



# Asymptotic iteration and variational methods for Gaussian potential

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**Abstract.** In this paper we studied the approximate solutions of radial Schrödinger equation with the attractive Gaussian potential. We used asymptotic iteration method and variational method to obtain energy eigenvalues for any  $n$  and  $l$  quantum numbers. Our results are in good agreement with the other studies.

**Keywords.** Gaussian potential; asymptotic iteration method; variational method.

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## 1. Introduction

Schrödinger equation of a particle with mass  $m$  and potential  $V$  can be written as

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}). \quad (1)$$

Here  $\psi(\vec{r})$  is the wave function and  $E$  is the energy eigenvalue. Since its invention at the beginning of 1900s, the Schrödinger equation is applied to electrons, protons, neutrons, quarks, etc. Solution of the Schrödinger equation is an important issue in physics, mathematics, chemistry and also in biology.

The solutions of the Schrödinger equation have always been a challenge. Many attempts have been made to solve the Schrödinger equation either analytically or approximately. The solutions of Schrödinger equation are important to understand the energy spectrum and system evolution in time (in the case of time-dependent Schrödinger equation). If one gets energy and wave function of the related system, it is possible to have a description about that system. The general framework is to solve the Schrödinger equation with the potential  $V(r)$ . In most of the cases, it is not always possible to obtain an accurate solution. For example, the Morse potential [1],  $V(r) = D_e[e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}]$ , where  $D_e$  is the association energy,  $r_e$  is the equilibrium distance and  $a$  is the potential parameter, has no exact solutions. In that case, approximate solutions are sought to describe the system. Besides that, some potentials such as harmonic oscillator potential, Coulomb

potential, Morse potential [2], Eckart potential [3], Woods–Saxon potential [4] and Kratzer potential [5] are exactly solvable within the framework of Schrödinger equation.

The general method to solve the Schrödinger equation is to transform it into a well-known ordinary differential equation which has solutions in terms of Hermit, Legendre, Bessel or in any other form of hypergeometric functions. These generally appear in undergraduate/graduate quantum mechanics textbooks [6–9]. An alternative method is supersymmetric quantum mechanics (SUSY-QM). In SUSY-QM, the Hamiltonian of the system is factorised. The other method is Nikiforov–Uvarov in which one can transform the Schrödinger equation with a specific potential into a hypergeometric-type second-order differential equation. This method can be described as by-hand method, as one can see all the steps in the solution. Perturbation and variational methods can also be used to find solutions. Of course, there is no one way to solve eigenvalue equations such as Schrödinger equation. There is a rich literature on this subject.

In this paper, we shall seek solutions of Gaussian potential by asymptotic iteration and variational methods. Variational methods for Gaussian potential have been studied before with different wave functions but to the best of our knowledge, a study of asymptotic iteration method for Gaussian potential has not been reported. In §2, we shall introduce the Gaussian potential. In §3 and §4, the asymptotic iteration and variational methods are given, respectively. In the last section,

these methods are applied to Gaussian potential and we present our results.

## 2. Gaussian potential

Gaussian potential is in the form

$$V(r) = -Ae^{-\lambda r^2}, \quad (2)$$

where  $A$  is the depth of the potential and  $\lambda$  is a parameter. It is an attractive potential. Gaussian potential was used as a model in nucleon–nucleon scattering theory by Buck *et al* [10]. The eigenvalues of Gaussian potential were first obtained by Buck in an unpublished paper in 1977 via direct numerical integration. Stephenson [11] obtained the eigenvalues of the three-dimensional Schrödinger equation with a radial Gaussian potential by using the Liouville–Green uniform asymptotic method. Bessis *et al* [12] studied energies and eigenfunctions of the Schrödinger equation with a radial Gaussian potential by using a perturbational and variational treatment on a conveniently chosen basis of the transformed Jacobi functions. Lai [13] obtained the energy eigenvalues of the Gaussian potential for various eigenstates within the framework of the hypervirial-Pade scheme. Cohen [14] obtained the eigenvalues and approximate eigenfunctions from a first-order perturbation treatment based on a scaled harmonic oscillator model.  $1/N$  expansion was applied to Gaussian potential by Chatterjee [15]. Köksal [16] used a combination of perturbation theory and supersymmetric quantum theory for bound state energies of an electron confined in an attractive Gaussian potential.

This work is devoted to obtain eigenvalues of the radial Schrödinger equation with the Gaussian potential

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2m}{\hbar^2} \left( E - V(r) - \frac{l(l+1)}{2mr^2} \right) R_{nl}(r) = 0, \quad (3)$$

where  $m$  is the mass of the particle. Inserting Gaussian potential into eq. (3), the radial Schrödinger equation takes the following form:

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2m}{\hbar^2} \left( E + Ae^{-r^2} - \frac{l(l+1)}{2mr^2} \right) R_{nl}(r) = 0, \quad (4)$$

where we took  $\lambda = 1$ . This form of Schrödinger equation cannot be solved analytically.

## 3. Asymptotic iteration method

The asymptotic iteration method was introduced to solve the second-order homogeneous linear differential equations of the form

$$y''(x) = \lambda_0(x)y'(x) + s_0(x)y_0(x), \quad (5)$$

where  $\lambda_0(x) \neq 0$  and the variables  $\lambda_0(x)$  and  $s_0(x)$  have sufficiently many derivatives [17]. This differential equation has the following solution:

$$y(x) = \exp\left(-\int^x \alpha dt\right) \times \left[ C_2 + C_1 \int^x \exp\left(\int^t (\lambda_0(\tau) + 2\alpha(\tau)) d\tau\right) dt \right], \quad (6)$$

where

$$\frac{s_k(x)}{\lambda_k(x)} = \frac{s_{k-1}(x)}{\lambda_{k-1}(x)} \equiv \alpha(x) \quad (7)$$

for sufficiently large  $k$ . In eq. (7),  $s_k(x)$  and  $\lambda_k(x)$  are defined as follows:

$$\begin{aligned} \lambda_k(x) &= \lambda'_{k-1}(x) + s_{k-1}(x) + \lambda_0(x)\lambda_{k-1}(x), \\ s_n(x) &= s'_{k-1}(x) + s_0(x)\lambda_{k-1}(x), \quad k = 1, 2, 3, \dots \end{aligned} \quad (8)$$

The convergence (quantisation) condition can be defined as

$$\begin{aligned} \delta_k(x) &= \lambda_k(x)s_{k-1}(x) - \lambda_{k-1}(x)s_k(x) = 0, \\ k &= 1, 2, 3, \dots \end{aligned} \quad (9)$$

For a given radial potential, it is possible to convert the radial Schrödinger equation to eq. (5). Once this form has been obtained, it is easy to see  $s_0(x)$  and  $\lambda_0(x)$  and calculate  $s_k(x)$  and  $\lambda_k(x)$  by using eq. (8). Eigenvalues are obtained from the quantisation (convergence) condition,  $\delta_k(x) = 0$ .

### 3.1 Asymptotic iteration method (AIM) for Gaussian potential

We have said that eq. (4) cannot be solved exactly. One way to solve this differential equation is to use the Taylor expansion. If we expand the Gaussian potential near the origin, we get

$$V(r) = -A + Ar^2 - \frac{Ar^4}{2} + \frac{Ar^6}{6} - \frac{Ar^8}{24} + \frac{Ar^{10}}{120} + O(r^{11}). \quad (10)$$

In principle, one can truncate this series at higher powers. But, as it is an asymptotic expansion, major contributions come from the first few terms. Putting

**Table 1.** The convergence of the eigenvalues for different  $\beta$  values with  $n = 0$  and  $l = 0$ .  $k$  is the iteration number.

$k$	$\beta = 5$	$\beta = 10$	$\beta = 15$	$\beta = 20$	$\beta = 25$
5	341.836822674	341.863607546	340.893507947	337.720033882	332.697776132
10	341.895185264	341.894773908	341.840149675	341.367656610	340.065208776
15	341.895181270	341.895177621	341.891722431	341.825947031	341.515599948
20	341.895182710	341.895183501	341.894944170	341.886006151	341.817565584
25	341.895182759	341.894765159	341.895345639	341.897695810	341.870927989
30	341.895185517	341.910303257	342.154549418	342.727071834	355.888111258
35	341.895475114	341.910303265	341.894010908	342.733072138	353.522636070

this expansion into the radial Schrödinger equation and defining  $\epsilon = 2m E_n/\hbar^2$  and  $\tilde{A} = 2mA/\hbar^2$ , one can get

$$\frac{d^2 R_{nl}(r)}{dr^2} + \left\{ \epsilon - \tilde{A} \left[ 1 - r^2 + \frac{r^4}{2} - \frac{r^6}{6} + \frac{r^8}{24} - \frac{r^{10}}{20} \right] + \frac{l(l+1)}{r^2} \right\} R_{nl}(r) = 0. \tag{11}$$

This is a second-order linear differential equation and in order to solve this equation via AIM, we should transform this into eq. (5). Karakoc and Boztosun [18], solved the Schrödinger equation with Yukawa potential  $V(r) = -(A/r) \exp(-\alpha r)$  via AIM by suggesting a wave function of the form  $R_{nl}(r) = r \exp(-\beta r) f_{nl}(r)$ . In the present work, regarding the shape of the potential, we propose a wave function of the form

$$R_{nl}(r) = r^{l+1} \exp(-\beta r^2) f_{nl}(r). \tag{12}$$

Inserting this wave function into eq. (11), we have the second-order linear homogeneous differential equation as

$$\frac{d^2 f_{nl}(r)}{dr^2} = \left( -\frac{2(L+1)}{r} + 4\beta r \right) \frac{df_{nl}(r)}{dr} + \left[ \frac{1}{120} A(r^{10} - 5r^8 + 20r^6 - 60r^4 + 120r^2 - 120) - \epsilon + 2\beta(2L - 2\beta r^2 + 3) \right] f_{nl}(r). \tag{13}$$

By comparing eq. (13) with eq. (5), we see that AIM can be applied and  $\lambda_0(x)$  and  $s_0(x)$  can be written as follows:

$$\lambda_0(x) = \left( -\frac{2(L+1)}{r} + 4\beta r \right),$$

$$s_0(x) = \left[ \frac{1}{120} A(r^{10} - 5r^8 + 20r^6 - 60r^4 + 120r^2 - 120) - \epsilon + 2\beta(2L - 2\beta r^2 + 3) \right]. \tag{14}$$

At this point, we should mention an important concept about AIM. If the potential is exactly solvable around  $x_0$ , the solution can be obtained when the iteration number  $k$  equals the principal quantum number (radial quantum number)  $n$ . If the potential is not exactly solvable, for iteration number  $k$  bigger than radial quantum number  $n$ , a suitable  $x$  is chosen and energy eigenvalues can be obtained [17]. Energy eigenvalues can be obtained by the quantisation condition (9). The quantisation condition depends on  $x$  but the energy eigenvalues obtained from this condition should be independent of the choice of  $x$ . This suitable choice of  $x$  minimises the potential or maximises the wave function, eq. (12). In the AIM method, the wave function can be written as

$$R(x) = f(x)g(x), \tag{15}$$

where  $f(x)$  represents the asymptotic behaviour. In our case,  $f(x) = x^{l+1} \exp(-\beta x^2)$  and  $x = \sqrt{l+1}/\sqrt{2}\sqrt{\beta}$ .  $\beta$  is an arbitrary parameter related to the convergence [19]. In table 1, the convergence for different values of  $\beta$  is shown.

As can be seen in table 1,  $\beta = 5$  and 10 gave more sensical results. The energy eigenvalues in this paper are obtained with  $\beta = 10$  because the solutions are very close after two iterations. The results are shown in table 2.

#### 4. Variational method

Variational method, known as Rayleigh–Ritz method, is very useful for obtaining the energy eigenvalues and eigenstates of the related system. This method is used when the perturbation theory cannot be applied, i.e. Hamiltonian cannot be written simply as  $H = H_0 + V$ , where  $H_0$  is the Hamiltonian which can be solved exactly. In this method, we have a system that is solvable and have energy eigenvalue and eigenfunction of one state, generally the ground state. By having these,

**Table 2.** Energy eigenvalues of the Gaussian potential in units  $\hbar = 1, m = 0.5$ .

<i>n</i>	1	AIM	Variational	[10]	[11]	[12] <sup>a</sup>	[13]	[15] <sup>b</sup>
0	0	341.895	341.895	341.9	341.6	341.895	341.895	341.895
	1	304.464	304.748	304.5	304.2	304.463	304.463	304.463
	2	268.111	268.235	268.1	267.9	268.111	268.111	268.111
	3	232.873	233.090	232.9	232.6	232.875	232.875	232.875
	4	198.796	198.925	198.8	198.5	198.797	198.798	198.798
	5	165.982	166.174	165.9	165.7	165.925	165.928	165.928
	6	134.321	134.450	134.3	134.1	134.317	134.323	134.323
1	0	269.643	269.644	269.7	269.4	269.644	269.644	269.644
	1	235.469	235.696	235.5	235.2	235.450	235.450	235.451
	2	202.415	202.592	202.4	202.2	202.431	202.431	202.432
	3	170.566	170.933	170.4	170.6	170.639	170.639	170.640
	4	140.028	140.249	140.1	139.9	140.134	140.135	140.136
	5	110.745	111.105	111.0	110.7	110.989	110.993	110.994
	6	83.359	83.426	83.3	83.0	83.295	83.306	83.307
2	0	203.958	203.983	204.0	203.7	203.983	203.983	203.997
	1	173.222	173.483	173.3	173.0	173.244	173.244	173.257
	2	143.669	143.923	143.8	143.6	143.808	143.809	143.821
	3	115.588	115.869	115.8	115.5	115.752	115.754	115.765
	4	88.992	89.281	89.2	88.9	89.169	89.175	89.184
	5	63.077	64.305	64.2	63.9	64.180	64.196	64.202
	6	39.874	40.169	41.0	40.7	40.950	40.989	40.990
3	0	145.133	145.377	145.4	145.1	145.377	145.378	145.431
	1	118.718	118.636	118.4	118.1	118.381	118.384	118.432
	2	92.089	92.733	92.9	92.6	92.873	92.878	92.919
	3	67.624	68.843	69.0	68.7	68.973	68.984	69.013
	4	46.950	46.692	46.9	46.6	46.846	46.868	46.881
	5	26.736	26.594	26.8	26.5	26.727	26.778	26.768
	6	9.667	8.953	9.1	8.8	8.995	9.126	9.080
4	0	93.497	94.456	94.5	94.2	94.454	94.458	94.582
	1	71.881	71.904	71.6	71.4	71.617	71.624	71.720
	2	49.021	50.842	50.6	50.3	50.557	50.568	50.623
	3	31.536	31.793	31.5	31.3	31.499	31.521	31.518
	4	14.252	14.042	14.9	14.6	14.794	14.851	14.768
	5	1.182	1.369			1.1	1.295	1.030

<sup>a</sup>Variational.

<sup>b</sup>Shifted 1/*N* expansion.

one can get energy eigenvalues and eigenfunctions of higher states.

The Hamiltonian of the Gaussian potential is

$$H = \frac{p^2}{2\mu} + V(r) = \frac{p^2}{2\mu} - Ae^{-r^2}, \tag{16}$$

where *p* is the relative momentum and  $\mu$  is the reduced mass of the two particles,  $\mu = m_1m_2/(m_1 + m_2)$ . In our case  $m_1 = m_2$ . In order to obtain energy eigenvalues, we have solved the radial Schrödinger equation with the Hamiltonian above using the variational method

$$E = \frac{\langle R(r)|H|R(r) \rangle}{\langle \psi|\psi \rangle} \equiv \langle H \rangle. \tag{17}$$

We used the radial part of the three-dimensional harmonic oscillator wave function as a trial function:

$$R_{nl} = N \left(\frac{r}{b}\right)^l L_n^{l+(1/2)}\left(\frac{r^2}{b^2}\right) e^{-(r^2/b^2)} \tag{18}$$

with  $L_n^{l+(1/2)}(x)$  being the associated Laguerre polynomials and normalisation constant

$$|N|^2 = \frac{2n!}{b^3\sqrt{\pi}} \frac{2^{2n+2l+1}}{(2n + 2l + 1)!} (n + l)!. \tag{19}$$

In eq. (18), *b* is treated as the variational parameter which is determined by minimising the expectation value of the Hamiltonian for each state. After having *b* value, it was used in the wave function to obtain energy

eigenvalues. The results of the variational method are given in table 2.

## 5. Results and discussion

In this paper, we solved the radial Schrödinger equation with the radial Gaussian potential via asymptotic iteration and variational methods. Gaussian potential was studied before using variational, perturbation, hypervirial-Pade and  $1/N$  expansion methods mentioned before as well as direct numerical integration in [20].

Bessis *et al* [12] studied the Gaussian potential with square integrable eigenfunctions in terms of Jacobi polynomial. In the present work, we used rather a different wave function in terms of Laguerre polynomials. The variational method is a cumbersome method to obtain energy eigenvalues and eigenfunctions. It contains tedious calculations. If we do not know exact results of a given Hamiltonian, the variational method can be used. We choose a wave function which mimics the actual unknown wave function of the system. This wave function can depend on some parameters. In some cases the trial wave function can be normalised to one so that the number of unknown parameters can be decreased. The expectation value of the Hamiltonian is calculated. The expectation value of the Hamiltonian must be bigger than the ground state,  $\langle H \rangle > E_0$  where  $E_0$  is the ground state energy of the system which is exactly solvable. There is no *a priori* reason for the choice of trial wave function. One must be careful about the behaviour of the wave function at asymptotic ranges.

We have solved the radial Gaussian potential for any  $n$ ,  $l$  and  $A$  in the framework of AIM by transforming the Schrödinger equation into a second-order differential equation in the form of eq. (5). In AIM, there is no constraint on the potential parameter values which makes the AIM easy to implement.

The energy eigenvalues obtained by AIM and variational methods are in good agreement with the other results given in table 2.

## 6. Conclusion

Schrödinger equation, which is an eigenvalue equation, can be solved analytically and approximately.

Interactions under a potential function generally make the Schrödinger equation solvable only by approximation methods. For example, Wentzel–Kramers–Brillouin (WKB) method, shifted  $1/N$  expansion method, Pade method and Nikiforov–Uvaranov method are used to solve the Schrödinger equation approximately.

Asymptotic iteration method deals with the second-order linear homogeneous differential equations. If one has a wave function with appropriate boundary conditions, AIM can be applied for such problems. In this manner eigenvalues can be obtained with a good accuracy. The AIM can be extended to study other interacting potentials together with the other methods.

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