APPLYING VARIATION PRINCIPLE TO 3D QUANTUM HARMONIC OSCILLATOR SYSTEM*

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Abstract

Quantum system with 3D harmonic oscillator well is one of the few problems in quantum mechanics that can be solved analytically. In this work, variational principle is applied to calculate eigenvalues and eigenstates of 3D harmonic oscillator system. The trial wave function is chosen as a linear superposition of Gaussian basis function of the form $r^{m_i}e^{-\frac{r^2}{b_i^2}}$. To validate the variational results, a numerical approach known as Numerov method is also used to calculate energy values and wave functions. The calculated values are further compared with analytical solutions. The results demonstrate that for a basis size of twelve, the energy values for low-lying states up to N = 15 agree very well with the analytical results, making this work suitable for applications to low-lying energy states.

Keywords: 3D harmonic oscillator, variational principle, Numerov method

Introduction

Variational principle, one of the famous approximation methods in quantum mechanics, states that for a quantum system represented by any trial wave function $|\psi\rangle$ with Hamiltonian H, the true ground state energy is less than or equal to the expectation value of the Hamiltonian with respect to trial wave function. Therefore, for a system of known Hamiltonian, it is useful to determine the upper bound energy eigenvalue. Mathematically, it can be expressed as follows.

$$E_0 \leq \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

where $\langle\psi|H|\psi\rangle$ is the expectation value of the Hamiltonian with respect to trial wave function. According to the principle, true ground state energy is achieved only when trial wave function exactly matches true ground state wave function.

Variational principle is often applied in determining ground state energy. But it could also be extended to higher energy states which is also known as generalized Rayleigh– Ritz method [Yasuyuki S, 1998)]. In mathematical form, it could be expressed as follows.

$$E_n \leq \frac{\langle\psi_n|H|\psi_n\rangle}{\langle\psi_n|\psi_n\rangle}, (n = 0, 2, 3, \ldots)$$

To apply variational principle in practical calculation, trial wave function is initially constructed with adjustable parameters which are later varied to minimize energy value. Trial wave function could take any form or any function, but it must satisfy properties of a well-behaved wave function such as square-integrability and convergence at infinity.

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In this work, gaussian basis which is in the form of $r^{m_i}e^{-\frac{r^2}{b_i^2}}$ is chosen as trial basis state. Here, m_i and b_i are known as variational parameters. The parameter b_i is linked to gaussian fall off distance. It determines how far the spatial extent of a gaussian is. Larger b_i represents broader gaussian distribution and smaller b_i results in narrow gaussian width with rapid decay. Therefore, b_i is important parameter in controlling the width of the gaussian basis function. For second parameter m_i, as the value is increased, the peak of the gaussian distribution moves toward larger value of r. The value of m_i determines the peak position of the gaussian basis along the radial axis. The higher m_i value, the more gaussian distribution is translated away from the origin.

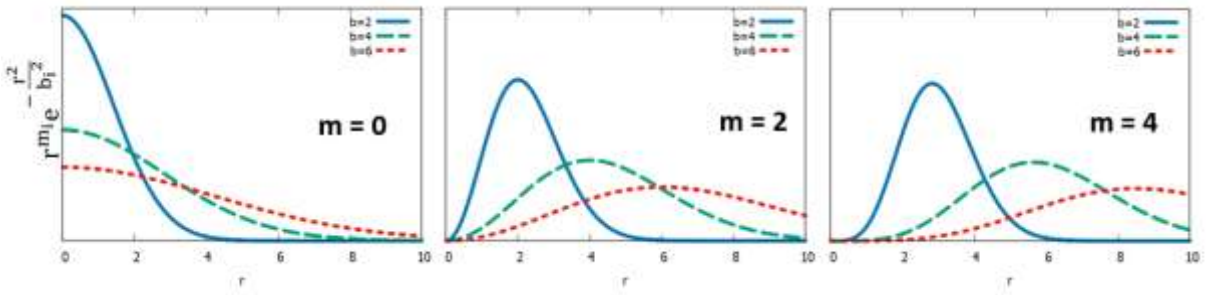

Figure 1. Basis states for various m_i and b_i values

Our trial wave function which is linear combination of chosen gaussian can now be written as $R(r) = \sum_{i=1}^{n} c_i r^{m_i} e^{-\frac{r^2}{b_i^2}}$. Here, n is the number of basis states, c_i is the expansion coefficient in the linear combination of the basis states. It quantifies the contribution of each basis state to the overall wavefunction.

Numerov method, which is also applied in this work, is a mathematical tool which can be used to solve second order differential equation of the form:

$$\frac{d^2y}{dx^2} = g(x)y(x) + s(x)$$

Schrodinger equation which can be written as $\frac{d^2\psi}{dr^2} + k^2(r)\psi = 0$, is an example of such equation and can be solved by using Numerov method. In this equation, the value of k which contains energy value reflects the curvature of the wave function. Setting the energy higher than the actual value gives wave function in higher nodes. On contrary, lower energy value results in equal or fewer number of nodes. By counting the number of nodes and comparing with desired number, one can estimate the energy eigenvalue of a quantum system.

In essence, variational principle gives theoretical framework to get a better estimation of wave function. Whereas, Numerov method is a numerical technique used to solve second order differential equation.

Numerical Calculations for 3D Harmonic Oscillator

Harmonic oscillator potential well is central potential which is expressed as $V(r) = \frac{1}{2}m\omega^2 r^2$. In this work, using natural units, Hamiltonian operator of harmonic oscillator potential can be written as follows.

$$H = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + \frac{1}{2}r^2$$

For central potential, which depends only on radial distance, wave function can be written as $\psi(r,\theta,\phi) = R(r)Y_{lm}(\theta,\phi) = \frac{U(r)}{r}Y_{lm}(\theta,\phi)$. Our trial wave function for radial part is already chosen as $R(r) = \sum_{i=1}^{n} c_i r^{m_i} e^{-\frac{r^2}{b_i^2}}$. Accordingly, new basis can be written as $u_i(r) = r^{m_i+1} e^{-\frac{r^2}{b_i^2}}$ and new wave function U(r) is a linear combination of these new 'n' number of basis states.

By solving generalized eigenvalue equation which is in matrix form of $Hc = ESc$ [Yasuyuki S, 1998], energy eigenvalues, E and wave function U(r) can be calculated. Here, H is Hamiltonian operator whose matrix element is given by $\langle u_i(r)|H|u_j(r)\rangle$, S is overlap matrix with matrix elements given by $\langle u_i(r)|u_j(r)\rangle$ which reduces to identity matrix for orthonormal basis states, c is a n-dimensional column vector with i^{th} component corresponding to c_i and E is energy eigenvalue. By adjusting parameters in the chosen basis, lower energy values can be obtained. According to the variational principle, the lower energy eigenvalues, the closer our trial wave function is to the true wave function.

Algorithm for applying variational principle

1. Staring with one single basis state, parameter values of m_1 and b_1 are initialized.
2. Overlap matrix elements and Hamiltonian matrix elements are calculated. The use of gaussian basis simplifies computation of matrix elements.
3. Generalized eigenvalue equation $Hc = ESc$, in matrix form, is solved by using DGGEV subroutine under LAPACK library [Joshua I, 2018]. This step provides energy eigenvalue E and corresponding expansion coefficient c_i.
4. The parameter b_1 is updated to minimize energy eigenvalue. It is found that choosing b_1 value of 1.41 gives optimal ground state energy value in the calculation.
5. Once optimal parameter b_1 is determined, the number of basis states is increased with m_i assigned as i-1 for each additional term. Adding higher values of m_i corresponds to shift of Gaussian peak away from the origin. The number of basis states is increased until energy convergence criterion is satisfied
6. The wave function corresponding to the calculated energy eigenvalue is calculated and normalized.

For the Numerov calculation, the second order differential equation in the form of radial equation for central potential, $\left(-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + \frac{1}{2}r^2\right)U(r) = EU(r)$ is solved [Nouredine Z, 2009]. Different values of l correspond to different effective potential wells. To solve this second order differential equation, recursion relations known as Numerov forward and Numerov backward calculations are employed to determine the wave function at successive points. For second order differential equation of the form $\frac{d^2U(r)}{dr^2} + k^2(r)U(r) = 0$, Numerov forward and Numerov backward relations can be expressed as follows respectively.

$$U(r+h) = \frac{2\left[1 - \frac{5}{12}h^2k(r)^2\right]U(r) - \left[1 + \frac{1}{12}h^2k(r-h)^2\right]U(r-h)}{1 + \frac{1}{12}h^2k^2(x+h)}$$

$$U(r-h) = \frac{2\left[1 - \frac{5}{12}h^2k(r)^2\right]U(r) - \left[1 + \frac{1}{12}h^2k(r+h)^2\right]U(r+h)}{1 + \frac{1}{12}h^2k^2(x+h)}$$

The above two equations indicate that the value of the wave function at a given point can be determined from its values at two successive neighboring points separated by a small radial step size 'h'. To achieve high-order accuracy, the value of h must be chosen sufficiently small. To initialize the wave function, the asymptotic forms are applied: near the origin $U(r) \sim r^{l+1}$ and at large distances, $U(r) \sim e^{-k^2(r)}$ correspondingly.

In the calculation, the number of nodes obtained from the Numerov method is counted and compared with expected number of nodes for a given state. By evaluating the difference in number of nodes, trial energy value is updated iteratively by using bisection method.

Algorithm for applying Numerov Method

1. Start with trial energy value E which is taken as top of the well in the program.
2. Numerov forward recursion relation is used to calculate wave function at each radial point and number of nodes is counted.
3. Calculated number of nodes is compared with expected number of nodes. If calculated number of nodes exceeds the desired number, trial energy is too high and upper bound of the energy bracket is updated. If the computed number of nodes is smaller, the trial energy is low and lower bound is updated. The Bi-section method is applied iteratively to refine energy values until energy convergence criterion is satisfied.
4. Once the desired energy value is obtained, Numerov backward recursion is applied. At the classical turning point, wave function values calculated by using Numerov backward and forward recursion relations are matched to ensure wave function continuity.
5. The resulting wave function is then normalized.

Result and Discussion

Some low-lying energy eigenvalues and eigen states for different n and l quantum numbers calculated by using variational method and the Numerov method are presented in the tables. Additionally, analytical results are also provided. Calculated energy eigenstates are for l = 0, 1, 2, and 3 and for each l value first four low lying energy values are presented.

Eigenvalue analysis

For the variational method, calculated eigenvalues by using basis number of four, eight and twelve are compared. With basis size of four and eight, very low level eigen states agree well with the analytical results. However, as energy levels become higher, discrepancy becomes significantly larger. As the basis size is increased to twelve, this discrepancy is significantly reduced, and results are in much closer agreement with the analytical values. For comparison, energy values calculated by using Numerov method are also included in the tables.

Table 1. Calculated energy values by using variational principle, Numerov method and analytical result for l = 0

n	l	Energy values by using variational method of different basis states			Energy values by using Numerov method	Analytical result $(N + 1\frac{1}{2})$ N = 2n + 1
		4 basis states	8 basis states	12 basis states		
0	0	1.5000	1.5000	1.5000	0.5000	0.5000
1	0	3.5000	3.5000	3.5000	3.5000	3.5000
2	0	5.5330	5.5000	5.5000	5.5000	5.5000
3	0	11.0791	7.5000	7.5000	7.5000	7.5000

Table 2. Calculated energy values by using variational principle, Numerov method and analytical result for l = 1

n	l	Energy values by using variational method of different basis states			Energy values by using Numerov method	Analytical result $(N + 1\frac{1}{2})$ N = 2n + 1
		4 basis states	8 basis states	12 basis states		
0	1	2.5000	2.5000	2.5000	2.5000	2.5000
1	1	4.5000	4.5000	4.5000	4.5000	4.5000
2	1	7.0537	6.5000	6.5000	6.5000	6.5000
3	1	34.8303	8.5000	8.5000	8.5000	8.5000

Table 3. Calculated energy values by using variational principle, Numerov method and analytical result for l = 2

n	l	Energy values by using variational method of different basis states			Energy values by using Numerov method	Analytical result $(N + 1\frac{1}{2})$ N = 2n + 1
		4 basis states	8 basis states	12 basis states		
0	2	3.5000	3.5000	3.5000	3.5000	3.5000
1	2	5.5320	3.5000	5.5000	5.5000	5.5000
2	2	10.5275	7.5000	7.5000	7.5000	7.5000
3	2	83.8682	9.5012	9.5000	9.5000	9.5000

Table 4. Calculated energy values by using variational principle, Numerov method and analytical result for l = 3

n	l	Energy values by using variational method of different basis states			Energy values by using Numerov method	Analytical result $(N + 1\frac{1}{2})$ N = 2n + 1
		4 basis states	8 basis states	12 basis states		
0	3	4.5000	4.5000	4.5000	4.5000	4.5000
1	3	6.8507	6.5000	6.5000	6.5000	6.5000
2	3	16.2851	8.5000	8.5000	8.5000	8.5000
3	3	157.6074	10.5275	10.5000	10.5000	10.5000

Eigen state analysis

Calculated wave functions by using variational principle with basis size of twelve, Numerov method and analytical solutions of the first six low lying energy states are illustrated in the graphs. The green thick line, dark dashed line and pink line correspond to variational result, Numerov result and analytical results correspondingly. Since variational results in this work produce low lying energy values very well, calculated eigen states yield strong agreement with analytical results. The calculated wave functions are shown in the following graphs.

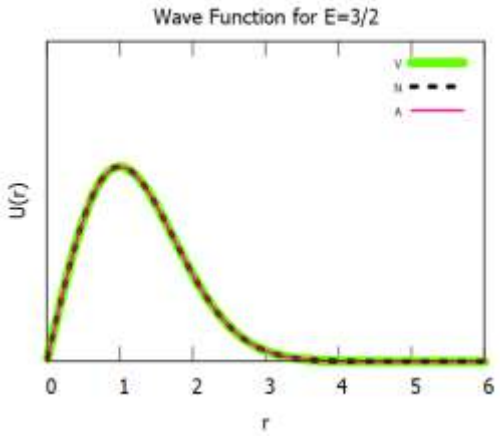

Figure 2. Wave function for N = 0 (n = 0, l = 0)

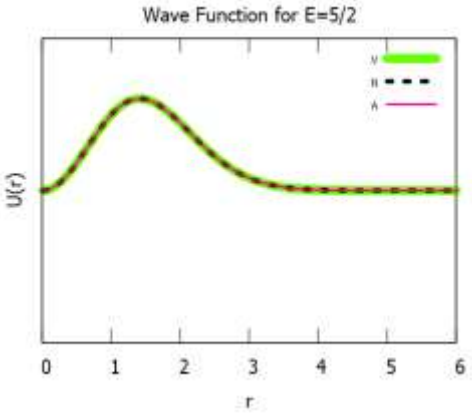

Figure 3. Wave function for N = 1 (n = 0, l = 1)

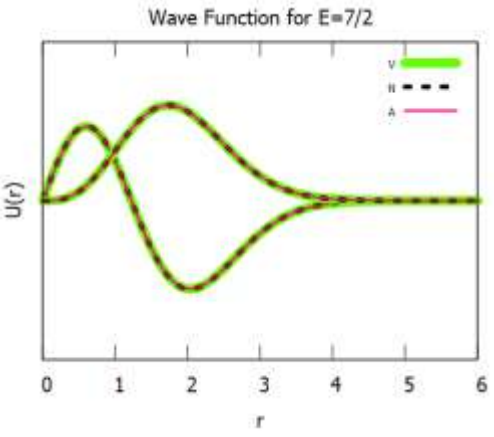

Figure 4. Wave function for N = 2 (n = 0, l = 2 and n = 1, l = 0)

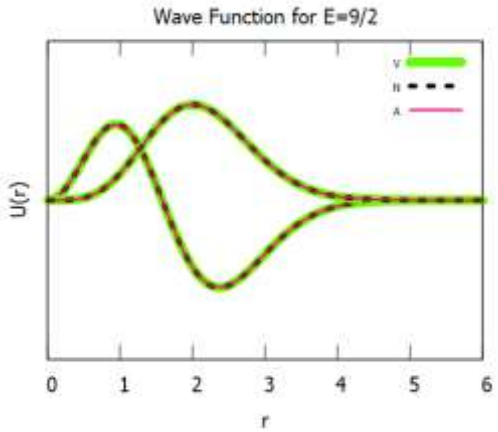

Figure 5. Wave function for N = 3 (n = 1, l = 1 and n = 0, l = 3)

Energy discrepancy of variation result

By using chosen trial wave function with twelve number of basis states, higher energy level states are also calculated and the discrepancy values with analytical results are presented. From the following graphs it could be seen that at low lying levels up to N = 15, variational calculation with chosen gaussian basis of twelve states could produce energy values quite well. But as the system goes to higher levels than N = 15, the discrepancy value begins to be significant and appears to be increasing as the energy levels get higher.

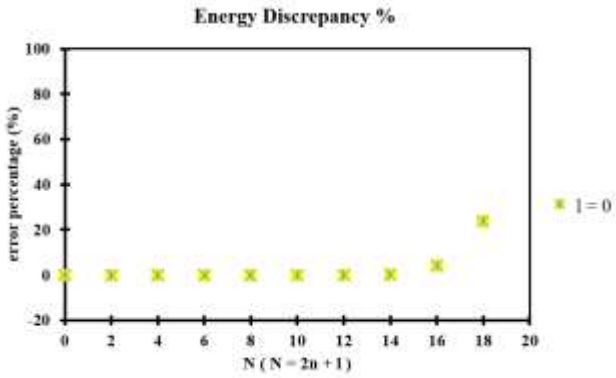

Figure 6. Energy discrepancy for various N values of fixed l = 0

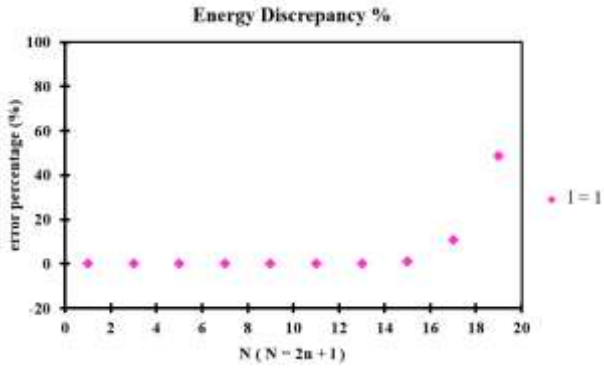

Figure 7. Energy discrepancy for various N values of fixed l = 1

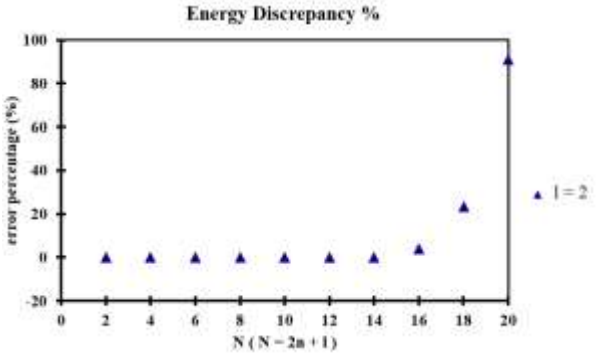

Figure 8. Energy discrepancy for various N values of fixed l = 2

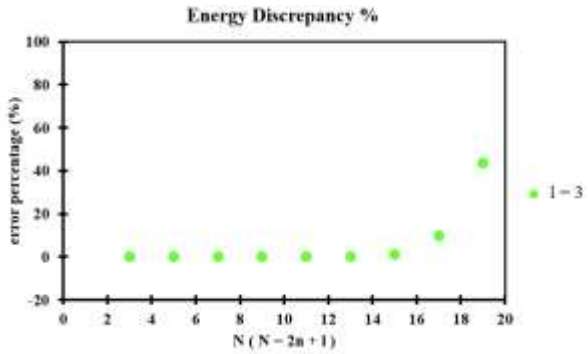

Figure 9. Energy discrepancy for various N values of fixed l = 3

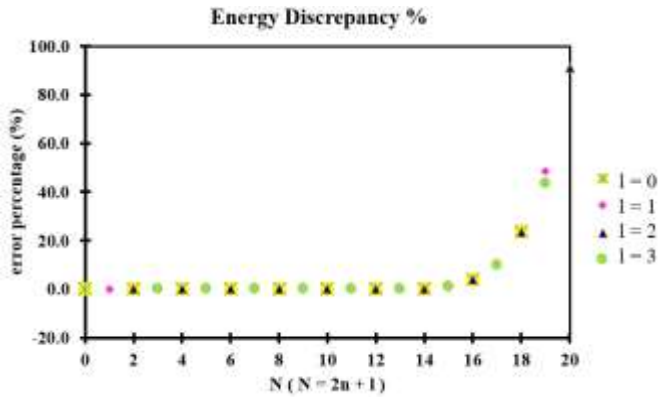

Figure 10. Energy discrepancy for various N values of l = 0, 1, 2 and 3

Conclusion

In this work, low lying energy levels of 3D quantum harmonic oscillator are calculated by using both variational principle and Numerov method. The results are compared with corresponding analytical solutions. For variational calculation, taking linear combination of gaussian basis as trial wave function demonstrated that a basis size of twelve is sufficient to accurately reproduce the low-lying levels of this system up to N = 15. The variational parameters chosen in this work are b_i = 1.41 and m_i starts from 0 to 11. The energy values computed by using Numerov method showed good agreement with analytical results for all considered states. Wave functions of first six low lying energy levels are also plotted, comparing the results obtained from variational method with Numerov method and analytical results. Since the variational results provide similar energy eigenvalues as analytical results, the wave functions appear to coincide.

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