it is more accurate and realistic. Besides, the WKB method gives approximately a wave function. In the new method, the wave function is exact because there is no approximation. That is why the theoretical calculated half-life values match better with the experimental values. From these, we conclude that the transmission coefficient given in Equation(73) is more correct and realistic. By using the new transmission coefficient and half-life formulas, the half-life values of nuclei can easily be calculated. The general transmission coefficient formula can be used for the other tunneling phenomenon such as the cold emission from the metals, tunneling diode, and Josephson joint, reactions in the sun, scanning tunneling microscope, quantum traps and such.

VIII. Scattering Theory

a) Calculation of the scattering amplitudes

Let us consider a spherical wave progressing at the direction of Ozaxis from left to right, and arriving to a central potential field, sitting at the origin of theOxyz coordinate system. When we consider scattering, we shall assume that the interaction between the scattering particle and the scatter can be represented by an effective central potential energy function U(r), where r is the relative radial variable. The effective potential U(r)can include attractive and repulsive parts. Such a central potential is schematically represented in Figure7. The total energy of the incoming particle beam is E and the incoming particle beam can be represented by the spherical wave. This progressive spherical wave progress from right to left and arrives to the point $r = r_1$in Figure7. We divide the potential region into four zones and examine the motion of particle beam into these four zones.

Zone I is the region before the effective potential from where free particle comes; zone II, III, and IV are the effective potential regions where the particle beam is affected. These regions may include attractive and repulsive potential segments. Zone IV is the region where the particle beam is not able to penetrate because the potential is infinite. So, the wave function is zero in this region. These are presented with four regions along with the central potentials in Figure 7.

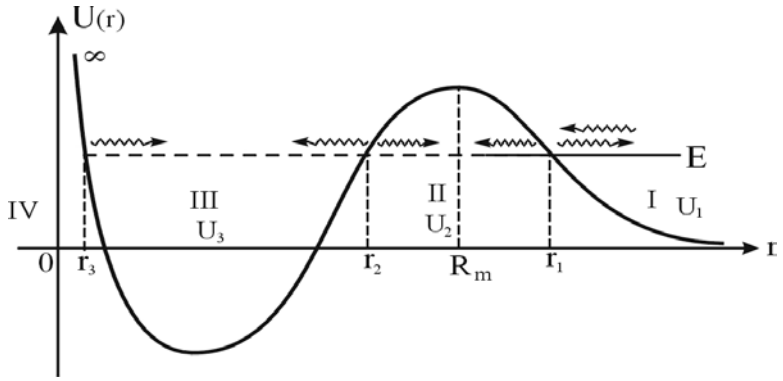


Figure 7: General schematic representation of scattering by central potential

We assume that $r = r_1$ and $r = r_2$at the interface between zone I and II, and zone II and III, respectively. The effective potential segments in the zones are represented as $U_1(r)$, $U_2(r)$ and $U_3(r)$ according to the zone numbers. The effective potential $U_4(r)$can be assumed infinite since the particle does not enter into this region. The central potential can be taken as zero at much far from the zone I so that the particle is free in that region and the effective potential is composed of only the centrifugal term due to the incoming particle angular momentum or spin. The Coulomb interaction potential should also be added to $U_1(r)$if that is available. The total energy of the incoming particle and the centrifugal term are always positive and the latter is less than the former. According to the functions given in Equations(52a)-(52f), the following functions are determined for the zones that are taken into account as follows:

In the zone I: $E > 0$, $U_1(r) > 0$ *and* $E > U_1(r)$; $k = i\, m_1\sqrt{E} = i\, K$; $(K = m_1\sqrt{E})$;

$$G_1(r) = i\, m_1 \int \sqrt{U_1(r)}\, dr = i\, Q_1(r); \left[m_1 = \sqrt{\frac{2\,m}{\hbar^2}}\ ,\ Q_1(r) = m_1 \int \sqrt{U_1(r)}\ dr\right].$$

In the zone II: $E > 0$, $U_2(r) > 0$ *and* $E < U_2(r)$, $k = m_1\sqrt{E} = K$;

$$G_2(r) = m_1 \int \sqrt{U_2(r)}\, dr = Q_2(r)\,; \left[k = m_1\sqrt{E} = K, \qquad m_1 = \sqrt{\frac{2\,m}{\hbar^2}}\right]$$

In the zone III, the conditions $E < 0$(This zone corresponds to the bound state. So, the negative energy should be taken), $U_3(r) < 0$ *and* $E > U_3(r)$leads to the expressions below:

$$k = i\, m_1\sqrt{E} = i\, m_1\sqrt{-|E|} = \pm K\,, \quad \left[K = m_1\sqrt{|E|}\right]$$

$$G_3(r) = i\, m_1 \int \sqrt{U_3(r)}\, dr = i\, m_1 \int \sqrt{-|U_3(r)|}\, dr = \pm\ Q_3(r)$$

The wave function in zone I should vanish at large distance. Under these circumstances, the radial wave functions in the three zones can be put in the forms below with regard to the general functions given in Equations(52a)-(52f):

$$F_1(r) = A_1 e^{i\,K\,r - Q_1(r)} + e^{-i\,K\,r - Q_0(r)}\ ; [B_1 = 1,\ Q_1(r) > 0,\ \ Q_0(r) > 0\ ] \quad (77a)$$

$$F_2(r) = A_2 e^{K\,r \pm i\,Q_2(r)} + B_2 e^{-K\,r \mp i\,Q_2(r)} \quad (77b)$$

$$F_3(r) = A_3 e^{-K\,r \pm i\,Q_3(r)} + B_3 e^{K\,r \mp i\,Q_3(r)} \quad (77c)$$

The wave function in zone IV vanishes since the effective potential in this region is infinite. Here, $Q_0(r)$ is the function resulting from the angular momentum of the incoming particle. This function $Q_0(r)$ can also be taken as zero because it does not have any contribution to the calculation of the scattering cross-section as it will be seen soon.

The potential in zone III can also be complex in some cases (usually called the optical potential). If $U_3(r)$ is the optical potential, it can be written as follows:

$$U_3(r) = |U_3(r)|e^{i\,\emptyset} = U_{31}(r) + i\,U_{32}(r) = \sqrt{U_{31}^2(r) + U_{32}^2(r)}e^{i\,\emptyset} \quad (78a)$$

Here, $\tan(\emptyset) = \frac{U_{32}(r)}{U_{31}(r)}$, $\emptyset = \arctan\left[\frac{U_{32}(r)}{U_{31}(r)}\right]$; $k = i\, m_1\sqrt{E} = i\, m_1\sqrt{-|E|} = K$, $\left[K = m_1\sqrt{|E|}\right]$;$G_3(r) = i\, m_1 \int \sqrt{U_3(r)}\, dr = i\, m_1 \int \sqrt{-|U_3(r)|}\, dr = \pm\ Q_3(r)$

$$Q_3(r) = \int \sqrt{|U_3(r)|}\, dr = m_1 \int \sqrt{\sqrt{U_{31}^2(r) + U_{32}^2(r)}}\ dr$$

$$Q_3(r) = m_1 \int \sqrt[4]{U_{31}^2(r) + U_{32}^2(r)}\, dr \quad (78b)$$

In Equations(77a) - (78b), the functions $Q_p(r)$ can also be written briefly as follows:

$$Q_p(r) = m_1 \int \sqrt{|U_p(r)|}\, dr\,, \quad [p = 0, 1, 2, 3]$$

The terms containing A_1 and B_1 in the functions in Equations(77a)-(77c) give outgoing and incoming waves, respectively. We assume that the amplitude of incoming

wave at the boundary of zone I and II is constant. The second (77b) and the third (77c) functions represent the states of the wave in the effective region of the potential. Applying the continuity conditions on $F_p(r_j)$ and $F_p'(r_j)$, $[p, j = 1, 2, 3]$ functions, the coefficients A_i and B_i in Equations(77a)-(77c) can be determined. These conditions at the boundary points of the three zones can be written in the following form:

Notes

$$F_1(r_1) = F_2(r_1)\ ;\quad F_1'(r_1) = F_2'(r_1);\ F_2(r_2) = F_3(r_2)\ ;\quad F_2'(r_2) = F_3'(r_2) \tag{79}$$

$$F_3(r_3) + \frac{F_3'(r_3)}{K} = 0\ ;\ Q_p'(r_j) = K\ ,\qquad (p, j = 1,2,3)$$

The coefficients A_1, A_2, B_2, A_3, B_3 in the functions given in Equations(77a)-(77c) can be found by solving five linear equations, which can be obtained by using the conditions given in Equation(79) for each of the functions given in Equations(77a)-(77c).The essential coefficient for the scattering cross section is A_1, as described below. Therefore, there is no need to give other coefficients here. TheA_1coefficient, which isobtained from four equations, is computed by taking into account the lower and upper signs in the exponential expressions in Equation(79) as follows:

i. *The A_1 coefficient found using the lower signs*

$$A_1 = \frac{1}{2}(1+i)e^{-2\,i\,K\,r_1 - Q_0(r_1) + Q_1(r_1)}\left\{-1 + (2-i)e^{[2\,K\,(r_3 - r_1) + 2\,i\,[Q_2(r_1) - Q_2(r_2) + Q_3(r_2) - Q_3(r_3)]}\right\} \tag{80a}$$

ii. *The A_1 coefficient, found using the upper signs*

$$A_1 = \frac{(1+i)e^{2(1-i)K\,r_1 - Q_0(r_1) + Q_1(r_1) + 2\,i\,[Q_2(r_1) + Q_3(r_2)]}}{(2+i)e^{[2\,K\,r_3 + 2\,i\,[Q_2(r_2) + Q_3(r_3)]} - e^{[2\,K\,r_1 + 2\,i\,[Q_2(r_1) + Q_3(r_2)]}} \tag{80b}$$

The terms with A_1in the functions given in Equations (77a)-(77c) representing the outgoing wave from the center of potential, includes both the scattered by the potential and the incoming wave. Therefore, we must subtract away the latter to find the amplitude of only the scattered wave. Thus, we obtain the scattering amplitude and radial wave function representing the scattered wave as follows:

$$C_s(r_1) = A_1 e^{-Q_1(r_1)} - e^{-Q_0(r_1)}\ ,\ \text{(scattering amplitude)} \tag{81a}$$

$$R_s(r) = \frac{F_s(r)}{r} = C_s(r_1)\frac{e^{i\,K\,r}}{r} = \left[A_1 e^{-Q_1(r_1)} - e^{-Q_0(r_1)}\right]\frac{e^{i\,K\,r}}{r} \tag{81b}$$

Equations(81a) and (81b) represent the elastic scattering wave by the potential.

b) Calculation of particle currents

i. *Calculation of the scattered particle current*

Using Equation(81b) and the equation $J_s(r) = \frac{\hbar}{2\,m\,i}\left[R_s^*(r)\frac{dR_s(r)}{dr} - R_s(r)\frac{dR_s^*(r)}{dr}\right]$, the current of scattered particles per unit area at $r = r_1$pointcan be found as follows:

$$J_s(r_1) = \frac{1}{r_1^2}\frac{\hbar K}{m}|C_s(r_1)|^2 \tag{82}$$

ii. *Calculation of incoming particle current*

The radial wave function of the incoming beam, passing through zone I and toward zone II, can be written as:

$$R_g(r) = \frac{F_g(r)}{r} = \frac{1}{r} e^{-i\,K\,r - Q_0(r_1)} = C_g(r_1)\frac{e^{-i\,K\,r}}{r}\ ,\ \left[C_g(r_1) = e^{-Q_0(r_1)}\right].$$

Here, $C_g(r_1) = e^{-Q_0(r_1)}$ represents the amplitude of the incoming wave. The incident current per unite area at $r = r_1$point can be obtained in the way that is applied to the current equation:

$$J_g(r_1) = \frac{1}{r_1^2}\frac{\hbar K}{m}|C_g(r_1)|^2 = \frac{1}{r_1^2}\frac{\hbar K}{m} e^{-2\,Q_0(r_1)} \tag{83}$$

c) Calculations of scattering cross-sections

i. *Calculation of elastic scattering differential cross-section*

The probability per unit differential surface of a sphere of radius r_1, that an incident particle is scattered into the differential surface area on the sphere of radius r_1 , $dS = r_1^2\, d\Omega$, $[d\Omega = \sin(\theta)\, d\theta\, d\phi\,]$ is expressed as the ratio of the scattered current to the incident current, that is:

$$\frac{d\sigma_s}{dS} = \frac{d\sigma_s}{r_1^2 d\Omega} = \frac{J_s(r_1)}{J_g(r_1)} \quad \rightarrow \quad \frac{d\sigma_s}{d\Omega} = \frac{J_s(r_1)}{J_g(r_1)} r_1^2 \tag{84}$$

The differential elastic cross-section can be expressed in a simple form by putting Equations(82) and (83) into Equation(84) as follows:

$$\frac{d\sigma_s}{d\Omega} = \frac{C_s(r_1)C_s^*(r_1)}{C_g(r_1)C_g^*(r_1)} r_1^2 = \frac{|C_s(r_1)|^2}{|C_g(r_1)|^2} r_1^2 \tag{85}$$

Since the scattering is azimuthally symmetrical, the angle ϕ can be integrated out so that the expression given in Equations(84) and (85) can be written as follows:

$$\frac{d\sigma_s}{d\theta} = 2\,\pi\,\frac{J_s(r_1)}{J_g(r_1)} r_1^2 \sin(\theta) = 2\,\pi \frac{|C_s(r_1)|^2}{|C_g(r_1)|^2} r_1^2 \sin(\theta) \tag{86}$$

The expressions (86) show the elastic scattering differential cross sections in the angle$d\theta$ which is usually measured experimentally.

ii. *Calculation of differential inelastic or reaction (no-elastic) cross-section*

Differential reaction (capture of particle, emission of particle, inelastic collision…) cross- section per the solid angle can be found through the difference between the incoming current and the outgoing current divided by the former. By analogy with Equation(86), the differential reaction cross-section can be expressed as follows:

$$\frac{d\sigma_r}{d\theta} = 2\,\pi\,\frac{[J_g(r_1) - J_s(r_1)]}{J_g(r_1)} r_1^2 \sin(\theta) = 2\,\pi \frac{[|C_g(r_1)|^2 - |C_s(r_1)|^2]}{|C_g(r_1)|^2} r_1^2 \sin(\theta) \tag{87}$$

iii. *Calculation of total cross sections*

The total elastic scattering cross section is the total probability to be elastic scattered in any direction and it can be determined through the integral of differential cross-section given in Equation(85) as follows:

$$\sigma_s = \int d\sigma_s = \int \frac{d\sigma_s}{d\Omega} d\Omega = \iint \frac{J_s(r_1)}{J_g(r_1)} r_1^2 \sin(\theta)\, d\,\theta\, d\phi$$

$$\sigma_s = 4\,\pi\, r_1^2 \frac{J_s(r_1)}{J_g(r_1)} = 4\,\pi\, r_1^2 \frac{|C_s(r_1)|^2}{|C_g(r_1)|^2} \tag{88}$$

By analogy with Equation(88), the total reaction cross-section can be expressed as follows:

$$\sigma_r = 4\,\pi\,r_1^2\,\frac{[J_g(r_1)-J_s(r_1)]}{J_g(r_1)} = 4\,\pi\,r_1^2 - \sigma_s \tag{89}$$

In Equation(89), it is seen that if$J_s(r_1) = J_g(r_1)$, then $\sigma_r = 0$, full-elastic scattering; if $J_s(r_1) > J_g(r_1)$, then $\sigma_r < 0$, it is taken out of the particle from the target (emission of particle from target) and if $J_s(r_1) < J_g(r_1)$, then $\sigma_r > 0$,it is captured (absorbed) the particle by the target. The total scattering cross-section, including all process [elastic plus reaction (all of no-elastic events)]:

$$\sigma_t = \sigma_s + \sigma_r = 4\,\pi\,r_1^2\,\frac{J_s(r_1)}{J_g(r_1)} + 4\,\pi\,r_1^2\,\frac{[J_g(r_1)-J_s(r_1)]}{J_g(r_1)} = 4\,\pi\,r_1^2 \tag{90}$$

Then the cross-sections σ_s , σ_r , σ_t can be expressed through theA_1 coefficients given in Equations(80a) and(80b).

σ_s elastic scattering cross-section found using the coefficient (80a) is as follows:

$$X_1 = 3\,e^{4\,Kr_1} + 5\,e^{4\,Kr_3} + 2\,e^{4\,Kr_1}[\cos(2\,K\,r_1) + \sin(2\,K\,r_1)]$$

$$X_2 = -2\,e^{2\,K\,(r_1+r_3)}[3\cos\big(2(Kr_1 - Y)\big) + 2\cos(2\,Y) + \sin\big(2(Kr_1 - Y)\big) + \sin(2\,Y)]$$

$$\frac{\sigma_s}{4\,\pi\,r_1^2} = \frac{1}{2}e^{-4\,K\,r_1}\{X_1 + X_2\} \tag{91a}$$

σ_s elastic scattering cross-section found using the coefficient (80b)is as follows:

$$P_1 = 3\,e^{4\,K\,r_1} + 5\,e^{4\,K\,r_3} + 2\,e^{4\,K\,r_1}[\cos(2Kr_1) + \sin\,(2Kr_1)]$$

$$P_2 = -2\,e^{2\,K(\,r_1+r_3)}[3\,\cos(2Kr_1 - 2\,Y) + 2\,\cos(2\,Y) + \sin(2Kr_1 - 2\,Y) + \sin\,(2Y)]$$

$$P_3 = e^{4\,K\,r_1} + 5\,e^{4\,K\,r_3} - 2\,e^{2\,K(r_1+r_3)}[2\,\cos(2Y) + \sin\,(2Y)]$$

$$\frac{\sigma_s}{4\,\pi\,r_1^2} = \frac{P_1+P_2}{P_3} \tag{91b}$$

In both cases, the reaction and total scattering cross-section σ_r and σ_t are as follows:

$$\frac{\sigma_r}{4\,\pi\,r_1^2} = 1 - \frac{\sigma_s}{4\,\pi\,r_1^2} \text{ and } \frac{\sigma_t}{4\,\pi\,r_1^2} = \frac{\sigma_s}{4\,\pi\,r_1^2} + \frac{\sigma_r}{4\,\pi\,r_1^2} = 1 \text{ or} \sigma_t = 4\,\pi\,r_1^2 \tag{91c}$$

In these expressions, Y is given by the following equation:

$$Y = Q_2(r_1) - Q_2(r_2) + Q_3(r_2) - Q_3(r_3) = m_1\int_{r_2}^{r_1}\sqrt{|U_2(r)|}\,dr + m_1\int_{r_3}^{r_2}\sqrt{|U_3(r)|}\,dr \tag{91d}$$

The integrals in Equation(91d) can be solved numerically if the functions$Q_2(r)$ and $Q_3(r)$cannot be calculated analytically. It can be seen from these formulas given in Equations(91a)-(91d) that the scattering cross-sections (σ_s and σ_r) depend on the total energy E [with K(E)], Y integral and the effective radius r_1 , r_2 , $r_3$of the scatter potential, separately, but total scattering cross-section $\sigma_t = \sigma_s + \sigma_r$ only depends on the parameter r_1, so the energy E .Here, $r_1$can be considered as impact or collision parameter, classically.

d) Examples of the calculation of scattering cross-section

i. *Model potentials, wave functions and their ingredients*

To calculate a scattering cross-section, a model potential should be considered. Here as an example, we consider the Wood-Saxon shape potential plus the spin-orbit, centrifugal and Coulomb potentials. The potential zones are defined in Figure7 and shown in Figure8 for these model potentials. Wood-Saxon potential depends on three parameters,(V_0, a_c, R_c). The calculations have been thus performed with these potentials. The scattering affects only relative motion. In the center of mass reference frame (CM), the scattering cross-section of the incoming (incident or projectile) particle $\sigma(\Omega)$ depends on the energy $E_r = M_t E_L/(M_p + M_t)$, where M_p and M_t respectively mass of incident (projectile) and target particles; E_L, Laboratory;and E_r, relative energies.The boundary values of the potential zones taken in the calculations: the maximum potential energy occurs at the distance$r_2 = R_m = R_0(A_p^{1/3} + A_t^{1/3})$, the addition of the projectile (incident particle) radius to the target radius provided that they are spherical, where A_p and $A_t$are the mass number of the projectile and the target, respectively. The zones and r_k, $(k = 1,2,3)$ values are shown in Figure8. The effective potential energy is as follows:

$$U(r) = V_{ws}(r) + V_{LSJ}(r) + V_S(r) + V_c(r) \tag{92}$$

$$V_{ws}(r) = -\frac{V_0}{1+\mathrm{Exp}\,[(r-R_c)/a_c]}, \text{ Wood-Saxon potential}$$

$$V_{LSJ}(r) = -\frac{\hbar^2}{2\,M_i^2 c^2}\frac{1}{r}\frac{dV_{ws}(r)}{dr} <\vec{L}.\vec{S}>, \text{ spin-orbit potential}$$

$$<\vec{L}.\vec{S}> = \frac{1}{2}[J(J+1) - L(L+1) - S(S+1)]$$

$$V_S(r) = \frac{b}{r^2}\ ;\ [\,b = \frac{\hbar^2 L\,(L+1)}{2\,M_i}\,], \text{ (centrifugal potential),}$$

$$V_c(r) = \frac{C_c}{r}\ ,\ [C_c = (Z_p e)(Z_t e) = Z_p Z_t e^2], \text{ (potential energy of Coulomb)}$$

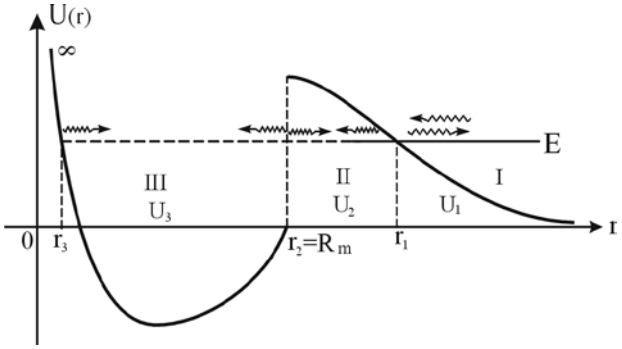


Figure 8: Effective Wood-Saxon potential and Coulomb potential zones used in the calculations

Here, $[L, S, J]$ are the relative orbital, spin and total angular momentum quantum numbers between the target and projectile, respectively. M_i is the reduced mass of the target and projectile. $R_c = R_0 A_t^{1/3}$, (R_0 is parameter). If

$r_{sc} = [C_c + \sqrt{C_c^2 + 4\,b\,E_r}\,]/[2\,E_r]$ is the positive root of the following equation: $E_r = \frac{b}{r^2} + \frac{C_c}{r} = V_s(r) + V_c(r)$ and $r_2 = R_m$, then we get $r_1 = r_2 + r_{sc} = r_2 + \left[C_c + \sqrt{C_c^2 + 4\,b\,E_r}\right]/[2\,E_r]$. Z_p and Z_t are the charge numbers of the projectile and the target, respectively. The r_3 value is determined by equalizing $V_s(r)$ to E_r. Consequently, (r_3, r_2, r_1) values are obtained as follows:

$$r_3 = \sqrt{b/E_r}; r_2 = R_m = R_0\left(A_p^{\frac{1}{3}} + A_t^{\frac{1}{3}}\right)\ ; r_1 = r_2 + \frac{C_c + \sqrt{C_c^2 + 4\,b\,E_r}}{2\,E_r}$$

The wave functions for zones 1-3 used in the calculation can be expressed in the following ways, respectively:

$$Q_0(r) = m_\hbar \int \sqrt{\frac{\hbar^2 L_0(L_0+1)}{2\,M_i\,r^2}}\ dr = \sqrt{L_0(L_0+1)}\,\ln(r)$$

$$Q_1(r) = m_\hbar \int \sqrt{\frac{C_c}{r} + \frac{b}{r^2}}\ dr = 2\,m_\hbar \left\{\sqrt{b + C_c\,r} - \sqrt{b}\ \operatorname{arctanh}\left[\sqrt{\frac{b + C_c\,r}{b}}\right]\right\}$$

$$Q_2(r) = m_\hbar \int \sqrt{\frac{C_c}{r} + \frac{b}{r^2}}\ dr = 2\,m_\hbar \left\{\sqrt{b + C_c\,r} - \sqrt{b}\ \operatorname{arctanh}\left[\sqrt{\frac{b + C_c\,r}{b}}\right]\right\}$$

$$Q_3(r) = m_\hbar \int \sqrt{|U_3(r)|}\ dr = m_\hbar \int \sqrt{|V_{ws}(r) + V_{LSJ}(r) + V_S(r)|}\ dr \qquad (93)$$

Here, $m_\hbar = \sqrt{2M_i}/\hbar$ and L_0 is the angular momentum of the incident particle.

It is seen from Equation(91c)that even though σ_s and $\sigma_r$have changed with the parameters V_0 and a_c; $\sigma_t = \sigma_s + \sigma_r$ has not changed for a certain value of R_0. In other words, the total cross-section does not depend on the parameters V_0 and a_c, and therefore, does not also depend on the potential. So, R_0 parameter can be obtained from the solution of the equation $4\pi r_1^2 = \sigma_t^{exp}$ as follows (σ_t^{exp} is experimental total cross-section):

$$R_0 = \frac{-\sqrt{\pi}\,10\left[C_c + \sqrt{C_c^2 + 4\,b\,E_r}\right] + E_r\sqrt{10\,\sigma_t^{exp}}}{20\,E_r\sqrt{\pi}\left[\sqrt[3]{A_p} + \sqrt[3]{A_t}\right]} \qquad (94)$$

To calculate σ_s and $\sigma_r$separately, the parameter V_0 in the range 20-60 by step 0.0001 and a_c in the range 0.40-0.60 by step 0.01 have been changed in the potential until $\sigma_r^{cal} > 0$ and round $[\sigma_r^{exp}]$ =round $[\sigma_r^{cal}]$ and floor $[\sigma_r^{exp}]$ = floor $[\sigma_r^{cal}]$″, during the calculations. So, rough V_0 and a_c values have been found. Then, with these approximate values, $\{\sigma_s^{exp} = \sigma_s^{cal}$ and $\sigma_r^{exp} = \sigma_r^{cal}\}$ system of equations hasbeen solved and the exact values of parameters V_0 and $a_c$have been found. With these V_0 and a_c parameters, the exact σ_s and $\sigma_r$have been recalculated. We have taken in the calculations the following values:

$e^2 = 1.439976$ MeV fm ; $M_u = 931.502$ MeV $/c^2; \hbar\,c = 197.329$ MeV fm .

ii. *Thermal neutron cross-sections*

For example, thermal neutron ($E_L = 0.025$ eV) scattering cross-sections for some targets have been calculated and compared with the measured values. In calculation, even nuclei have been taken as targets because of their angular momentums are zero. So, the relative angular momentums are those of the projectile, they are $L = 0$, $S = 1/2$, $J = 1/2$ for neutron. For the calculations of σ_s, σ_r and σ_t, the formulas given in Equation(84) which has been obtained by the lower sign functions. The results are compared with the measured total cross-sections in Table 10. The experimental values have been taken from [15]. It is seen that agreements are fairly good as seen in Table 10. In this table, first column: target; the second column: from top to down(R_0, V_0, a_c) parameters, respectively; the third column: from top to down(R_c, $R_m = r_2$, r_1), respectively; the fourth column: cross-sections; the fifth column: values of calculation; and the sixth column: values of experiment.

Table 10: [n (0 , 1) + Xn (Z , N)] Thermal neutron cross-section comparisons with those measured

Target**Xn (Z, N)**	**R_0 V_0 a_c**	**R_c R_m r_1**	Cross-sections(**mb**)	Calculations(**mb**)	Experiment(**mb**)
H (1,2)	2.29845	2.89586	$\sigma_s \rightarrow$	3390	3390±12
	21.3275	5.19431	$\sigma_r \rightarrow$	0.519	0.519±0.007
	0.40	5.19431	$\sigma_t \rightarrow$	3390.52	3390.52
C (6,12)	1.86896	4.27885	$\sigma_s \rightarrow$	4746	4746±2
	35.2934	6.14781	$\sigma_r \rightarrow$	3.53	3.53±0.07
	0.40	6.14781	$\sigma_t \rightarrow$	4749.53	4749.53
O (8,16)	1.5543	3.91659	$\sigma_s \rightarrow$	3761	3761±6
	41.2421	5.47089	$\sigma_r \rightarrow$	0.190	0.190±0.019
	0.40	5.47089	$\sigma_t \rightarrow$	3761.19	3761.19
Si (14,28)	1.02922	3.12533	$\sigma_s \rightarrow$	1992	1992±6
	21.3192	4.15456	$\sigma_r \rightarrow$	177	177±5
	0.40	4.15456	$\sigma_t \rightarrow$	2169	2169
Ca (20,40)	1.1803	4.03655	$\sigma_s \rightarrow$	3010	3010±8
	39.0960	5.21685	$\sigma_r \rightarrow$	410	410±20
	0.40	5.21685	$\sigma_t \rightarrow$	3420	3420

iii. ^3_2He *Cross-sections on some targetsin the intermediate energy*

The cross-sectionsσ_t at three different energies of$^3_2$Hehave been calculated for 5 different targets[$^9_4$Be, $^{12}_6$C, $^{16}_8$O, $^{28}_{14}$Si, $^{40}_{20}$Ca]. The calculated cross-sections have been compared with those measured taken from [15, 16]. The comparisons are made in the way that is described above and given in Table 11. In this table: Xn [Z, N] target; E_L laboratory energy of projectile; σ_t^{cal} calculated total cross-section; σ_t^{exp} experimental measured total cross-section. There is no need for relative angular momentums here.

Ref

15. Mughabghab, S. F.; Divadeenam, M.; Holden, N. E., Neutron Cross Sections 1/A, 1981, Academic Press.

Table 11: [He [2 , 3] + Xn [Z , N] Total cross-section comparison with those measured

Xn [Z, N]	E_L(MeV)	R_0(fm)	R_c(fm)	R_m(fm)	r_1 (fm)	σ_t^{cal} (mb)	σ_t^{exp}(mb)
Be[4,9]	96.4	0.673279	1.40048	2.37051	2.53101	805	805±30
	137.8	0.623868	1.29770	2.19747	2.30905	670	670±30
	167.3	0.607056	1.26273	2.13825	2.23016	625	625±30
C[6,12]	96.4	0.620244	1.42000	2.31455	2.53885	810	810±40
	137.8	0.594922	1.36203	2.22006	2.37697	710	710±30
	167.3	0.572480	1.31065	2.13631	2.26556	645	645±35
O[8,16]	96.4	0.631332	1.59086	2.50140	2.78546	975	975±35
	137.8	0.606261	1.52768	2.40206	2.60079	850	850±50
	167.3	0.595506	1.50058	2.35945	2.52313	800	800±25
Si[14,28]	96.4	0.600731	1.82417	2.69058	3.15392	1250	1250±65
	137.8	0.603057	1.83124	2.70099	3.02513	1150	1150±70
	167.3	0.590377	1.79273	2.64420	2.91119	1065	1065±40
Ca[20,40]	96.4	0.544438	1.86195	2.64717	3.28976	1360	1360±90
	137.8	0.563942	1.92866	2.74200	3.19154	1280	1280±85
	167.3	0.565988	1.93565	2.75195	3.12222	1225	1225±75

The calculation of cross sections through solution of radial SE (RSE) by the partial wave expansion is very difficult. In many cases, some approximations are needed for these kinds of solutions. In the present study, firstly, differential elastic scattering, inelastic (or reaction) scattering and total cross-sections have been calculated without using any approximation. These calculations have been performed using a simple method, improved for the solution of RSE, for an incident particle being in a central field of any form. We have obtained the general formulas of the scattering amplitudes and elastic, inelastic (no-elastic) and total scattering cross-sections. Secondly, we have made some applications. In these applications, the potentials have been assumed to have Saxon-Woods shape plus spin-orbit interaction, centrifugal and Coulomb potentials. These potentials are very complex potentials. Calculations with these are not easy. However, it is very easy to make calculations with our method. With these potentials, first, for the thermal neutrons; the elastic, inelastic (neutron radiative capture), and total scattering cross-sections of different targets have been calculated. Then, total scattering cross-sections for $^3_2$He particles of three different energies on 5 targets have been calculated. The calculated results have been compared with experimental results. The results calculated have given satisfactory agreement with the available experimental results. More cross section calculations can be found in [17].

The calculations have also shown that the total cross-sections depend on the mean potential range. Thus, it is also proved that the total cross-sections can be calculated easily using even very complex potentials. The same calculations have also been performed using optical potentials, but the results have not been included here due

Ref

17. Erbil, H. H.; Selvi, A. S.; Kunduracl, T., IREPHY, 2013, 7, 230-238.

to getting the same scattering distance and cross-sections. The use of two parameters is seen to be enough in the agreement of the calculated results with the measured results, whereas this agreement is ensured using more parameters in the partial wave expansion method.

IX. Conclusion and Some Explanations

We have found a simple procedure for the general solution of the time-independent SE in one dimension without using any infinite series or other approximations. The wave functions, which are always periodic in the bound states, are given in Equations(52a)-(57). In our procedure of solution, there are two difficulties: one is to solve the equation $E = U(x)$ to find the energy; and the other is to integrate $\sqrt{U(x)}$, namely, to calculate $\int \sqrt{U(x)}\, dx$ to find the exact normalized wave function.If these calculations cannot be done analytically, then it should be done by numerical methods. To find the energy values, there is no need to calculate this integral, it is sufficient to find the classical turning points by solving the equation $E = U(x)$. Thus, there is no need to know the wave functions to find the energy values of the states; it is enough to know only the potential energy function.The SE has been solved for a particle in many potential wells and found their total energies and normalized wave functions were calculated as examples.

Using this simple procedure, the solution of the radial SE for spherically symmetric potentials without using any infinite series has been achieved in this study. The wave functions which are always periodicals are given in Equations(52a)-(57). By using this procedure, the radial SE has been solved for a particle found in many spherically symmetric central potential wells and two different solutions have been found. One of them is symmetric function and the other is anti symmetric function. From these expressions, it is observed that these functions are periodic and they are similar to each other in form for all potential wells. This simple solution was applied to relativistic, scattering and tunneling theories and it yielded good results.

The solution that we propose is a general solution. The points of view supporting the method we presented here is more realistic which are as follows:

As it is known, the SE is a second order differential equation with variable coefficients. The solutions of such equations are based generally on series method and special functions (Hermit, Bessel ...) in quantum physics. In the expanding of power series, the consecutive relations between the coefficients of the series are found. Some approaches are taken to make the series convergent and by using them, the energy values and the wave functions are determined. In all of these solutions, one or more approximations are used. Some other methods such as perturbation, WKB, variation, etc. are also applied for solving the SE and approximate solutions are obtained. However, the solution that is proposed here is neither based on series methods nor special functions, and no approximation is used. We think that these solutions, which do not have any approach, are more realistic.

It is seen that the functions found with the known methods and with the present method are different in form. However, when we do numerical calculations, the results are not very different from each other and are consistent with their well-known values. For example the one dimensional harmonic oscillator, our result and the result obtained by the known methods are very close to each other, but they are not exactly same.

The SE, the fundamental equation of the quantum mechanics, is also known as the Schrödinger wave equation. In physics, the harmonic waves are represented with

Notes

periodic functions e.g. sin and cos. However, most of the known solutions of the SE are in the form of polynomials. Especially the solution of the harmonic oscillator should be periodic function. However, the known solution is polynomial. As it is seen in the functions given in Equations(5.1.3) and (5.1.4),our solution gives sin and cos functions, which makes it more realistic.

It is said that the quantum mechanics includes classical mechanics. Hence, the results of the classical mechanics should be obtained from the results found in quantum mechanics. As it is seen from the functions given in Equation(5.1.4), it is very difficult to obtain sin and cos functions from polynomials. However, the classical solutions could be easily obtained if $\Psi(x)$is taken very small in the functions given in Equation (5.1.3).

In quantum mechanics textbooks, it is said that all infinitely high potential wells are similar to each other. But when we look at their solutions, we see that all of the solutions are different in form; whereas our solutions are similar to each other in form for all such potential wells.

In the quantum mechanics, if there is no exact solution, sometimes, the variation principle is used to find the ground state energy. The calculations of variation are made with a trial function, and it is seen that the results are not very dependent on the trial function. However, the wave functions are not necessary to find the ground or excited state energy in our solutions. It is sufficient to know the classical turning points of the potential function.

Special conditions are not required in order to find energy values and the wave functions. The continuity of the wave functions and their derivatives at the classical turning points are enough.

The application of our procedure is very easy. Most of the problems that could not be solved analytically with the known methods can easily be solved using our procedure. A complete solution of the SE used in all branches of physics has been made. A problem that has been worked onby many theoretical physicists has easily been solved. We think that this solution is very useful and helpful for those physicists interested in quantum mechanics and applications.

Acknowledgements

I would like to express my sincere gratitude to my wife Özel and my daughters Işıl and Beril for their support and patience during my study and for their help in editing.

References

1. Erbil, H. H., Turkish Journal of Physics, 42, 2018, 527-572.
2. Erbil, H. H.;IREPHY Vol.1, 2007, N.4, 197-213.
3. Greiner, W., Quantum Mechanics, 1993, Springer-Verlag.
4. Cooper, F.; Khare, A., Sukhatme, U., Supersymmetry in Quantum Mechanics, 2001, World Scientific.
5. Erbil, H. H., IREPHY Vol.2, 2008, 1, 1-10.
6. Pal, M. K., The Theory of Nuclear Structure, 1983, Scientific and Academic Editions.
7. Erbil, H. H,; Kunduracı, T., IREPHY, 2012, 6, 269-278.
8. Erbil, H. H., IREPHY,2012, 6, 439-447.
9. Erbil, H. H., IREPHY,2012, 6, 144-152.
10. Erbil, H. H,; Ertik. H,; Şirin, H.; Kunduracı, T., IREPHY, 2012, 6 , 359-366.

11. Volya, A.; https://nucracker.volya.net/index.php?p=ws˙fft.
12. Messiah, A., Quantum Mechanics, 1958, North Holland.
13. Schwabl, F., Quantum Mechanics, 1995,Springer.
14. Krane, K. S., Introductory Nuclear Physics, 1988, John-Wiley & Sons.
15. Mughabghab, S. F.; Divadeenam, M.; Holden, N. E., Neutron Cross Sections 1/A, 1981, Academic Press.
16. Avrigeanu, M.; Von Oertzen W.; Fischer, U. ; Avrigeanu, V., Nuclear Physics A 2005, 759,327.
17. Erbil, H. H.; Selvi, A. S.; Kunduracı, T., IREPHY, 2013, 7, 230-238.
18. Chu, S. Y. F. ; Exström, L. P.; Firastone, R. B., The Lund/LBNL, Nuclear Data Search, Nucleardata. nuclear.lu.se/toi/index.asp, Summary drawings for A=1-277.
19. Erbil, H. H., IREPHY,2013, 7,376-384.
20. Erbil, H. H.;IREPHY Vol.1, 2007, N.4, 197-213.
21. Erbil, H. H., KuantumFiziği, 2001, Ege University.

Notes