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Solutions of the Schrödinger equation with the harmonic oscillator potential (HOP) in cylindrical basis

Abstract

In this paper, we have studied the Schrodinger equation in the cylindrical basis with harmonic oscillator using a Nikiforov–Uvarov technique. The energy eigenvalues and the normalized wave function for this system are also obtained. We have equally evaluated the probability current and the result shows that the oscillator propagates along the axis of symmetry of HOP.

Keywords: Schrödinger equation, harmonic oscillator potential, probability current, NU method, hermite polynomials.

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Introduction

Over the years, the Schrodinger Equation (SE) has proved an excellent tool for the study of quantum systems. The SE is solved in the non–relativistic limit both exactly and approximately. It is solved approximately for an arbitrary non–vanishing angular momentum quantum number, $l \neq 0$ and solved exactly for an s–wave $(l=0)$ by the path integral method,[1] operator algebraic method,[2] or power series method.[3–4]These are however traditional methods of solving the SE analytically.

Alternatively, it can be solved by the NU method,[5] shifted $1/N$ expression,[6] supersymmetric quantum mechanics,[7] and a host of other methods.[8–9] We use the NU method in this work and compare our results with those obtained by Greiner et al.[10]

Various authors have studied the Harmonic Oscillator Potential (HOP). For example, Ikot et al.[11] derived the energy eigenvalues and eigenfunctions for the two–dimensional HOP in Cartesian and Polar coordinates using NU method. Wang et al.[12] determined the viral theorem for a class of quantum nonlinear harmonic oscillators, Amore & Fernandez[13] studied the two–particle harmonic oscillator in a one–dimensional box and Greiner & Maruhn[10] obtained the energy eigenvalues and eigenfunctions of the HOP in cylindrical basis by factorization method.

However, it must be noted that the choice of basis set is a matter of whether the spin–orbit coupling or the deformation of the potential is more important. In practice this depends on deformation near spherical shapes. But the spin–orbit coupling splits the levels much more than the deformation, while for large deformation the cylindrical basis is closer to the true states.[10] In cylindrical basis (ρ,ϕ,z), the HOP is of the form:[10]

$$V(\rho,z)=\frac{\omega^2}{2}\left(z^2+\rho^2\right), \qquad (1)$$

Where ω is the frequency of the oscillator.

The Nikiforov–Uvarov (NU) method

The NU method[5] is used for solving any linear, second–order differential equation of the hypergeometric type:

$$\psi_n''(s)+\frac{\tilde{\tau}(s)}{\sigma(s)}\psi_n'(s)+\frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi_n(s)=0, \qquad (2)$$

Where $\sigma(s)$ and $\tilde{\tau}(s)$ are polynomials of at most, second–degree and $\tilde{\tau}(s)$ is a first degree polynomial. The primes denote derivatives with respect to the variable *s*. The function $\psi_n(s)$ can be decomposed as

$$\psi_n(s)=\varphi_n(s)y_n(s), \qquad (3)$$

So that equation (2) takes the hyper geometric from

$$\sigma(s)y_n''(s)+\tau(s)y_n'(s)+\lambda y_n(s)=0 \qquad (4)$$

Where the function $\varphi_n(s)$ is obtained from the logarithmic derivative

$$\frac{\varphi'(s)}{\varphi_n(s)}=\frac{\pi(s)}{\sigma(s)} \qquad (5)$$

Here, $\pi(s)$ is a first–degree polynomial defined as

$$\pi(s)=\frac{\sigma'(s)-\tilde{\tau}(s)}{2}\pm\sqrt{\left(\frac{\sigma'(s)-\tilde{\tau}(s)}{2}\right)^2-\tilde{\sigma}(s)+k\sigma(s)}, \qquad (6)$$

Where *k* is obtained under the condition that the discriminant of the root function of order 2 is set to zero, so as to ensure that $\pi(s)$ is a first degree polynomial.

The other part $y_n(s)$ is the hypergeometric type function whose polynomial solutions are given by the Rodrigues relation

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n}\left[\sigma^n(s)\rho(s)\right], \tag{7}$$

Where B_n is a normalization constant and $\rho(s)$ is the weight function given by

$$\rho(s) = \exp\left[\int\left(\frac{\tau(s) - \sigma'(s)}{\sigma(s)}\right)ds\right] \tag{8}$$

By computing

$$\tau(s) = \tau(s) + 2\pi(s), \tag{9}$$

Subject to the condition

$$\tau'(s) < 0 \tag{10}$$

and equating

$$\lambda = \lambda_n = -n\tau(s) - \frac{n(n-1)}{2}\sigma''(s), \quad n = 0,1,2,..., \tag{11}$$

with

$$\lambda = k + \pi'(s), \tag{12}$$

the energy eigenvalues equation is obtained.

Solutions of the Schrödinger equation (SE) in cylindrical coordinates

In orthogonal curvilinear coordinates q_i, with scale factors h_i the SE for a particle of mass M having energy E, interacting with a potential $V(q_i)$ is given by

$$\frac{-\hbar^2}{2M}\left[\left(\prod_{i=1}^{n} h_i\right)^{-1} \sum_{i=1}^{n} \frac{\partial}{\partial q_i}\left(\frac{\prod_{i=1}^{n} h_i}{h_i^2}\frac{\partial\psi(q_i)}{\partial q_i}\right)\right] + V(q_i)\psi(q_i) = E\psi(q_i) \tag{13}$$

With the identifications[14]

$h_1 = 1, h_2 = \rho, h_3 = 1, q_1 = \rho, q_{2j} = \phi, q_3 = z_j\, n = 3$ and with the potential (1), Equation (13) takes the form[10]

$$\left[\frac{-\hbar^2}{2M}\left(\frac{\partial^2}{\partial z^2} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{\partial^2}{\partial\phi^2}\right) + \frac{\omega^2}{2}\left(z^2 + \rho^2\right)\right]\psi(\rho,\phi,z) = E\psi(\rho,\phi,z) \tag{14}$$

By using the decomposition

$$\psi(\rho,\phi,z) = \zeta(z)\chi(\rho)\eta(\phi) \tag{15}$$

Equation (14) reduces to the following equations:

$$\left(\frac{d^2}{d\phi^2} + \mu^2\right)\eta(\phi) = 0 \tag{16}$$

$$\left(\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} - \frac{M^2\omega^2\rho^2}{\hbar} - \frac{\mu^2}{\rho^2} + \frac{2M\Lambda}{\hbar^2}\right)\chi(\rho) = 0 \tag{17}$$

$$\left(\frac{d^2}{dz^2} - \frac{M^2\omega^2 z^2}{\hbar^2} + \frac{2M(E-\Lambda)}{\hbar^2}\right)\zeta(z) = 0, \tag{18}$$

Where μ and Λ are separation constants.

Solution of the ϕ – equation

The ϕ –equation is easily solved to give

$$\eta_\mu(\phi) = \frac{1}{\sqrt{2\pi}}e^{i\mu\phi}, \quad \mu = 0, \pm 1, \pm 2, ... \tag{19}$$

Solution of the ρ – *equation*

By using the transformation $\rho^2 \to s$, Equation (17) reduces to the hyper geometric form

$$\chi''(s) + \frac{\chi'(s)}{s} + \frac{1}{s^2}\left[\frac{-\beta^2\delta^2 - \mu^2}{4} + \alpha s\right]\chi(s) = 0, \tag{20}$$

Where

$$\beta = \frac{M\omega}{\hbar}$$

$$\alpha = \frac{M\Lambda}{2\hbar^2}$$

Comparing Equation (20) with Equation (2), we obtain the following polynomials

$$\sigma(s) = s, \tilde{\tau}(s) = 1, \tilde{\sigma}(s) = -\frac{\beta^2 s^2 \mu^2}{4} + \alpha s, \pi(s) = \pm\sqrt{\frac{\beta^2 s^2 \mu^2}{4} - \alpha s + ks} \tag{21}$$

On setting the discriminate of $\pi(s)$ to zero, we obtain the following expressions for $\pi(s)$

$$\pi(s) = \pm\begin{cases} \dfrac{\beta s + \mu}{2}, for\, k_+ = \alpha + \dfrac{\beta\mu}{2} \\ \dfrac{\beta s - \mu}{2}, for\, k_- = \alpha - \dfrac{\beta\mu}{2} \end{cases} \tag{22}$$

so that

$$\pi(s) = -\frac{\beta s + \mu}{2}, k = k_- = \alpha - \frac{\beta\mu}{2} \tag{23}$$

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and

$$\tau(s) = 1 + \mu - \beta s, \tau'(s) = -\beta < 0, \; since \beta > 0 \quad (24)$$

Thus,

$$\lambda = \alpha - \frac{\beta\mu}{2} - \frac{\beta}{2}, \quad (25)$$

and using (11),

$$\lambda = \lambda_n = n\beta \quad (26)$$

Equating (25) and (26) yields the condition for Λ :

$$\Lambda = \hbar\omega\left(2n + |\mu| + 1\right) \quad (27)$$

Using Equations (21, 23 & 5), we obtain the function $\phi(s)$ as

$$\varphi(s) = \alpha_\mu s^{|\mu|/2} e^{\beta s/2}, \quad (28)$$

Where α_μ is the integration constant. The weight function is obtained using Equations (24, 21 & 8) as

$$\rho(s) = b_\mu e^{-\beta s} s^{|\mu|}, \quad (29)$$

Thus, we obtain the other part of the wave function $y_n(s)$ as

$$y_n(s) = N e^{\beta s} s^{-|\mu|} \frac{d^n}{ds^n}\left[s^{n+|\mu|} e^{-\beta s}\right] = N_{n\rho} L_{n\rho}^{|\mu|}(\beta s), \quad (30)$$

Where $L_n^{|\mu|}(\xi)$ are the associated Laquerre polynomials.

Thus,

$$\chi(s) = N_{n_\rho} s^{|\mu|/2} e^{-\beta s/2} L_{n_\rho}^{|\mu|}(\beta s), \quad (31)$$

or

$$\chi(\rho) = N_{n_\rho} \rho^{|\mu|/2} e^{-\beta\rho/2} L_{n_\rho}^{|\mu|}(\beta\rho^2), \quad (32)$$

Where n_p is the number of quanta in the ρ – direction.

Solution of the z–equation

By using the transformation $z^2 \to s$, Equation (18) reads

$$\xi''(s) + \frac{\xi'(s)}{2s} + \frac{1}{4s^2}\left[-\beta^2 s^2 + ys\right]\xi(s) = 0, \quad (33)$$

with the identification

$$\gamma = \frac{2M(E - \Lambda)}{\hbar^2}$$

Following the same procedure in subsection, we obtain the following:

$$\sigma(s) = 2s, \; \tilde{\tau}\sigma(s) = -\beta^2 s^2 + \gamma s, \quad (34)$$

with

$$\pi(s) = \frac{1}{2} \pm \begin{cases} \beta s + \frac{1}{2}, \; for \; k_+ = \frac{\gamma + \beta}{2} \\ \beta s - \frac{1}{2}, \; for \; k_- = \frac{\gamma - \beta}{2} \end{cases} \quad (35)$$

so that

$$\pi(s) = -\beta s + 1, \; \tau(s) = 3 - 2\beta s. \quad (36)$$

Thus,

$$\lambda = k + \pi'(s) = \frac{\gamma - \beta}{2} - \beta = \lambda_n = 2n\beta$$

and

$$E - \Lambda = \hbar\omega\left(2n + \frac{3}{2}\right) \quad (37)$$

Using the condition (27), the energy eigenvalues of the system become

$$E = \hbar\omega\left(n_z + 2n_\rho + |\mu| + \frac{3}{2}\right) \quad (38)$$

where

$$n_2 = 2n_\rho + 1.$$

This is a unique result and we note that n_ρ counts twice because it contains two oscillator directions and the angular momentum projection, μ contributes to the energy because of the centrifugal potential.

The wave function $\varphi(s)$ is obtained as

$$\varphi(s) = a_{n_i} e^{-\beta s/2} \quad (39)$$

and the weight function

$$\rho(s) = b_{n_i}\sqrt{s} e^{-\beta s}, \quad (40)$$

so that

$$Y_{n_i}(s) = Ne^{-\beta s/2} L_{n_z}^{1/2}(\beta s). \quad (41)$$

Consequently,

$$\zeta(z) = Nze^{-\beta z^2/2} L_{n_z}^{1/2}(\beta z^2). \quad (42)$$

Using the relation[15,16]

$$H_{2n+1}(x) = (-1)^n 2^{2n+1} n! x L_n^{1/2}(x^2), \quad (43)$$

we obtain

$$\zeta(z) = N_{n_i} e^{-\beta z^2/2} H_{n_z}\left(\sqrt{\beta} z\right), \quad (44)$$

Where $H_{n_z}(\zeta)$ are the Hermite Polynomials of order n_z .

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Thus, the complete wave function for the HOP in cylindrical basis is expressed as

$$\psi_{n_z n_\rho \mu}(z,\rho,\phi) = N_{n_z n_\rho \mu} e^{-\beta/2(z^2+\rho^2)} H_{n_z}\left(\sqrt{\rho z}\right)\rho^{|\mu|} L_{n_\rho}^{|\mu|}\left(\beta\rho^2\right)e^{i\mu\phi} \quad (45)$$

Equations (45, 38 & 27) are the same as those obtained by Greiner et al.[10] By using the normalization condition[17–19]

$$\int |\psi|^2 d\tau = 1, \quad (46)$$

together with the relations[16,20]

$$\int_0^\infty dx e^{-x} x^m L_n^m(x) = \frac{(n+m)!}{n!}\delta_{n'n} \quad (47)$$

$$\int_{-\infty}^\infty dx e^{-x^2} H_{n'}(x) H_n(x) = 2^n n! \sqrt{x}\delta_{n'n}, \quad (48)$$

we obtain the normalization constant $N_{nzn_\upsilon\mu}$ as

$$N_{n_z n_\rho \mu} = \sqrt{\frac{(n_\rho + |\mu|)!}{2^{n_z+2}\beta^{|\mu|+1/2}\pi^{3/2} n_\rho! n_z!}} \quad (49)$$

Thus,

$$\psi_{n_z n_\rho \mu}(z,\rho,\phi) = \sqrt{\frac{(n_\rho + |\mu|)!}{2^{n_z+2}\beta^{|\mu|+1/2}\pi^{3/2} n_\rho! n_z!}} e^{-\beta/2(z^2+\rho^2)} H_{n_z}\left(\sqrt{\beta z}\right)\rho^{|\mu|} L_{n_\rho}^{|\mu|}\left(\beta\rho^2\right)e^{i\mu\phi} \quad (50)$$

The probability current

The probability current is defined as[17]

$$J = \frac{i\hbar}{2M}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right) \quad (51)$$

or in cylindrical coordinates

$$J(z,\rho,\phi) = \frac{i\hbar}{2M}\left\{\left(\psi\partial_\rho^* - \psi^*\partial_\rho\right)\hat{\rho} + \frac{1}{\rho}\left(\psi\partial_\phi^* - \psi^*\partial_\phi\right)\hat{\phi} + \left(\psi\partial_z^* - \psi^*\partial_z\right)\hat{z}\right\}, \quad (52)$$

where we have adopted the notation

$$\partial_a \equiv \frac{\partial\psi}{\partial a}, \partial_a^* \equiv \frac{\partial\psi^*}{\partial a} \quad (53)$$

Using the relations[16,20]

$$\frac{d^m}{dx^m}\left\{H_n(x)\right\} = \frac{2^m n!}{(n-m)!}H_{n-m}(x), \; for \; m < n \quad (54)$$

and

$$\frac{d}{dx}\left\{L_n^m(x)\right\} = -L_{n-1}^{m+1}(x), \quad (55)$$

we obtain the following derivatives:

$$\partial_\rho^* = \psi^*\left(-\beta\rho + \frac{|\mu|}{\rho}\right) - 2\beta N_{n_z n_\rho \mu}\rho^{|\mu|+1} e^{-\beta/2(z^2+\rho^2)} H_{n_z}\left(\sqrt{\beta z}\right) L_{n_\rho-1}^{|\mu|+1}\left(\beta\rho^2\right)e^{-i\mu\rho} \quad (56)$$

$$\frac{\partial_\rho^*}{\rho} = \frac{i|\mu|}{\rho}\psi \quad (57)$$

$$\partial_z^* = -\psi^*\beta z + 2n\sqrt{\beta}\, e^{-\beta/2(z^2+\rho^2)} N_{n_z n_\rho \mu}\rho^{|\mu|} L_n^{|\mu|}\left(\beta\rho^2\right) H_{n-1}\left(\sqrt{\beta\rho}\right)e^{-i\mu\phi} \quad (58)$$

Taking the conjugate of the above derivatives, we obtain expressing for $\partial_\rho, \frac{1}{\rho}\partial_\phi, \partial_z$. Thus, the probability current for the harmonic oscillator in cylindrical basis becomes

$$\vec{J}(z,\rho,\phi) = \frac{|\mu|\hbar}{M\rho}\left|\psi_{n_z n_\rho \mu}\right|^2\hat{\phi} = \frac{|\mu|\hbar}{M\rho}\left(\frac{(n\rho+|\mu|)!}{2^{n_z+2}\beta^{|\mu|+1/2}\pi^{3/2} n\rho!}\right)e^{-\beta(z^2+\rho^2)}\rho^{|\mu|} H_{n_z}\left(\sqrt{\beta z}\right) L_{n_\rho}^{|\mu|}\left(\beta\rho^2\right)\hat{\phi} \quad (59)$$

This indicates that the oscillator propagates along the axis of symmetry of the HOP.

Conclusion

We have obtained analytically the energy eigenvalues and normalized eigenfunctions of the SE with the HOP in cylindrical basis using a quite different powerful mathematical tool: Nikiforov–Uvarov method. Our results are in good agreement with those obtained by Greiner et al.[10] As an application of our results we have also determined the probability current of the HOP in cylindrical basis.

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Conflict of interest

Authors declare that there is no conflict of interest.

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