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

Abstract

In this paper, we have studied the Schrödinger 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.

Introduction

Over the years, the Schrödinger 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 ≠ 0 and solved exactly for an s–wave (l = 0) by the path integral method,1 operator algebraic method,2 or power series method.3–8 These are however traditional methods of solving the SE analytically.

Alternatively, it can be solved by the NU method,9 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 virial theorem for a class of quantum nonlinear harmonic oscillators, Amore & Fernandez13 studied the two–particle harmonic oscillator in a one–dimensional box and Greiner & Maruhn14 obtained the energy eigenvalues and eigenfunctions of the HOP in cylindrical basis by factorization method.

However, it must be noticed 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

\[ V(\rho, z) = \frac{\omega^2}{2}(z^2 + \rho^2), \]

Where \( \omega \) is the frequency of the oscillator.

The nikiforov–uvarov (NU) method

The NU method10 is used for solving any linear, second–order differential equation of the hypergeometric type:

\[ \psi''_n(s) + \frac{\tau(s)}{\sigma(s)} \psi'_n(s) + \frac{\sigma(s)}{\sigma^2(s)} \psi_n(s) = 0, \]

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

\[ \psi_n(s) = \varphi_n(s) y_n(s), \]

So that equation (2) takes the hyper geometric from

\[ \sigma(s) y'_n(s) + \tau(s) y'_n(s) + \lambda y_n(s) = 0 \]

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

\[ \frac{\varphi'(s)}{\varphi_n(s)} = \frac{\pi(s)}{\sigma(s)} \]

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

\[ \pi(s) = \frac{\sigma'(s) - \tau(s)}{2} \left[ \frac{(\sigma'(s) - \tau(s))^2}{2} - \sigma(s) + k\sigma(s) \right], \]

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

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

\[ \rho(s) = \exp \left[ j \left( \tau(s) - \sigma(s) \right) \frac{ds}{\sigma(s)} \right], \]  
(8)

By computing \( \tau(s) = \tau(s) + 2 \pi(s) \),

\[ \tau'(s) < 0 \]  
(9)

Subject to the condition

\[ \tau'(s) < 0 \]  
(10)

and equating

\[ \lambda = \lambda_n = -n \pi \left( s - \frac{n(n-1)}{2} \sigma(s) \right), \quad n = 0, 1, 2, \ldots \]  
(11)

with

\[ \lambda = k + \pi(s) \],

(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 \( V(q) \) is given by

\[ -\frac{\hbar^2}{2M} \left( \sum_{i=1}^{n} h_i \nabla_i \right)^2 + V(q) \psi(q) = E \psi(q) \]  
(13)

With the identifications \( h_1 = \rho, h_2 = \sigma, h_3 = s, q_1 = \rho, q_2 = \phi, q_3 = z, n = 3 \) and with the potential (1), Equation (13) takes the form

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

By using the decomposition

\[ \psi(\rho, \phi, z) = \zeta(z) \chi(\rho) \eta(\phi) \]  
(15)

Equation (14) reduces to the following equations:

\[ \frac{d^2}{d\phi^2} + \mu^2 \chi(\rho) \eta(\phi) = 0 \]  
(16)

\[ \frac{d^2}{d\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} - \frac{M_\omega^2 \rho^2}{\hbar^2} - \frac{\mu^2}{\rho^2} + \frac{2MA}{\hbar^2} \chi(\rho) \]  
(17)

\[ \frac{d^2}{dz^2} - \frac{M_\omega^2 z^2}{\hbar^2} + \frac{2M(E - \Lambda)}{\hbar^2} \zeta(z) = 0, \]  
(18)

Where \( \mu \) and \( \Lambda \) are separation constants.

**Solution of the \( \phi \)–equation**

The \( \phi \)–equation is easily solved to give

\[ \eta(\phi) = \frac{1}{\sqrt{2\pi}} e^{i\mu \phi}, \quad \mu = 0, \pm 1, \pm 2, \ldots \]  
(19)

**Solution of the \( \rho \)–equation**

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

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

Where

\[ \beta = \frac{M_\omega}{h} \]

\[ \alpha = \frac{MA}{2h^2} \]

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

\[ \sigma(s) = s, \tau(s) = 1, \sigma(s) = -\beta^2 s^2 - \mu^2 + \alpha s, \pi(s) = \pm \sqrt{\beta^2 s^2 + \mu^2 - \alpha s + ks} \]  
(21)

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

\[ \pi(s) = \pm \frac{\beta s + \mu}{2}, \quad \text{for} \quad k_+ = \alpha + \frac{\beta \mu}{2} \]  
(22)

\[ \pi(s) = \pm \frac{\beta s - \mu}{2}, \quad \text{for} \quad k_- = \alpha - \frac{\beta \mu}{2} \]  
(23)

\[ \pi(s) = -\frac{\beta s + \mu}{2}, \quad k = k_- = \alpha - \frac{\beta \mu}{2} \]  
(24)

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\[ \tau(s) = 1 + \mu - \beta s, \tau'(s) = -\beta < 0, \text{ since } \beta > 0 \] \hspace{1cm} (24)

Thus,
\[ \lambda = \alpha - \frac{\beta \mu}{2} - \frac{\beta}{2}, \] \hspace{1cm} (25)

and using (11),
\[ \lambda = \lambda_n = n\beta \] \hspace{1cm} (26)

Equating (25) and (26) yields the condition for \( \Lambda \):
\[ \Lambda = \hbar \omega \left( 2n + |\mu| + 1 \right) \] \hspace{1cm} (27)

Using Equations (21, 23 & 5), we obtain the function \( \varphi(s) \) as
\[ \varphi(s) = \alpha \rho^{1/2} e^{-\rho s/2}, \] \hspace{1cm} (28)

Where \( \alpha \rho \) is the integration constant. The weight function is obtained using Equations (24, 21 & 8) as
\[ \rho(s) = \beta \rho e^{-\rho s}, \] \hspace{1cm} (29)

Thus, we obtain the other part of the wave function \( \gamma(s) \) as
\[ \gamma(s) = N \left( \frac{d^n}{ds^n} \left[ s^n \rho s e^{-\rho s} \right] \right) = N \rho^{1/2} \left( \frac{\partial^n}{\partial \rho^n} \right) \left( \beta \rho s \right), \] \hspace{1cm} (30)

Where \( \rho^{1/2}(\beta) \) are the associated Laguerre polynomials.

Thus,
\[ \chi(s) = N \rho^{1/2} e^{-\rho s/2} \rho^{1/2} \left( \beta \rho s \right), \] \hspace{1cm} (31)

or
\[ \chi(s) = N \rho^{1/2} e^{-\rho s/2} \rho^{1/2} \left( \beta \rho^2 s \right), \] \hspace{1cm} (32)

Where \( \rho \) is the number of quanta in the \( \rho \) direction.

**Solution of the z-equation**

By using the transformation \( z^2 \rightarrow s \), Equation (18) reads
\[ \frac{\zeta''(s)}{2s} + \frac{\zeta'(s)}{4s} + \left[ -\beta^2 s^2 + \gamma s \right] \zeta(s) = 0, \] \hspace{1cm} (33)

with the identification
\[ \gamma = \frac{2M(E - \Lambda)}{\hbar^2} \]

Following the same procedure in subsection, we obtain the following:
\[ \sigma(s) = 2s, \quad \tau(s) = -\beta^2 s^2 + \gamma s, \] \hspace{1cm} (34)

with
\[ \pi(s) = \frac{1}{2} \left( \beta s + \frac{1}{2}, \text{ for } k = \frac{\gamma + \beta}{2} \right) \]

so that
\[ \pi(s) = -\beta s + 1, \quad \tau(s) = 3 - 2\beta s. \] \hspace{1cm} (36)

Thus,
\[ \lambda = k + \pi(s) = \frac{\gamma - \beta}{2} - \beta = \lambda_n = 2n\beta \]

and
\[ E - \Lambda = \hbar \omega \left( 2n + \frac{3}{2} \right) \] \hspace{1cm} (37)

Using the condition (27), the energy eigenvalues of the system become
\[ E = \hbar \omega \left( n + \frac{3}{2} \right) \]

where
\[ n_2 = 2n_1 + 1. \]

This is a unique result and we note that \( n_1 \) counts twice because it contains two oscillator directions and the angular momentum projection, \( \mu \) contributes to the energy because of the centrifugal potential.

The wave function \( \varphi(s) \) is obtained as
\[ \varphi(s) = a \rho e^{-\rho s/2} \]

and the weight function
\[ \rho(s) = b \rho e^{-\rho s/2}, \]

so that
\[ Y_n(s) = Ne^{-\rho s/2} \rho^{1/2} \left( \beta \rho s \right). \] \hspace{1cm} (41)

Consequently,
\[ \zeta(z) = N \rho e^{-\rho^2 z/2} \rho^{1/2} \left( \beta \rho^2 s \right). \] \hspace{1cm} (42)

Using the relation \( ^{15,16} \)
\[ H_{2n+1}(x) = (-1)^n 2^{2n+1} n! x^{1/2} \left( x^2 \right). \] \hspace{1cm} (43)

we obtain
\[ \zeta(z) = N \rho e^{-\rho^2 z/2} H_{n_2} \left( \sqrt{\beta} z \right). \] \hspace{1cm} (44)

Where \( H_{n_2} \) are the Hermite Polynomials of order \( n_2 \).
Thus, the complete wave function for the HOP in cylindrical basis is expressed as

$$\psi_{n_z n_r n_\theta n_\phi}(x, \rho, \phi, \theta) = N_{n_z n_r n_\theta n_\phi} e^{-\frac{\rho}{2}(x^2 + \rho^2)} H_n \left( \sqrt{\rho^2} \rho \right) \beta \rho H_{n_\theta} \left( \beta \rho \right) e^{i\rho \phi}$$

Equations (45, 38 & 27) are the same as those obtained by Greiner et al.\textsuperscript{10} By using the normalization condition\textsuperscript{13–19}

$$\int \psi^* \psi \, d\tau = 1,$$

we obtain the normalization constant $N_{n_z n_r n_\theta n_\phi}$ as

$$N_{n_z n_r n_\theta n_\phi} = \frac{\sqrt{\sqrt{2^{n_\theta + 1/2} \pi^{3/2} n_\theta ! n_\phi ! \beta^{n_\phi + 1/2} \beta^{n_\theta + 1/2}}} H_n \left( \sqrt{\rho^2} \rho \right) \beta \rho H_{n_\theta} \left( \beta \rho \right)}{\sqrt{2^{n_r + 1/2} \pi^{3/2} n_r ! n_\theta !}}.$$

Thus,

$$\psi_{n_z n_r n_\theta n_\phi}(x, \rho, \phi, \theta) = \frac{\sqrt{\sqrt{2^{n_\theta + 1/2} \pi^{3/2} n_\theta ! n_\phi ! \beta^{n_\phi + 1/2} \beta^{n_\theta + 1/2}}} H_n \left( \sqrt{\rho^2} \rho \right) \beta \rho H_{n_\theta} \left( \beta \rho \right)}{\sqrt{2^{n_r + 1/2} \pi^{3/2} n_r ! n_\theta !}} e^{-\frac{\rho}{2}(x^2 + \rho^2)}.$$

### The probability current

The probability current is defined as\textsuperscript{17}

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

or in cylindrical coordinates

$$j(z, \rho, \phi, \theta) = \frac{i\hbar}{2M} \left( \left( \psi_r \hat{\rho} + \psi_\rho \hat{\rho} \right) \hat{\rho} + \frac{1}{\rho} \left( \psi_\rho \hat{\rho} + \psi_\phi \hat{\phi} \right) \hat{\phi} + \left( \psi_\phi \hat{\phi} + \psi_\theta \hat{\theta} \right) \hat{\theta} \right),$$

where we have adopted the notation

$$\partial_a = \frac{\partial}{\partial a}, \quad \partial_a^* = \frac{\partial^*}{\partial a^*}.$$

Using the relations\textsuperscript{16,20}

$$\frac{d^m}{dx} H_n(x) = \frac{2^m n!}{(n-m)!} H_{n-m}(x), \text{ for } m < n$$

and

$$\frac{d}{dx}(n_\theta^m(x)) = -L_{n-1}^m(x),$$

we obtain the following derivatives:

$$\partial_\rho^* = \psi^* \left( -\beta \rho + \frac{\beta^2}{\rho} \right),$$

$$\partial_\rho = \frac{\beta}{\rho},$$

$$\partial_\phi = -\beta \rho + 2 n \sqrt{\rho} e^{-\beta \rho^2 / 2} n_{z+n_\theta} \rho H_{n_\theta} \left( \beta \rho \right) H_{n+1} \left( \beta \rho \right) e^{-\beta \rho^2 / 2}.$$


