Research Article

Oscillations through a barrier tunneling potential for a particle in a central potential (double potential well)

Abstract

In some molecules such as ammonia, double vibrations are observed at small energies. These small vibrations are thought to arise from double well potentials. To explain these small energy gaps, double potential wells are investigated, and complex calculations are made. Until recently, since the exact solution of the Schrödinger equation was not known, approximate solutions were always obtained. The exact solution of the Schrödinger equation is now known. In previous studies, a simple procedure for the general solution of the radial Schrödinger Equation has been found for spherical symmetric potentials without making any approximation. In this article, the Schrodinger equation was solved with this new solution method. It has been applied to the oscillations through a barrier tunneling potential for a particle in a central quadratic deformed potential well (double potential well). It is seen that there is no need to look for complex potentials to explain the double wells observed in small vibrations in ammonia and similar molecules, they were compared with experimentally measured energies. The results were found to be fully compatible. It has been seen that there can always be double well potentials at small energies for all molecules, atomic nuclei, and similar particles with angular momentum other than zero.

Keywords: central potentials, radial equation, spherical symmetric potential, oscillations through a barrier tunneling, double potential well, small vibrations

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Introduction

Although the radial Schrödinger Equation (SE) for some simple spherical symmetric potential is solved, an exact solution is not possible in complicated situations, and it must be then resorted to approximation methods. For the calculation of stationary states and energy eigenvalues, these methods include perturbation theory, the variational method and the WKB approximation. Perturbation theory is applicable if the Hamiltonian differs from an exactly solvable part by a small amount. The variational method gives a good estimate of the ground state energy if one has a qualitative idea of the form of the wave function and the WKB method is applicable in the nearly classical limit. In one of the previous studies, it has been achieved a simple method for the exact general solution of the radial SE for spherically symmetric potential well of any form without making any approximation. This simple solution method has been applied to many spherical symmetric potential.[1,2] In this study, we have applied this simple method to solve the oscillations through a barrier of potential (double potential well). It was applied to the ammonia molecule, and it was seen that the values calculated with experimental measurements agreed very well. It is seen that there is no need to look for complex potentials to explain the double wells observed in small vibrations in ammonia and similar molecules, and that there will be double wells in small vibrations in all molecules, atomic nuclei, and similar particles with non-zero angular momentum.

Radial Schrodinger equations for spherical symmetric potentials and their solution (general solution)

The SE in three dimensions is given as follows:

$$\Delta \psi(\vec{r}) + \frac{2m}{\hbar^2}\left[E - V(\vec{r})\right]\psi(\vec{r}) = 0 \tag{1}$$

Where, E and V are the total and potential energies, respectively, m is the mass or reduced mass of particle. The spherical polar coordinates (r, θ, ϕ) are given as follows:

$$X = r\sin(\theta)\cos(\phi), \ y = r\sin(\theta)\sin(\phi), \ z = r\cos(\theta)$$

These coordinates appropriate for the symmetry of the problem. The Equation (1), expressed in these coordinates, is as follows:

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right]\psi(r,\theta,\phi) + \frac{1}{r^2}\widehat{\mathscr{L}^2}(\theta,\phi)\psi(r,\theta,\phi) + \frac{2m}{\hbar^2}[E - V(r,\theta,\phi)]\psi(r,\theta,\phi) = 0$$

$$\widehat{\mathscr{L}^2}(\theta,\phi) = \frac{\partial^2}{\partial\theta^2} + \cot g(\theta)\frac{\partial}{\partial\theta} + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2} \tag{2}$$

The potential energy of a particle which moves in a central and spherically symmetric field of force depends only upon the distance r between the particle and the center of force. Thus, the potential energy should be such as $V(r,\theta,\phi) = V(r)$. Solution of the Equation (2) can be found by the method of separation of variables. To apply this method, it is assumed that the solution is in the form of

$$\Psi(r,\theta,\phi) = R(r)Y(\theta,\phi) = R(r)|jm> \tag{3}$$

in which $R(r)$ is independent of the angles, and $Y(\theta,\phi)$ and $|jm>$ are independent of r. By substituting Equation (3) into Equation (2) and rearranging, the following Equation is obtained. In the Equation (3), m is not mass, it is magnetic quantum number.

$$\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right]R(r)+\left\{\frac{2m}{\hbar^2}\left[E-V(r)\right]-\frac{C}{r^2}\right\}R(r)=0 \qquad (4)$$

$$\mathcal{L}^2(\theta,\phi)\,Y(\theta,\phi)+C\,Y(\theta,\phi)=0 \qquad (5)$$

Here, C is a constant. Equation (5) is independent of the total energy E and of the potential energy $V(r)$, therefore, the angular dependence of the wave functions is determined by the property of spherical symmetry, and admissible solutions of Equation (5) are valid for every spherically symmetric system regardless of the special form of the potential function. The solutions of the Equation (5) can be found in any quantum mechanics and mathematical physics text−books and the solutions are known as spherical harmonic functions, $Y(\theta,\phi)=Y_{\ell,\mu}(\theta,\phi)$, where $C=\ell(\ell+1),\ell=0,1,2,3,...$ are positive integer numbers and $\mu=-\ell,\,-\ell+1,...0...+\ell$. Equation (4) is the radial SE (**S**chrödinger **E**quation). Substituting $C=\ell(\ell+1)$ and $R(r)=F(r)/r$ into Equation (4), the radial wave Equation is obtained as follow:

$$\left\{\frac{d^2}{dr^2}+\frac{2m}{\hbar^2}\left[E-U(r)\right]\right\}F(r)=0 \; ;$$

$$\frac{d^2F(r)}{dr^2}+[\alpha-U_e(r)=0 \qquad (6)$$

Here $\alpha=\frac{2m}{\hbar^2}E$; $U(r)=V(r)+\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}$ is the effective potential energy, and $U_e(r)=\frac{2m}{\hbar^2}U(r)$. here m is mass or reduced mass of particle.

Equation (6) is one dimensional differential equation. The solution of this one-dimensional differential equation has been given in.[1,2] The $F(r)$ functions have been found by using the same procedure that is explained in these references. Two of these solutions are given as follows:

$$F(r)=\cosh[k\; r]\;[A\,e^{i\,G(r)}+B\;e^{-iG(r)}]\;;$$

$$F(r)=\sinh[k\; r]\;[A\,e^{i\,G(r)}+B\;e^{-iG(r)}] \qquad (7)$$

Here,

For $\alpha>U_e(r)$, (bound state), $k=\sqrt{-\alpha}$,$G(r)=\int\sqrt{-U_e(r)}dr$; [$G(r)$ real function]. For $\alpha>U_e(r)$, (unbound state), $k=\sqrt{\alpha}$, $G(r)=\int\sqrt{-U_e(r)}\,dr$. r_1 and r_2 are the roots of the following Equation:

$$\alpha-U_e(r)=0\; or\; E-U(r)=0 \qquad (8)$$

In some cases, using the following quantities can provide more conveniences:

$$d=r_2-r_1,\;(r_1<r_2);\;r_0=(r_1+r_2)/2;\;r_1=r_0-d/2\;;r_2=r_0+d/2.$$

If one takes $(r-r_0)$ instead of **r** in the above functions, these can also be used when obtaining the solutions of the Equation (6). The **A and B** coefficients of the functions are determined by using the boundary and normalization conditions.

In bound states (in the wells), the normalized wave functions are as follows [$G(r)$ is taken as real function]:

$$F_s(r)=A\cos[k\; r]e^{\pm i\; G(r)}$$

$$F_a(r)=B\sin[k\; r]e^{\pm i\; G(r)} \qquad (9)$$

or

$$F_s(r)=A\cos[k(r-r_0)]e^{\pm i\; G(r-r0)}$$

$$F_a(r)=B\sin[k(r-r_0)]e^{\pm i\; G(r-r0)} \qquad (10)$$

$$A=B=\sqrt{2/d}=\sqrt{2K/q};\;;\;(s:\text{ symmetric; a: antisymmetric}).$$

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

$$K\;[r_2(E)-r_1(E)]=Kd=q\;;$$

$$K=\sqrt{|\alpha|}=\sqrt{\frac{2\,m}{\hbar^2}|E|}\;. \qquad (11)$$

Equation (11) is the quantization condition of energy in bound states. For $q=2$, the ground state (minimum energy) occurs; for $q=n\pi,\,(n=1,2,3,...)$, the excited states occur. We have symmetric states for odd integer values of **n** and antisymmetric states for even integer values of n .

Solution of Schrodinger equation in double potential wells

Consider a particle with mass or reduced mass m is in the central potential of $V(r)$ in a coordinate system at the point $(0,0)$ of the coordinate start. The variable r of the potential in this coordinate system is always positive. If the spin of the particle is also considered, the total angular momentum quantum number j should be taken instead of ℓ. Thus, the effective potential is $U(r)=V(r)+b/r^2;[b=\hbar^2\,j(j+1)/(2m)]$. This effective potential is usually a parabolic function in the bound states. In the bound states, the total energy is always negative and consequently the effective potential is also negative. Therefore, $U(r)<0$ should be in the bound states. When mass m vibrates in this effective potential, the term b of the potential creates an obstacle that tries to prevent vibration motion. This potential comes from the rotation of the mass m, that is, from the centrifugal motion. If there is no rotation, this term is zero. The solution of the Equation $U(r)=-E\; or\; |U(r)|=E$ are r_1,r_2,r_3 and r_4 values, depending on E. If the values $(r_3\text{ and }r_4)$ are real and non-zero, there is a potential barrier in the potential well. If this Equation is solved at a point $r=r_0$, these roots are written also as follows: $r_1=r_0-d_1/2$ and $r_2=r_0+d_1/2$ and $r_3=r_0-d_2/2$ and $r_4=r_0-d_3/2$. Here $d_1=(r_2-r_1),d_3=(r_4-r_3)$ and $r_0=(r_1+r_2)/2=(r_3+r_4)/2$. If the origin of the coordinate system is taken as the point r_0, these are $r_1=-d_1/2$ and $r_2=-d_1/2\,'$ and $r_3=-d_3/2$ and $r_4=-d_3/2$. The points $r_1\text{ and }r_2$, and $r_3\text{ and }r_4$ are the classic turning points of the $U(r)$ potential. Since $U(r_1)=U(r_2)\; and\; U(r_3)=U(r_4)$ are equal at the potential of the classical turning points. Thus, the following Equations can be written:

$$U(-d_1/2)+U(+d_1/2)=2E$$

$$U(-d_3/2)+U(+d_3/2)=2E$$

Since $E=m_h\;q^2/d_i^2(E)$,$\left(m_h=\frac{\hbar^2}{2\,m}\right)$.

these Equations can also be written as follows:

$$U(-d_1/2)+U(+d_1+2)=2m_h\;q^2/d_i^2(E)$$

$$U(-d_3/2)+U(+d_3+2)=2m_h\;q^2/d_3^2(E)$$

The solution of these two Equations has the same energy. It is therefore sufficient to solve one of these two Equations to find the energy values. When these Equations cannot be solved analytically, numerical solutions are made, and energy values are found. When one of these two Equations is solved, two energies based on q are obtained. One of these energies $(+)$ and the other $(-)$ becomes and their absolute values are equal. The $(-)$ sign indicates that the particle is bound. For $q = 2,$ the ground state (minimum energy) occurs; for $q = n\pi, (n = 1,2,3,...),$ the excited states occur. We have symmetric states for odd integer values of n and antisymmetric states for even integer values of n. This problem is useful in some cases if it is solved in two wells.

Conversion of potential into two parts (double well)

Solutions become easier when you divide a given potential into two parts. This separation process will be given here. If the potential is given as $V(r) = V_0(r) - V_{00}, [V_0(r) > 0 \; and \; V_{00} > 0],$ the effective potential is $U(r) = V_0(r) - V_{00} + \dfrac{b}{r^2} < 0$ in the bound states. Here, $-V_{00}$ is the depth of the potential well. Let us find the maximum and minimum values of this effective potential $U(r)$ et the roots of the Equation $U'(r) = 0,$ $r_{m1} \; and \; r_{m2}$ be. $r_0 = (r_{m1} + r_{m1})/2$ is the point where the potential receives the smallest values $U(r_{m1}) \; and \; U(r_{m2})$ and the largest value $U(r_0)$. Let $U_0 = U(r_0) - V_{00}$.Thus $U(r) = V_0(r) - U + \dfrac{b}{r^2} < 0$ can be written. By solving this $U(r)$ potential directly, energy values and wave functions can be found. However, if this potential is divided into two parts with an obstacle in the middle, there may be some convenience. The obstacle in the two potential wells comes from rotational energy and the potential $[V_0(r) - U_0]$. Therefore, the $U(r)$ potential can be written as the sum of two parts as follows:

$$U(r) = V_0(r) - U_0 + \frac{b}{r^2} = U_w(r) + U_b(r);$$

$$[U_w(r) = V_0(r) - U_0 \; ; \; U_b(r) = \frac{b}{r^2}] \qquad (12)$$

Here, the $U_w(r)$ potential is the vibration part of the $U(r)$ potential, and the $U_b(r)$ potential is total of the rotational and the other obstacle potential parts of the potential $U(r)$. U_0 is the depth of the potential well. If the coordinate start is taken at the point $(r_0, -U_0),$ in this new coordinate system, $U_b(r) = \dfrac{b}{r^2}$ and $U_w(r) = V_0(r)$. Thus, the effective potential is written as follows:

$$U(r) = V_0(r) + \frac{b}{r^2} = U_w(r) + U_b(r);$$

$$[U_w(r) = V_0(r) \; ; \; U_b(r) = \frac{b}{r^2}] \qquad (13)$$

The graph of this potential is shown in Figure 1. (Shape of the U(r) function $(r_0, -U_0)$ in the coordinate system). In this way, three domains I, II, III are obtained. Thus, by solving the Equation (13), E energy values are found.
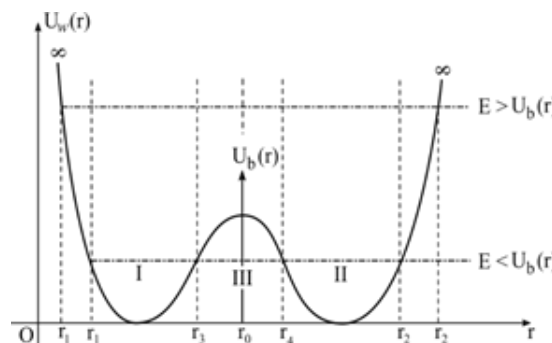

Figure 1 The plot of the potential $U(r)$ in the form of two wells; the points r_1, r_2, r_3, r_4 are classic turning points.

Solution of the equation of [U (r) =E$_q$]

The functions $U_w(r) \; and \; U_b(r)$ are symmetrical functions according to point r_0. The $U_b(r)$ function is an obstacle function located in the midpoint of the well $U_w(r)$ function. The quantities (r_1, r_2, r_3, r_4) that are the solution of the Equation $U(r) = E$ are depending on r_0. As seen in Figure 1, the roots of the Equation, $U(r) = E$ are (r_1, r_2, r_3, r_4) and the roots of $U_b(r) = E$ are $(r_3, r_4),$ the roots of $U_w(r) = E$ are (r_1, r_2). From there, the following values are obtained:

$$\frac{r_1 + r_2}{2} = \frac{r_3 + r_4}{2} = 0 \; ; d_1 = r_3 - r_1 \; ; d_2 = r_2 - r_4 \; ; d_1 = d_2 \; ; d_3 = r_4 - r_3 \; ; d = r_2 - r_1$$

$[d_1, d_2, d_3]$ are respectively the widths of the regions (I,II,III) Since $d_1 = d_2$, it is sufficient to make a solution in one of the regions (I) and (II). Particle is unbound in the region $(III),$ it cannot remain in this area continuously, it can pass from region II to region I or from region I to region II by tunneling with equal probability. Here the probability of passing coefficient is calculated.

Example: Three axial deformed harmonic oscillator potential (anisotropic harmonic oscillator potential) (Nilson model in the nuclear physics)

Effective potential

The nucleus is assumed to have a spherical shape in the shell model. 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 that the deformed shell model. In deformed shell model calculations, it is used the three-dimensional anisotropic harmonic oscillator potential which is given as follows:

$$V_0(x, y, z) = \frac{1}{2}\mu\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_Z^2 Z^2\right) \qquad (14)$$

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 $\omega_X = \omega_y = \omega_\perp \neq \omega_z$ 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 $\omega_x, \omega_y, \omega_z$ relate to the deformation parameters ε *and* γ by the following expressions:

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

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

$$\omega_z = \omega_0(\varepsilon,\gamma)\left[1 - \frac{2}{3}\varepsilon\cos(\gamma)\right] \tag{15}$$

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

$$\omega_x\omega_y\omega_z = \omega_{00}^3 \tag{16}$$

From Equation (16), we get the following value:

$$\omega_0(\varepsilon,\gamma) = 3\omega_{00}[27 = 9\varepsilon^2 - 2\varepsilon^3\cos(3\gamma)]^{-1/3} \tag{17}$$

As can be seen from Equation (17), if $\varepsilon = 0$, isotropic state is obtained. Let us express the potential given in Equation (14) the following spherical coordinates:

$$\text{x} = r\sin(\theta)\cos(\phi), \quad y = r\sin(\theta)\sin(\phi), \ z = r\cos(\theta) \tag{18}$$

If the potential given in Equation (14) is calculated by considering Equations (15), (16) and (17), the following function is obtained:

$$V_0(r,\varepsilon,\gamma) = \frac{1}{2}\mu\omega_{00}^2 r^2[A(\varepsilon,\gamma)\sin^2(\theta)\cos^2(\phi) + B(\varepsilon,\gamma)\sin^2(\phi)\sin^2(\phi) + C(\varepsilon,\gamma)\cos^2(\theta)] \tag{19}$$

$$A(\varepsilon,\gamma) = \frac{\left[3 + 2\varepsilon\sin\left(\frac{\pi}{6} + \gamma\right)\right]^2}{\left[27 = 9\varepsilon^2 - 2\varepsilon^3\cos(3\gamma)\right]^{2/3}}; \ B(\varepsilon,\gamma) = \frac{\left[3 + 2\varepsilon\sin\left(\frac{\pi}{6} - \gamma\right)\right]^2}{\left[27 - 9\varepsilon^2 - 2\varepsilon^3\cos(3\gamma)\right]^{2/3}}; \ C(\varepsilon,\gamma) = \frac{\left[3 - 2\varepsilon\cos(\gamma)\right]^2}{\left[27 - 9\varepsilon^2 - 2\varepsilon^3\cos(3\gamma)\right]^{2/3}}; \tag{20}$$

$$\beta^2 = A(\varepsilon,\gamma)\sin^2(\theta)\cos^2(\phi) + B(\varepsilon,\gamma)\sin^2(\theta)\sin^2(\phi) + C(\varepsilon,\gamma)\cos^2(\theta)$$

$$\beta^2 = A(\varepsilon,\gamma)\left[1 - \cos^2(\theta)\right]\cos^2(\phi) + B(\varepsilon,\gamma)\left[1 - \cos^2(\theta)\right][1 - \cos^2(\phi)] + C(\varepsilon,\gamma)\cos^2(\theta)$$

$$\beta^2 = B(\varepsilon,\gamma)\left[C(\varepsilon,\gamma) - B(\varepsilon,\gamma) - \{A(\varepsilon,\gamma) - B(\varepsilon,\gamma)\}\cos^2(\phi)\right]\cos^2(\theta) + \left[A(\varepsilon,\gamma) - B(\varepsilon,\gamma)\right]\cos^2(\theta) \tag{21}$$

If γ is exceedingly small, then $\sin(\gamma) \approx 0$ and A ≈ B (symmetric ellipsoid form) can be taken. Thus, β^2 can be taken as follows:

$$\beta^2 = B(\varepsilon,\gamma) + \left[C(\varepsilon,\gamma) - B(\varepsilon,\gamma)\right]\cos^2(\theta) = B(\varepsilon,\gamma) + \left[C(\varepsilon,\gamma) - B(\varepsilon,\gamma)\right]\left[\frac{1}{3} + \frac{2}{3}\sqrt{\frac{4\pi}{5}}Y_0^2\right] \tag{22}$$

Y_0^2 is spherical harmonic function. Thus, the anisotropic harmonic oscillator potential becomes as follows:

$$V_0(r,\varepsilon,\gamma) = \frac{1}{2}\mu\omega_{00}^2 r^2\beta^2(\varepsilon,\gamma) \tag{23}$$

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

$$U(r,\varepsilon,\gamma) = V_0(r,\varepsilon,\gamma) + \frac{\hbar^2}{2\mu r^2}j(j+1) = \frac{1}{2}\mu\omega_{00}^2 r^2\beta^2(\varepsilon,\gamma) + \frac{\hbar^2}{2\mu r^2}j(j+1) \tag{24}$$

Here, ω_{00} is the isotropic oscillator angular frequency and j total angular momentum quantum number. The Coulomb potential must be added to the potential given in Equation (24) when the charged particle levels are calculated. The Coulomb potential in the spherical case, neglecting the effect of the surface, is as follows:

$$V_c(r) = \frac{(Z-1)e^2}{r}\begin{cases}\dfrac{3\,r}{2\,R_0} - \dfrac{1}{2}\left(\dfrac{r}{R_0}\right)^2, & for \ r \leq R_0 \\ 1 & , \ for \ r > R_0\end{cases}$$

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

$$V_c(r) = b_c + a_c\,r^2 \ ;\left[a_c = -\frac{(Z-1)e^2}{2R_0^3}, \ b_c = \frac{3(Z-1)e^2}{2R_0}\right] \tag{25}$$

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

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

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

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

$$V_c(r) = b_c(\varepsilon) + a_c\,r^2\ ;$$

$$[a_c = -\frac{(Z-1)e^2}{2R_0^3}, \ b_c(\varepsilon) = \frac{3(Z-1)e^2}{2R_0}\left(-8.9723 - 3.3241\,\varepsilon + 8.14235\sqrt{1.5+\varepsilon}\right) \tag{26}$$

It is seen that for $\varepsilon = 0$, Equation (26) is equal to Equation (25). On the other hand, the total wave function is $\psi(r,\theta\phi) = R(r)\left|\ell jm\right> = \frac{F(r)}{r}\left|\ell jm\right>$ and the radial SE is written as follows:

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

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$$\frac{d^2 F(r)}{dr^2}\Big|\ell jm> + \frac{2\mu}{\hbar^2} F(r)\Big[E - U(r,\varepsilon,\gamma)\Big]\Big|\ell jm >= 0 \qquad (27)$$

In Equation (27), $\Big[E - U(r,\varepsilon,\gamma)\Big]\Big|\ell jm >$ is calculated as follows:

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

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

$$\beta^2(\varepsilon,\gamma)\Big|\ell jm > = \beta^2\Big|\ell jm > = \left\{B(\varepsilon,\gamma) + \Big[C(\varepsilon,\gamma) - B(\varepsilon,\gamma)\Big]\Big[\frac{1}{3} + \frac{2}{3}\sqrt{\frac{4\pi}{5}}Y_0^2\Big]\right\}\Big|\ell jm > \quad (28)$$

$$\beta^2(\varepsilon,\gamma)\Big|\ell jm > = \beta^2\Big|\ell jm > = \left\{B(\varepsilon,\gamma) + \Big[C(\varepsilon,\gamma) - B(\varepsilon,\gamma)\Big]\cos^2(\theta)\right\}\Big|\ell jm >$$

If we calculate $Y_0^2\big|\ell jm\rangle = a_{20}\big|\ell jm\rangle$ in Equation (28), by the Wigner-Eckart theorem, we have found the following value:

$$a_{20}(\ell,j,m) - \sqrt{\frac{\pi}{2\ell+1}}\frac{j + j^2 - 3m^2}{2j(j+1)} = a_{20}$$

Thus, $\beta^2(\varepsilon,\gamma,a_{20})$ are written as follows:

$$\beta^2(\varepsilon,\gamma,a_{20}) = B(\varepsilon,\gamma) + \Big[C(\varepsilon,\gamma) - B(\varepsilon,\gamma)\Big]\left[\frac{1}{3} + \frac{2}{3}\sqrt{\frac{4\pi}{5}}a_{20}\right] \qquad (29)$$

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

$$U(r;\varepsilon,\gamma,a_{20}) = \frac{1}{2}\mu\omega_{00}^2\beta^2(\varepsilon,\gamma,a_{00})r^2 + \frac{\hbar^2}{2\mu r^2}j(j+1) = ar^2 + \frac{b}{r^2} = U(r) \qquad (30)$$

$$a = \frac{1}{0}\mu\omega_{00}^2\beta^2(\varepsilon,\gamma,a_{20}) = \frac{1}{2}\mu\omega^2; b = \frac{\hbar^2}{2\mu}j(j+1); \omega^2 = \omega_{00}^2\beta^2(\varepsilon,\gamma,a_{20}) \qquad (31)$$

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

Solution of the equation of [U (r) =E_q]

Consider $U_w(r) = a\,r^2$ and $U_b(r) = \frac{\hbar^2}{2\mu}\frac{j(j+1)}{r^2} = \frac{b}{r^2}, \left[b = m_h\,j(j+1),\ m_h = \frac{\hbar^2}{2\mu}\right]$.

Thus, according to (30), we have:

$$U(r) = V_0(r) + \frac{b}{r^2} = U_w(r) + U_b(r);$$

$$\left[U_w(r) = V_0(r) = a\,r^2\ ; U_b(r) = \frac{b}{r^2}\right].$$

Solution of the Equation $U(r) = E_q$ gives the following r values:

$$r_1 = -\sqrt{\frac{E_q + \sqrt{E_q^2 - 4\,a\,b}}{2\,a}};\ r_2 = \sqrt{\frac{E_q + \sqrt{E_q^2 - 4\,a\,b}}{2\,a}};$$

$$r_3 = -\sqrt{\frac{E_q - \sqrt{E_q^2 - 4\,a\,b}}{2\,a}}\ ;\ r_4 = \sqrt{\frac{E_q - \sqrt{E_q^2 - 4\,a\,b}}{2\,a}}.$$

$$\frac{r_1 + r_2}{2} = \frac{r_3 + r_4}{2} = r_0 = 0\ ;\ d_1 = r_3 - r_1\ ;\ d_2 = r_2 - r_4\ ;\ d_1 = d_2\ ;\ d_3 = r_4 - r_3\ ;\ d = r_2 - r_1.$$

Now, we will solve this problem in three cases as follows.

Solution of the case E_b > U_b (r)

In this case, the following equation can be written according to the quantization condition of energy:

$$K\,d = E_q\ \text{ or } K^2 d^2 = E_q^2\ ; \left[K = \sqrt{\frac{2\,\mu\,E_q}{\hbar^2}}\right]$$

The following energy value is obtained from the solution of this equation.

$$E_q = \frac{\sqrt{a}\ \hbar^2 q^2}{2\sqrt{2\,\mu}\sqrt{\hbar^2 q^2 - 8\,\mu\,b}}\ ; [E_q > U_b(r)] \qquad (32)$$

If the energy E_q does not depend on the angular momentum quantum number j, i.e., rotation, energy is purely vibrational energy.

In this case, $b = 0$ and $E_q = \frac{1}{2}\hbar\,\omega$.

Solution of the case E_q < U_b (r)

In this case, since $d_1 = d_2$, equal energy values are obtained in (I) and (II) regions. So, the following equation can be written according to the quantization condition of energy:

$$K\,d_1 = E_q\ \text{ or } K^2 d_1^2 = E_q^2\ ; \left[K = \sqrt{\frac{2\,\mu\,E_q}{\hbar^2}}\right]$$

The following energy values are obtained from the solution of this equation.

$$E_q^{(1)} = \frac{\sqrt{a\,\mu\left(4b\,\mu + \hbar^2 q^2\right) + \delta(a,b,q)}}{\mu}\ ;$$

$$E_q^{(2)} = \frac{\sqrt{a\,\mu\left(4b\,\mu + \hbar^2 q^2\right) - \delta(a,b,q)}}{\mu} \qquad (33)$$

$$\delta = 2\sqrt{2a^2 b\,\mu^3\left(2\,b\,\mu + \hbar^2 q^2\right)}$$

If the values of b are put in place, the following values depending on (a, j, q) are obtained:

$$E_{q1}(a,j,q) = \frac{\sqrt{a\hbar^2\left(2j + 2j^2 + q^2\right)\mu + \delta}}{\mu}\ ;$$

$$E_{q2}(a,j,q) = \frac{\sqrt{a\hbar^2\left(2j + 2j^2 + q^2\right)\mu - \delta}}{\mu}. \qquad (34)$$

$$\delta(a,j,q) = 2a\hbar^2\mu\sqrt{j(1+j)\left(j + j^2 + q^2\right)}$$

Then, in case $E_q < U_b(r)$, there are two equal energy values in regions (I) and (II). As seen in Figure 1, the $U_b(r)$ barrier potential located between (I) and (II) potential wells divides the energy of the particle into two. While the particle is oscillating in these wells, when the particle reaches the r_3 (or r_4) point, some of its energy passes from the III region to the II (or I) region by tunneling, and some of it is reflected from the r_3 (or r_4) point. This transition is equally likely for both parties. (This passing probability will be calculated below). Thus, the potential barrier divides the energy of the particle in two. The rotational potential due to angular momentum always splits the energy into two parts. This phenomenon may be a way to find the angular momentum of a particle. When $j = 0,(\delta = 0)$ in (34), there is only one energy. So, the $U_b(r)$ barrier cuts a single energy into two parts. These double energy splits are observed at small vibrations in some molecules such as ammonia. Many double wells are proposed to explain these energy splits, although there is no need for them. Because this energy splitting occurs in small vibrations for all particles with angular momentum.

Solution of the case E_q = U (r), [In one potential well]

We consider the effective potential given here as a whole. We will solve the two wells at the bottom of the potential well in general, without considering them separately.

$$U(r) = V_0(r) + \frac{b}{r^2} = U_w(r) + U_b(r);$$

$$\left[U_w(r) = V_0(r) ; U_b(r) = \frac{b}{r^2} ; V_0(r) = a\,r^2 \right]$$

Solution of the Equation $U(r) = E_q$ gives the following r values:

$$r_1 = -\sqrt{\frac{E_q + \sqrt{E_q^2 - 4ab}}{2a}} \; ; \; r_2 = \sqrt{\frac{E_q + \sqrt{E_q^2 - 4ab}}{2a}} \; ;$$

$$r_3 = -\sqrt{\frac{E_q - \sqrt{E_q^2 - 4ab}}{2a}} \; ; \; r_4 = \sqrt{\frac{E_q - \sqrt{E_q^2 - 4ab}}{2a}}$$

$$d_1 = r_2 - r_1 \; ; \; d_3 = r_4 - r_3 .$$

Positive root of Equation $d_1^2\left[U(r_1) + U(r_2)\right] = 2m_h q^2$ is

$$E_{q1} = \frac{\sqrt{a}\; m_h q^2}{2\sqrt{m_h q^2 - 4b}} = \frac{q^2\,\hbar\omega}{4\sqrt{q^2 - 4j(j+1)}} .$$

Positive root of Equation $d_3^2\left[U(r_3) + U(r_4)\right] = 2m_h q^2$ is

$$E_{q3} = \frac{\sqrt{a}\; m_h q^2}{2\sqrt{m_h q^2 - 4b}} = \frac{q^2\,\hbar\omega}{4\sqrt{q^2 - 4j(j+1)}} .$$

From here it is seen that $E_{q1} = E_{q3}$. Since the particle is not bound in zone III, so energy is obtained as follows.

$$E_q(q,j) = \frac{\sqrt{a}\; m_h q^2}{2\sqrt{m_h q^2 - 4b}} = \frac{q^2\,\hbar\omega}{4\sqrt{q^2 - 4j(j+1)}} \qquad (35)$$

It is seen that the energy of (32) and the energy of (35) are the same for $j = 0$. We have for $q = 2$, the minimum (ground) state energy; for the exited state energies. We have symmetric states for $q = n\,\pi$, $(n = 1,2,3...)$ odd integer values of n; antisymmetric states for even integer values of n.

Here the solutions are made for the potential $V_0(r) = a\,r^2$ and all solutions could be done analytically. If the potential is not a potential that can be solved analytically (as Saxon-Wood potential, trigonometric potentials etc.), numerical solutions can be made in the same way.

Finding wave functions

If the potential $U_w(r)$ potential is an isotropic harmonic oscillator potential, therefore, the mass or reduced mass m in zone (I) makes a harmonic motion. If there were no (III) barriers, there would be only one energy value. So, the energy value would be corrupt. With such a two-well solution, corruption is eliminated. Therefore, total energy would be 32 or (35) if there were not the $U_b(r)$ obstacle at the point r_0. According to the function (10), the radial normalized wave functions can be written as follows:

$$Q(r) = m_1 \int \sqrt{|U_w(r)|}\; dr = Q(r);$$

$$\left[m_1 = \sqrt{\frac{2m}{\hbar^2}} = \frac{\sqrt{2m}}{\hbar} \right] \qquad (36)$$

For the state of E_q, the independent of time and time dependent normalized wave functions are as follows, respectively:

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

$$F^a(r) = B\sin[K\,r]\, e^{\pm i\,Q(r)} .$$

$$F^s(r,t) = A\cos[K\,r]\, e^{\pm i\,Q(r)} e^{-\frac{i}{\hbar} E_q\, t} ;$$

$$F^a(r,t) = B\sin[K\,r]\, e^{\pm i\,Q(r)} e^{-\frac{i}{\hbar} E_q\, t} . \qquad (37)$$

$$A = B = \sqrt{2K/q} \; , \; K = \sqrt{\frac{2m}{\hbar^2} E_q} = m_1\sqrt{E_q} .$$

The independent of time and time-dependent total normalized wave functions are as follows, respectively:

$$\psi^s(r,\theta,\phi) = R(r)|jm> = \frac{F^s(r)}{r}|jm>;$$

$$\psi^a(r,\theta,\phi) = R(r)|jm> = \frac{F^a(r)}{r}|jm>$$

$$\psi^a(r,\theta,\phi,t) = R(r)|jm> = \frac{F^a(r)}{r}|jm> e^{-\frac{i}{\hbar} E_q\, t} ;$$

$$\psi^s(r,\theta,\phi,t) = R(r)|jm> = \frac{F^s(r)}{r}|jm>^{-\frac{i}{\hbar} E_q\, t} \qquad (38)$$

Let us consider a general solution of the type of time-depending functions:

$$\psi(r,t) = \frac{1}{\sqrt{2}}\left\{ \psi_s(r) e^{-i\,E_s t/\hbar} + \psi_a(r) e^{-i\,E_a t/\hbar} \right\} \qquad (39)$$

(a: antisymmetric; s: symmetric). Here, both states, symmetric and antisymmetric, are equally probable. Let us calculate the probability density of presence as follows:

$$\rho = \psi^*(r,t)\,\psi(r,t) = \frac{1}{2}\left\{ \psi_s^2 + \psi_a^2 + 2\,\psi_a\psi_s\cos\left[(E_a - E_s)t/\hbar\right] \right\} \qquad (40)$$

If the wave functions of the energy states E_{q1} and E_{q2} given in the formulas (34) are $\psi_{q1}(r)$ and $\psi_{q2}(r)$, respectively, and the general wavefunction and the probability density of presence will be as follows:

$$\psi(r,t) = \frac{1}{\sqrt{2}}\left\{ \psi_{q1}(r) e^{-i\,E_{q1}t/\hbar} + \psi_{q2}(r) e^{-i\,E_{q2}t/\hbar} \right\}$$

$$\rho = \psi^*(r,t)\,\psi(r,t) = \frac{1}{2}\left\{ \psi_{q1}^2 + \psi_{q2}^2 + 2\,\psi_{q1}\psi_{q2}\cos\left[(E_{q2} - E_{q1})t/\hbar\right] \right\}$$

When the cosine is equal to 1, we have $\rho = \frac{1}{2}(\psi_{q1} + \psi_{q2})^2$, and this corresponds to a state where the probability of finding the particle in domain I is maximum. When the cosine is equal to -1, we have $\rho = \frac{1}{2}(\psi_{q2} - \psi_{q1})^2$, and this corresponds to a state where the probability of finding the particle in domain I is minimum. The expression (39) and (40) must be interpreted by saying that it is a state where particle oscillates from the left bowl (domain I) to the right bowl (domain II). The frequency of this oscillation is $f = (E_{q2} - E_{q1})/h$. To perform such an oscillation corresponding to the energy variation ($E_{q2} - E_{q1}$), the particle must receive energy from the outside, for example by placing it in an electromagnetic field having the frequency f. Such an oscillation is not possible classically because the energy supplied $(E_{q2} - E_{q1})$ is insufficient for the particle to cross over the hump of the potential U_b. But, according to quantum mechanics, by tunneling through the III region, these oscillations are possible. It is observed similar states in ammonia (NH_3), and similar molecules which have the shape of a pyramid. This is called rotational symmetry. If $J = 0$, there is one energy value and one wave function; so, there is no energy splitting. If $J \neq 0$, there are always two energies and two wave functions; so, there is an energy splitting.

Calculation of the transmission coefficient through the zone (III)

The particle is unbound state in the region (III). From the solution of the $\left[U_b(r) = E_q \right]$; Equation, r_3 and r_4 values depending on E_q are obtained. The solution to this Equation (at the point r_0) gives the following values r_3 and r_4: $r_3 = r_0 - d_3/2$ and $r_4 = r_0 + d_3/2$. From here, the width of the obstacle d_3 is found: $d_3 = r_4 - r_3$. The energy E_q is found by the Equation (33). In the region III, $E_q < U_b(r)$, (unbound state), thus the particle cannot remain stable in zone (III), it can pass from region II to region I or from region I to region II by tunneling with equal probability. Here the probability of passing coefficient is calculated. The tunneling probability coefficient (or transmission coefficient) is given by the following formula:[3–5]

$$T = \frac{2}{cosh[2K\,d] + cos(2P)}$$

Here, the width of the potential barrier d, $K = m_1\sqrt{|E|}$, $m_1 = \sqrt{\frac{2m}{\hbar^2}}$, E energy, $Q(r) = m_1\int\sqrt{|U(r)|}\,dr$, $U(r)$ barrier potential and $P = Q(r_4) - Q(r_3)$. Here, according to our quantities, these quantities are as follows:

$$P = \sqrt{\frac{2m}{\hbar^2}}\int_{r_3}^{r_4}\sqrt{|U_b(r)|}\,dr = Q_b(r_4) - Q_b(r_3);$$

$$Q_b(r) = m_1\int\sqrt{|U_b(r)|}\,dr \;;\; K = m_1\sqrt{|E_q|} \;;\; d = d_3.$$

If $Q_b(r)$ is pair, $P = 0$. If $Q_b(r)$ is odd, $P = Real\left[Q_b(r_4) - Q_b(r_3) \right] = 0$. Thus, if $P = 0$, the coefficient transmission is obtained as follows:

$$T = \frac{2}{1 + cosh[2K\,d_3]} \;;\; \text{and If} \;\; d_3 = 0, \;\; T = 1.$$

In regions (I) and (II), energy satisfies the quantization condition $K\,d_1 = q$. In zone (III), the particle is not bound. But the energy will be equal at r_3 and r_4 points and $K\,d_3 = q$ quantization condition gets also in the (III) region. Therefore, it is $K\,d_1 = q = K\,d_3$. So, it is obtained as:

$$T = \frac{2}{1 + cosh[2K\,d_3]} = \frac{2}{1 + cosh[2q]} = T(q) \qquad (41)$$

Numerical calculations

The energy values of some triaxial harmonic oscillator states calculated according to the formula (34) are given in Table 1. In this table, the parameters are taken arbitrarily to see how the energy values vary according to these parameters.

Application to ammonia molecule (NH$_3$)

The ammonia molecule consists of one nitrogen and three hydrogen atoms. The effective potential curve becomes as shown in Figure 1. The hydrogen atoms define the orientation of ammonia. If the nitrogen atom is situated on the right side of potential barrier there is a chance that it can overcome the barrier and move to the other side. The movement of nitrogen atom consists of left and right vibrations and a slow drift between left and right zones of the potential. The classical turning points for the ground vibrational state, r_1 and r_3 or r_4 and r_2, are indicated as well in Figure 1. Due to tunneling through the potential barrier each vibrational level is split in two

symmetrical components. As seen from formula (34), masses are not needed to calculate energies. Masses are within the angular frequency ω. Therefore, from the Equation (31) $a = \frac{1}{2}\mu\omega^2{}_{00}\beta^2(\varepsilon,\gamma,a_{20}) = \frac{1}{2}\mu\omega^2$, and **a** must be explicitly calculated based on the mass (hence ω). But the mass is also calculated here to explain how the problem is. The masses and total angular momentums of hydrogen and nitrogen atoms are given as follows, respectively.

$$M_H = 1.007825u \;,\; J_H^+ = \frac{1}{2}^+ \text{ and } M_N = 14.003074\,u \;,\; J_N^+ = 1^+ \;;\; [u \text{ is atomic unit}]$$

$$1\,u = 931.502\,MeV/c^2 \;;\; c = 2.99792458 \times 10^{10}\,cm/s \;;\; h = 4.13570 \times 10^{-15} \times eV \times s \;;$$

$$\hbar = 6.58217 \times 10^{-16} \times eV \times s$$

The reduced mass of three hydrogen atoms and one nitrogen atoms is as follows:

$$m = \frac{3M_H M_N}{M_N + 3M_H}u = \frac{3M_H M_N}{M_N + 3M_H} \times 931.502\,MeV/c^2 \;;\; m_h = \frac{\hbar^2}{2m} = \frac{\hbar^2 c^2}{2m\,c^2}.$$

The relative total angular momentum of a hydrogen atom and other atoms are as follows:

$$\left| 1 - \frac{1}{2} \right| \le J \le 1 + \frac{1}{2} \;\rightarrow\; J = \frac{1}{2}\,,\,\frac{3}{2}$$

Since $J = \frac{3}{2}$ is not suitable for the smallest energy $(\text{for } q = 2)$, it is sufficient to take $J = \frac{1}{2}$. Since $q = 2$ for the smallest energy state $q = 2$ will be taken here. With these data, the following energy values are found by the formulas (34).

Ground state energy

According to the formulas (34): $E_{q1}(q,j) = E_{q2}(q,j) = E_{q1}(2,0) = E_{q2}(2,0) = \hbar\omega$.

According to the formula (35): $E_q(q,j) = E_q\left(2, \frac{1}{2} \right) = \hbar\omega$

(Since formula (34) gives the energy of the excited states, it is necessary to take $j = 0$ when using this formula when calculating the ground state energy).

Energies of excited states

According to the quantization condition of energy: $q = 2$ for the ground state, $q = n\,\pi$, $(n = 1, 2, 3...)$ for the excited states. The smallest energy (ground state energy) value measured in the ammonia molecule is $E_0 = 9.813 \times 10^{-5}$ eV ; $(\text{frequency} = 2.3789 \times 10^{10}$ Hz).[6] Some excited energy values calculated by taking this energy value as zero are given in Table 2. In this table, the first and second columns experimental energies; third, fifth and seventh columns q1 and q2 parameters giving the energy split Eq1 and Eq2 ; the fourth, sixth and eighth columns are the energies found by the parameters q1 and q2 , according to the formulas (34) . The q1 and q2 values are obtained by solving the equations Eq1 = Eexp and Eq2 = Eexp . As can be seen in Table 2, it is understood that the energy is divided into two parts in the small energy states observed in the ammonia molecule. The measured energies and the calculated energies are the same. Very complex double wells are sought to explain these small vibrations. However, if there is angular momentum other than zero, it is possible to observe small vibrations in each potential well. When the angular momentum is different from zero, splitting occurs even in high energy states, but it may not be possible to measure it because the difference between the splitting energy values is very small.

Table 1 Continued...

Table 1 Some energy values of the three-axial harmonic oscillator calculated according to (34), (unit $\hbar\omega_{00}$)

States $\|(\ell)\,jm>$ $q=2$	Eq1 $\varepsilon=0$ $\gamma=0^0$	Eq2 $\varepsilon=0$ $\gamma=0^0$	Eq1 $\varepsilon=0.35$ $\gamma=0^0$	Eq2 $\varepsilon=0.35$ $\gamma=0^0$	Eq1 $\varepsilon=0.35$ $\gamma=30^0$	Eq2 $\varepsilon=0.35$ $\gamma=30^0$
f 7 / 2 5 / 2	4.30371	4.98456	4.52261	5.23809	4.1478	4.80398
f 5 / 2 5 / 2	3.36143	5.04564	3.88143	5.82618	3.4523	5.18205
g 9 / 2 5 / 2	5.26168	5.64722	5.28032	5.66723	4.92295	5.28368
g 7 / 2 5 / 2	4.30371	4.98456	4.51152	5.22525	4.14115	4.79628
d 5 / 2 5 / 2	3.36143	5.04564	3.95404	5.93517	3.49732	5.24963
h 11 / 2 5 / 2	6.22978	6.48175	6.12706	6.37487	5.7554	5.98818
h 9 / 2 5 / 2	5.26168	5.64722	5.29317	5.68102	4.93054	5.29182
i 13 / 2 5 / 2	7.20478	7.38356	7.02208	7.19631	6.6188	6.78303

Table 2 Calculated vibrational energies in the double potential well of the ammonia molecule

Eexp (unit cm^{-1})	Eexp (unit eV)	$\gamma=0$ $\varepsilon=0.00$ $q_1,\,q_2$	Ecal (unit eV)	$\gamma=0$ $\varepsilon=0.10$ $q_1,\,q_2$	Ecal (unit eV)	$\gamma=0$ $\varepsilon=0.20$ $q_1,\,q_2$	Ecal (unit eV)
0.0	0.0	0.0				0.0	0.0
0.79340	9.813×10^{-5}	2.36603q1 1.22474	9.813×10^{-5}	2.35928 1.22474	9.813×10^{-5}	2.33860 1.22474	9.813×10^{-5}
932.400	0.115324	2351.26 2349.52	0.115324	2345.98 2344.25	0.115324	2329.97 2328.23	0.115324
968.1219	0.119742	2441.30 2439.57	0.119742	2435.83 2434.09	0.119742	2419.20 2417.47	0.119742
1597.50	0.197587	4027.84 4026.11	0.197587	4018.80 4017.07	0.197587	3991.36 3989.63	0.197587
1626.2747	0.201146	4100.37 4098.64	0.201146	4091.17 4089.44	0.201146	4063.24 4061.51	0.201146
1627.3724	0.201282	4103.14 4101.41	0.201282	4093.93 4092.20	0.201282	4065.98 4064.25	0.201282
1882.1775	0.232798	4745.45 4743.72	0.232798	4734.80 4733.07	0.232798	4702.48 4700.74	0.232798
2384.200	0.294890	6010.95 6009.22	0.294890	5997.46 5995.72	0.294890	5956.51 5954.78	0.294890
2540.5243	0.314226	6405.01 6403.28	0.314226	6390.63 6388.90	0.314226	6347.00 6345.27	0.314226
2586.1286	0.319866	6519.97 6518.24	0.319866	6505.34 6503.60	0.319866	6460.92 6459.19	0.319866
2895.5219	0.358133	7299.89 7298.16	0.358133	7283.50 7281.77	0.358133	7233.77 7232.04	0.358133
3189.40	0.394482	8040.70 8038.96	0.394482	8022.65 8020.91	0.394482	7967.87 7966.14	0.394482
3215.90	0.397760	8107.50 8105.76	0.397760	8089.30 8087.56	0.397760	8034.07 8032.33	0.397760
3217.5792	0.397967	8111.73 8110.00	0.397967	8093.52 8091.79	0.397967	8038.26 8036.53	0.397967
3240.1630	0.400761	8168.66 8166.93	0.400761	8150.32 8148.59	0.400761	8094.67 8092.94	0.400761
3241.5983	0.400938	8172.28 8170.55	0.400938	8153.93 8152.20	0.400938	8098.26 8096.53	0.400938

Conclusion

In previous studies, it has been achieved a simple method for the exact general solution of the radial SE for central potential well without using any approach. In this article, by using this simple procedure, the oscillations through a barrier of arbitrary form central potential for a particle in central potential well of any form was solved without any approach. It has been applied to a barrier of quadratic form potential which is found in the quadratic form of a potential wells. It seems that our results are very compatible because there is not any

approach in our solutions whereas there is some approach in classical solutions. Our wave functions and our solutions can be applied to the quantum tunneling of particles through potential barriers, and in the solutions of every problem using molecular, atomic, and nuclear wave functions. In the present study, these wave functions were applied to quantum tunneling in a double square well potential which is available in the ammonia molecule. Here, triaxial ellipsoid shaped potential energy was taken, but similar calculations can be made by taking other double-well potentials. If there is a non-zero angular momentum, that is, rotational motion in a quantum system, there is always a double potential well in the excited states. Conversely, there is a rotation if there are double potential wells in a quantum system. Here, the energies can be calculated and compared with the energies found experimentally by taking another suitable double potential well or by changing the å parameter. Such a study may be another research topic. Here we have shown how to calculate the double potential well.

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Conflicts of interest

The author declares there is no conflict of interest.

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