

## Iterative approach for the eigenvalue problems

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MS received 24 January 2010; revised 13 June 2010; accepted 30 June 2010

**Abstract.** An approximation method based on the iterative technique is developed within the framework of linear delta expansion (LDE) technique for the eigenvalues and eigenfunctions of the one-dimensional and three-dimensional realistic physical problems. This technique allows us to obtain the coefficient in the perturbation series for the eigenfunctions and the eigenvalues directly by knowing the eigenfunctions and the eigenvalues of the unperturbed problems in quantum mechanics. Examples are presented to support this. Hence, the LDE technique can be used for non-perturbative as well as perturbative systems to find approximate solutions of eigenvalue problems.

**Keywords.** Formulation of iterative technique for one dimension and applications; formulation of iterative technique for three dimensions and applications.

**PACS Nos** 03.65.Fd; 03.65.Ge; 03.65-w

### 1. Introduction

Quantum mechanics is supposed to solve the Schrödinger equations with different potentials. But realistic physical problems can never be solved exactly. Only for a few idealized problems, an exact solution of the Schrödinger equation exists. Normally, non-exactly solvable potentials have to be solved using an approximation method such as the perturbation theory (PT). This theory constitutes one of the most powerful tools available to study of quantum mechanics in the atom and molecules. The perturbation theory is applied to those cases in which the real system can be described by a small change in an exactly solvable idealized system.

The Rayleigh–Schrödinger (RS) perturbation technique is a standard approach to deal with bound-state problems of non-relativistic quantum mechanics. One typical difficulty associated with this method lies in the infinite sums that arise in all corrections in the way that one summation will occur in second-order correction, two summations will occur in third correction and so on. Higher eigenvalues involve summation over all possible eigenfunctions.

As opposed to this, the so-called logarithmic perturbation theory (LPT) [1] exists in another form of the perturbation theory in which the energy correction to any order is recast in an alternative simpler form. Here the knowledge of the unperturbed initial state is sufficient to compute the values for the energy corrections. Within the framework of LPT, the conventional way to solve a quantum mechanical bound-state problem consists of changing from the wave function to its logarithmic derivative and converting the time-independent Schrödinger equation into the nonlinear Riccati equation.

Utilizing an appropriate ansatz to the wave function, Ikhdair and Server [2] reproduced a single bound-state solution of the radial Schrödinger equation confining perturbed Coulomb problem. Dutta and Mukherjee [3] studied the analytical solution of the Schrödinger equation for the energy levels with a class of confining potentials [3] using Kato–Rellich perturbation theory of linear operations. Killingbeck [4] has calculated the energy eigenvalues of the confinement potential using hypervirial relations.

One interesting problem is to find out the higher excited states and the corresponding energy. Exact solution of Schrödinger equations provides all important information about the system concerned. But for physical systems, completely exactly solvable potentials are very few in number. Therefore, the quasi-exactly solvable potentials (QES) have received wide attention [5]. These QES models allow exact solutions only for a limited part of the energy spectrum. Thus, these potentials fill up the gap between the exactly solvable and non-solvable potentials and help to understand many physical phenomena. Moreover, QES problem has its own inner mathematical beauty – it can provide a good starting point for doing calculations perturbatively for complex systems.

Non-singular potentials are very much fascinating now-a-days because of their mathematical beauty like parity and time reversal symmetry (PT) [6] and its application in different branches of physics [7]. Recently, the study of anharmonic potentials have been much more desirable to physicists and mathematicians who want to understand newly discovered phenomena such as structural phase transitions, polaron formation in solids and the concept of false vacuo in field theory. Unfortunately, the study of these anharmonic potentials have not been carried out further.

In an interesting work, Amore *et al* [8] have presented the linear delta expansion (LDE) technique [9] to find approximate solutions to eigenvalue problems of non-perturbative nature. Here, our objective is to examine the simple perturbation formulae within the framework of LDE technique from which one can obtain all perturbation corrections to eigenvalue problems of perturbative nature in quantum mechanics for real QES systems. In the application of the present method to the ground state as well as the excited state, one requires the knowledge of the unperturbed eigenfunctions and eigenvalues. Hence, the present technique offers explicit expressions for the energy corrections and provides a clean route to the excited states. This simple technique provides a basis to develop a useful technique for the real QES problems.

In §2 and §3 we have developed the iterative formulation within the framework of LDE technique for both one- and three-dimensional systems, respectively and applied this technique for calculating the first- and second-order corrections for the ground state as well as the excited states for quantum mechanical QES potentials – quartic anharmonic, sextic, octic potentials in one dimension and harmonic oscillator plus non-singular

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potential, spherical anharmonic oscillator, Coulomb plus non-singular potential and perturbed Coulomb potential in three dimensions. Finally, we draw the conclusion in §4.

## **2. Formalism and applications**

### *2.1 Formulation of iterative technique for one-dimensional systems*

Many quantum mechanical problems are characterized by Hamiltonians ( $H$ ) for which it is difficult to solve the corresponding eigenvalue problem exactly. Fortunately, there exist physical situations where the unsolved Hamiltonian differs only slightly from the Hamiltonian ( $H_0$ ) for a problem that can be solved rigorously. The small difference  $H_p$  between  $H$  and  $H_0$  is referred to as a perturbation and the so-called perturbation theory provides useful techniques for constructing the eigenspectrum or the eigenfunction of the full Hamiltonian  $H$  by using the knowledge of the corresponding quantities for  $H_0$  and the smallness of  $H_p$ .

Consider the Schrödinger equation in one dimension

$$H\psi(x) = E\psi(x) \quad (1)$$

with

$$H = H_0 + H_p. \quad (2)$$

As already noted,  $H_0$  forms a simpler Hamiltonian, of which we know the spectrum, and  $H_p$  is a small perturbation to  $H_0$ . We are interested in generating the eigenvalues and eigenstates of  $H$  by LDE technique. In the traditional Rayleigh–Schrödinger perturbation theory, the wave function and energy eigenvalue of eq. (1) are expanded as

$$\psi(x) = \psi_0 + \lambda\psi_1(x) + \lambda^2\psi_2(x) + \dots \quad (3)$$

and

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \dots, \quad (4)$$

where  $\psi(x)$  and  $E_0$  stand for the eigenstates and eigenvalues of  $H_0$  while  $\psi_j(x)$  and  $E_j$  are the  $j$ th order corrections over  $\psi_0(x)$  and  $E_0$  respectively. Equations (1)–(4) provide a basis to compute the corrections of  $\psi_j(x)$  and  $E_j$ .

The derivation of the mathematical procedure to obtain the approximate solutions can be facilitated by writing the Schrödinger equation in the form

$$\frac{d^2\psi(x)}{dx^2} + \left( E - V_0(x) - V_p(x) \right) \psi(x) = 0, \quad (5)$$

Here, the potential  $V_0(x)$  is exactly solvable and  $V_p(x)$  is the perturbing potential of interest. Here,  $E$  denotes the energy. Throughout this paper, the unit system  $2m = \hbar = 1$  is chosen.

In order to calculate perturbation corrections of sufficiently larger order by means of LDE technique, we define the unnormalized  $n$ th bound state wave function of eq. (5) as

$$\psi_n(x) = e^{-f(x)}\Phi_n(x), \quad n = 0, 1, 2, 3, \dots \quad (6)$$

Here, the exponential function  $f(x)$  is known for the unperturbed potential  $V_0(x)$  and the eigenfunctions  $\Phi_n(x)$  will be determined. Substituting eq. (6) into eq. (5), we arrive at the differential equation

$$\begin{aligned} \Phi_n''(x) - 2f'(x)\Phi_n'(x) + (E_n - V_0(x) + f'^2(x) - f''(x))\Phi_n(x) \\ = V_p(x)\Phi_n(x). \end{aligned} \quad (7)$$

Following the spirit of our LDE technique, we have introduced in eq. (7)  $\delta$ , which is used as a power-counting device, and as a result we can rewrite eq. (7) as perturbative differential equation like

$$\begin{aligned} \Phi_n''(x) - 2f'(x)\Phi_n'(x) + (E_n - V_0(x) + f'^2(x) - f''(x))\Phi_n(x) \\ = \delta(V_p(x))\Phi_n(x). \end{aligned} \quad (8)$$

Here, we shall treat the right-hand side of eq. (8) as a perturbation. It is obvious that when  $\delta = 0$ , eq. (8) becomes an unperturbed problem. When  $\delta = 1$  it becomes the original eq. (7). So, when the embedding parameter  $\delta$  monotonically increases from zero to unity, the trivial problem is continuously deformed. The basic assumption is that the solution of eq. (8) can be written as a power series in  $\delta$  as

$$\Phi_n(x) = \sum_{j=0}^{\infty} \delta^j \phi_{nj}(x), \quad E_n = \sum_{j=0}^{\infty} \delta^j E_{nj}. \quad (9)$$

When  $\delta = 1$ , the best approximation for solutions are

$$\Phi_n(x) = \phi_{n0}(x) + \phi_{n1}(x) + \phi_{n2}(x) + \dots$$

and

$$E_n(x) = E_{n0}(x) + E_{n1}(x) + E_{n2}(x) + \dots,$$

where the solutions  $\phi_{n0}(x)$  as well as the eigenvalues  $E_{n0}$  stand for the unperturbed systems while  $\phi_{nj}(x)$  and  $E_{nj}$  are the  $j$ th-order corrections over  $\phi_n(x)$  and  $E_n$ , respectively. Substituting eq. (9) into eq. (8), one can generate a hierarchy of equations corresponding to the different order of  $\delta$  on both sides of eq. (8) as

$$\phi_{n0}''(x) - 2f'(x)\phi_{n0}'(x) + (E_{n0} - V_0(x) + f'^2(x) - f''(x))\phi_{n0}(x) = 0, \quad (10)$$

$$\begin{aligned} \phi_{n1}'' - 2f'(x)\phi_{n1}'(x) + (E_{n0} - V_0(x) + f'^2(x) - f''(x))\phi_{n1}(x) \\ = (V_p - E_{n1})\phi_{n0}(x) \end{aligned} \quad (11)$$

and

$$\begin{aligned} \phi_{n2}''(x) - 2f'(x)\phi_{n2}'(x) + (E_{n0} - V_0(x) + f'^2(x) - f''(x))\phi_{n2}(x) \\ = -E_{n2}\phi_{n0}(x) + (V_p - E_{n1})\phi_{n1}(x). \end{aligned} \quad (12)$$

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Equations (10)–(12) provide a basis to compute the corrections of  $\phi_{nj}(x)$  and  $E_{nj}$  – eq. (10) for the unperturbed system is a homogeneous differential equation whereas eqs (11), (12) and similar ones form a set of inhomogeneous differential equations for any state. Here, fortunately, the solution of eq. (10) is known. The main task of this paper is to solve eqs (11), (12) and so on by iterative method.

#### *2.2 Applications for one-dimensional systems*

In this section, we consider the applications of our method to anharmonic potentials of the form  $V(x) = x^2 + \lambda x^{2N}$  ( $N = 2, 3, 4, \dots$ ) to demonstrate how this technique can be used to determine the perturbation coefficients and exact results [3] recovered. For example, we consider the quartic, sextic and octic anharmonic oscillators because these are better choices to test a new method before applying them to more interesting problems.

For the unperturbed harmonic oscillator potential  $V(x) = x^2$ , the unnormalized solutions of Schrödinger equation are  $\psi_n(x) = e^{-\frac{1}{2}x^2} \phi_{n0}(x)$ , where the principal quantum number  $n = 0, 1, 2, 3, \dots$  and  $\phi_{n0}(x)$  are the polynomial of  $n$ th degree and is also a solution of eq. (6) with energy eigenvalues  $E_n = 2n + 1$ . The first three  $\phi_n(x)$  are  $\phi_{n=0,0} = 1$ ,  $\phi_{n=1,0}(x) = x$ ,  $\phi_{n=2,0}(x) = 2x^2 - 1$ .

**2.2.1 Quartic anharmonic oscillator:** As an illustration, let us consider the phenomenologically useful and methodically challenging quartic anharmonic oscillator which has a great deal of interest in the analytical investigation of the one-dimensional anharmonic oscillator because of their importance in molecular vibrations [10], solid state physics [11] and quantum field theory [12].

Here, we shall examine the ground state as well as excited states of the potential  $V(x) = x^2 + \lambda x^4$ .

**(i) Ground state ( $n = 0$ )**

Substituting the values of  $\phi_{00}(x) = 1$ ,  $E_{00} = 1$  and  $V_p(x) = \lambda x^4$  in eq. (11) and solving it, we have obtained the first-order correction of  $\phi_0(x)$  as

$$\phi_{01}(x) = -\frac{\lambda}{8}x^4 - \frac{3\lambda}{8}x^2 \quad (13)$$

and the corresponding correction of energy  $E_{01} = 3\lambda/4$ .

Substituting the above values of  $\phi_{01}(x)$  and  $E_{01}$  in eq. (12) and solving it, we get the second-order correction of  $\phi_0(x)$  as

$$\phi_{02}(x) = \frac{\lambda^2}{128}x^8 + \frac{13\lambda^2}{192}x^6 + \frac{31\lambda^2}{128}x^4 + \frac{21\lambda^2}{32}x^2 \quad (14)$$

and the second-order correction of energy  $E_{02} = -21\lambda^2/16$ .

**(ii) First excited state ( $n = 1$ )**

For the first excited state, the solution of eq. (11) for the values of  $\phi_{10}(x) = x$  and  $E_{10} = 3$  is

$$\phi_{11}(x) = -\frac{\lambda}{8}x^5 - \frac{5\lambda}{8}x^3 \quad (15)$$

which gives the first-order correction of  $\phi_1(x)$  and the corresponding correction of energy  $E_{11} = 15\lambda/4$ .

For the second-order correction, substituting the above values of  $\phi_{11}(x)$  and  $E_{11}$  in eq. (12) and solving it, we get the second-order correction of  $\phi_1(x)$  as

$$\phi_{12}(x) = \frac{\lambda^2}{128}x^9 + \frac{19\lambda^2}{192}x^7 + \frac{59\lambda^2}{128}x^5 + \frac{55\lambda^2}{32}x^3 \quad (16)$$

and the corresponding correction of energy  $E_{12} = -165\lambda^2/16$ .

(iii) *Second excited state* ( $n = 2$ )

For the second excited state, we put  $\phi_{20}(x) = 2x^2 - 1$  and  $E_{20} = 5$  in eq. (11) which gives the first-order correction of  $\phi_2(x)$  as

$$\phi_{21}(x) = -\frac{\lambda}{4}x^6 - \frac{13\lambda}{8}x^4 + \frac{39\lambda}{8}x^2 \quad (17)$$

and the corresponding correction of energy  $E_{21} = 39\lambda/4$ .

Now, for second-order correction, substituting the values of  $\phi_{21}(x)$  and  $E_{21}$  in eq. (12) and solving it, we get the second-order correction of  $\phi_2(x)$  as

$$\phi_{22}(x) = \frac{\lambda^2}{64}x^{10} + \frac{97\lambda^2}{384}x^8 + \frac{41\lambda^2}{48}x^6 + \frac{313\lambda^2}{128}x^4 - \frac{615\lambda^2}{64}x^2 \quad (18)$$

and correction of energy  $E_{22} = -615\lambda^2/16$ . Finally, we can write the energy eigenvalue of quartic anharmonic oscillator in general form as

$$E_n = (2n+1) + \frac{3}{4}(2n^2 + 2n+1)\lambda - \frac{1}{16}(34n^3 + 51n^2 + 59n + 21)\lambda^2 + O(\lambda^3) + \dots \quad (19)$$

**2.2.2 Sextic potential.** Here, we will examine the ground state as well as the excited states of sextic potential of the form  $V(x) = x^2 + \lambda x^6$ .

(i) *Ground state* ( $n = 0$ )

Substituting the values of  $\phi_{00}(x) = 1$ ,  $E_{00} = 1$  and  $V_p(x) = \lambda x^6$  into eq. (11) and solving it, we have obtained the first-order correction of  $\phi_0(x)$  as

$$\phi_{01}(x) = -\frac{\lambda}{12}x^6 - \frac{5\lambda}{16}x^4 - \frac{15\lambda}{16}x^2 \quad (20)$$

and the corresponding correction of energy  $E_{01} = 15\lambda/8$ .

Substituting the values of  $\phi_{01}(x)$  and  $E_{01}$  in eq. (12) and solving it, we get the second-order correction of  $\phi_0(x)$  as

$$\begin{aligned} \phi_{02}(x) = & \frac{\lambda^2}{288}x^{12} + \frac{37\lambda^2}{960}x^{10} + \frac{141\lambda^2}{512}x^8 + \frac{2931\lambda^2}{2304}x^6 \\ & + \frac{14430\lambda^2}{3072}x^4 + \frac{13980\lambda^2}{1024}x^2 \end{aligned} \quad (21)$$

and the second-order correction of energy  $E_{02} = -3495\lambda^2/128$ .

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(ii) *First excited state* ( $n = 1$ )

For the first excited state, for the values of  $\phi_{10}(x) = x$  and  $E_{10} = 3$ , the solution of eq. (11) is

$$\phi_{11}(x) = -\frac{\lambda}{12}x^7 - \frac{7\lambda}{16}x^5 - \frac{35\lambda}{16}x^3 \quad (22)$$

which gives the first-order correction of  $\phi_1(x)$  and the corresponding correction of energy  $E_{11} = 105\lambda/8$ .

For the second-order correction, substituting the values of  $\phi_{11}(x)$  and  $E_{12}$  and solving eq. (12), we get the second-order correction of  $\phi_1(x)$  as

$$\begin{aligned} \phi_{12}(x) = & \frac{\lambda^2}{288}x^{13} + \frac{47\lambda^2}{960}x^{11} + \frac{727\lambda^2}{1536}x^9 + \frac{6333\lambda^2}{2304}x^7 \\ & + \frac{42126\lambda^2}{3072}x^5 + \frac{188580\lambda^2}{3072}x^3 \end{aligned} \quad (23)$$

and the corresponding correction of energy  $E_{12} = -47145\lambda^2/128$ .

(iii) *Second excited state* ( $n = 2$ )

For the second excited state, for the values of  $\phi_{20}(x) = 2x^2 - 1$  and  $E_{20} = 5$ , eq. (12) gives the first-order correction of  $\phi_2(x)$  as

$$\phi_{21}(x) = -\frac{\lambda}{6}x^8 - \frac{25\lambda}{24}x^6 - \frac{125\lambda}{16}x^4 + \frac{375\lambda}{16}x^2 \quad (24)$$

and the corresponding correction of energy as  $E_{21} = 375\lambda/8$ .

Now, for second-order correction, substituting the values of  $\phi_{21}(x)$  and  $E_{21}$  in eq. (12) and solving it, we get the second-order correction of  $\phi_2(x)$  as

$$\begin{aligned} \phi_{22}(x) = & \frac{\lambda^2}{144}x^{14} + \frac{83\lambda^2}{720}x^{12} + \frac{5527\lambda^2}{3840}x^{10} + \frac{37743\lambda^2}{4608}x^8 \\ & + \frac{78692\lambda^2}{1536}x^6 + \frac{149855\lambda^2}{512}x^4 - \frac{295095\lambda^2}{256}x^2 \end{aligned} \quad (25)$$

and the correction of energy  $E_{22} = -295095\lambda^2/128$ .

**2.2.3 Octic potential.** Here, we shall examine the ground state as well as the first excited states of octic potential  $V(x) = x^2 + \lambda x^8$ .

(i) *Ground state* ( $n = 0$ )

Substituting the values of  $\phi_{00}(x) = 1$ ,  $E_{00} = 1$  and  $V_{1p}(x) = \lambda x^8$  into eq. (11) and solving it, we have obtained the first-order correction of  $\phi_0(x)$  as

$$\phi_{01}(x) = -\frac{\lambda}{16}x^8 - \frac{7\lambda}{24}x^6 - \frac{35\lambda}{32}x^4 - \frac{105\lambda}{32}x^2 \quad (26)$$

and the corresponding correction of energy  $E_{01} = 105\lambda/16$ .

Substituting the values of  $\phi_{01}(x)$  and  $E_{01}$  in eq. (12) and solving it, we get the second-order correction of  $\phi_0(x)$  as

$$\begin{aligned} \phi_{02}(x) = & \frac{\lambda^2}{512}x^{16} + \frac{73\lambda^2}{2688}x^{14} + \frac{8113\lambda^2}{32256}x^{12} + \frac{98063\lambda^2}{53760}x^{10} + \frac{146727\lambda^2}{14336}x^8 \\ & + \frac{146237\lambda^2}{3072}x^6 + \frac{363755\lambda^2}{2048}x^4 + \frac{67515\lambda^2}{128}x^2 \end{aligned} \quad (27)$$

and the second-order corrections of energy  $E_{02} = -67515\lambda^2/64$ .

(ii) *First excited state* ( $n = 1$ )

For the first excited state, for the values of  $\phi_{10}(x) = x$  and  $E_{10} = 3$ , the solution of eq. (11) is

$$\phi_{11}(x) = -\frac{\lambda}{16}x^9 - \frac{9\lambda}{24}x^7 - \frac{63\lambda}{32}x^5 - \frac{315\lambda}{32}x^3 \quad (28)$$

which gives the first-order correction of  $\phi_1(x)$  and the corresponding correction of energy  $E_{11} = 945\lambda/16$ .

For the second-order correction, substituting the values of  $\phi_{11}(x)$  and  $E_{12}$  and solving eq. (12), we get the second-order correction of  $\phi_1(x)$  as

$$\begin{aligned} \phi_{12}(x) = & \frac{\lambda^2}{512}x^{17} + \frac{29\lambda^2}{896}x^{15} + \frac{187\lambda^2}{512}x^{13} \\ & + \frac{8553\lambda^2}{2560}x^{11} + \frac{46569\lambda^2}{2048}x^9 + \frac{137817\lambda^2}{1024}x^7 \\ & + \frac{1417311\lambda^2}{2048}x^5 + \frac{424305\lambda^2}{128}x^3 \end{aligned} \quad (29)$$

and the corresponding correction of energy  $E_{12} = -1272915\lambda^2/64$ .

For perturbed harmonic oscillators, we note that exactly similar treatments must be given for the wider class of potentials of the form  $x^2 + \lambda x^{2N}$ , where  $\lambda$  is a small parameter ( $\lambda < 1$ ) and  $N = 3, 4, 5, \dots$ . It is observed that in the region  $0 < \lambda < 0.5$ , one can achieve high accuracy for the quartic, sextic as well as octic anharmonic oscillators. But it is more difficult to obtain high accuracy for  $\lambda > 0.5$ , and hence, small coupling parameter values yield excellent results. We have examined the ground state as well as the excited states for these potentials and seen that the energy eigenvalues coincide with those listed in [13,14].



### 3. Formulation for three-dimensional systems

We consider three-dimensional Schrödinger equation like

$$\frac{d^2\psi(r)}{dr^2} + (E - U_0(r) - V_p(r))\psi(r) = 0, \quad (30)$$

where  $U_0(r) = V_0(r) + (l(l+1))/r^2$ . Obviously, the potential  $V_0(r)$  is solvable and  $V_p(r)$  is the perturbing potential, where  $\psi \in L_2(0, \infty)$  and satisfies the condition  $\psi(0) = 0$  known as the Dirichlet boundary condition. Here,  $E$  denotes the energy. Considering the unnormalized wave function of the form

$$\psi(r) = r^{l+1}e^{-\alpha f(r)}\Phi_{nl}(r)$$

and substituting this wave function in eq. (30), we arrive at the differential equation as

$$\begin{aligned} \Phi_{nl}'' + \left( \frac{2(l+1)}{r} - 2\alpha f'(r) \right) \Phi_{nl}' \\ + \left( E_n - V_0(r) + \alpha^2 f'^2 - \frac{2\alpha(l+1)}{r} f'(r) \right. \\ \left. - \alpha f''(r) - V_p(r) \right) \Phi_{nl}(r) = 0. \end{aligned} \quad (31)$$

As before, following the spirit of our technique, we have introduced in eq. (31) a parameter  $\delta$ , which is used as a power-counting device, and we can rewrite eq. (31) as perturbative differential equation like

$$\begin{aligned} \Phi_{nl}''(r) + \left( \frac{2(l+1)}{r} - 2\alpha f'(r) \right) \Phi_{nl}' + \left( E_n - V_0(r) + \alpha^2 f'^2 \right. \\ \left. - \frac{2\alpha(l+1)}{r} f'(r) - \alpha f''(r) \right) \Phi_{nl}(r) = \delta (V_p(r)) \Phi_{nl}(r). \end{aligned} \quad (32)$$

Like one-dimensional case expanding the functions as  $\Phi_{nl,j}(r) = \sum_{j=0}^{\infty} \delta^j \phi_{nl,j}(r)$ ,  $E_n = \sum_{j=0}^{\infty} \delta^j E_{nj}$  and putting these values in eq. (32), one can generate a hierarchy of equations corresponding to the different order of  $\delta$  on both sides of eq. (32) as

$$\begin{aligned} \phi_{nl,0}''(r) + \left( \frac{2(l+1)}{r} - 2\alpha f'(r) \right) \phi_{nl,0}'(r) \\ + \left( E_{n0} - V_0(r) + \alpha^2 f'^2 - \frac{2\alpha(l+1)}{r} f'(r) \right. \\ \left. - \alpha f''(r) \right) \phi_{nl,0}(r) = 0 \end{aligned} \quad (33)$$

$$\begin{aligned} \phi_{nl,1}''(r) + \left( \frac{2(l+1)}{r} - 2\alpha f'(r) \right) \phi_{nl,1}'(r) + \left( E_{n0} - V_0(r) \right. \\ \left. + \alpha^2 f'^2 - \frac{2\alpha(l+1)}{r} f'(r) - \alpha f''(r) \right) \phi_{nl,1}(r) \\ = (V_p - E_{n1}) \phi_{nl,0}(r) \end{aligned} \quad (34)$$

and

$$\begin{aligned} \phi''_{nl,2}(r) + \left( \frac{2(l+1)}{r} - 2\alpha f'(r) \right) \phi'_{nl,2}(r) \\ + \left( E_{n0} - V_0(r) + \alpha^2 f'^2 - \frac{2\alpha(l+1)}{r} f'(r) - \alpha f''(r) \right) \phi_{nl,2}(r) \\ = -E_{n2} \phi_{nl,0}(r) + (V_p - E_{n1}) \phi_{nl,1}(r). \end{aligned} \quad (35)$$

### 3.1 Applications for three-dimensional systems

In most of the practical applications of quantum mechanics, one deals with the more complicated case involved the three-dimensional Schrödinger equation with the anharmonic oscillator potential. Here, we extend the above-mentioned formalism to the bound state problem for spherical anharmonic oscillator that has numerous applications in the theory of molecules and solid-state physics. For three dimensions, one can consider a bound state problem for a non-relativistic particle moving in a central potential of an anharmonic oscillator admitted bounded eigenfunctions and having in consequence a discrete energy spectrum.

To describe the technique, we restore the exact result for the wave functions and eigenvalues of the spherical harmonic oscillator as  $R_{n,l}(r) = r^{l+1} e^{-\alpha r^2} \phi_{nl,0}(r)$  and energy eigenvalue  $E_{n,l} = 2\alpha(4n + 2l + 3)$ . Here, the function  $\phi_{nl}(r) = {}_1F_1(-n, l + \frac{3}{2}; 2\alpha r^2)$  is the solution of eq. (33).

**3.1.1 Harmonic oscillator plus non-singular potentials.** It is desirable to study harmonic oscillator plus non-singular potentials to understand several physical phenomena such as structural phase transitions, polaron formation in solids etc. For this, we consider a harmonic oscillator plus non-singular potential [15]

$$V(r) = Br^2 - Dr + Er^3 + Cr^4, \quad (36)$$

where  $B = 4\alpha^2, C = 9\beta^2, D = 3\beta(2l + 4)$  and  $E = 12\alpha\beta$ .

(i) *Ground state* ( $n = 0$ )

For the first-order correction, substituting  $f(r) = r^2$  and  $\phi_{0l,0}(r) = 1$  in eqs (34) and (35) solving by iterative way, we get the first-order correction for the ground state wave function as

$$\phi_{0l,1}(r) = -\frac{C}{16\alpha} r^4 - \frac{E}{12\alpha} r^3 - \frac{C(2l+5)}{32\alpha^2} r^2 \quad (37)$$

and first- and second-order corrections of energy as

$$E_{01} = \frac{C(2l+3)(2l+5)}{16\alpha^2} \quad (38)$$

and

$$\begin{aligned} E_{02} = -\frac{C^2(4l+11)(2l+5)(2l+3)}{512\alpha^5} - \frac{E^2(2l+7)(2l+5)(2l+3)}{768\alpha^4} \\ + \frac{DE(2l+5)(2l+3)}{192\alpha^3}. \end{aligned} \quad (39)$$

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(ii) *First excited state* ( $n = 1$ )

Now, for the first excited state substituting  $\phi_{10} = 1 - (4\alpha r^2/(2l + 3))$  in eqs (34) and (35) solving by iterative way, we obtain the first-order correction of the eigenfunction as

$$\begin{aligned} \phi_{1l,1}(r) = & \frac{C}{4(2l+3)}r^6 + \frac{E}{3(2l+3)}r^5 + \frac{C(2l+15)}{16\alpha(2l+3)}r^4 \\ & + \left( \frac{5E(l+3)}{6\alpha(2l+3)} - \frac{E}{4\alpha} - \frac{D}{2l+3} \right) r^3 - \frac{C(2l+15)(2l+5)}{32\alpha^2(2l+3)}r^2 \\ & + \left( \frac{D(4l+9)}{4\alpha(2l+3)} + \frac{3E(l+2)}{8\alpha^2} - \frac{5E(l+2)(l+3)}{4\alpha^2(2l+3)} \right) r \end{aligned} \quad (40)$$

and first- and second-order corrections of energies as

$$E_{11} = \frac{C(2l+15)(2l+5)}{16\alpha^2} \quad (41)$$

and

$$\begin{aligned} E_{12} = & -\frac{D^2}{16\alpha^2} - \frac{ED(42(l+3)(l+2) + (2l+3)(4l+9))}{192\alpha^3} \\ & + \frac{C^2(4l+45)(2l+7)(2l+5)}{512\alpha^5} \\ & + \frac{E^2(2l+5)(3(4l+21)(2l+1) - 4(2l+9)(2l+7))}{768\alpha^4}, \end{aligned} \quad (42)$$

respectively.

3.1.2 *Spherical quartic anharmonic oscillator potential.* Quartic anharmonic interactions continue to remain a focus of attention. The Hamiltonian

$$H = \frac{p^2}{2m} + 4\alpha^2 r^2 + \lambda r^4$$

forms one of the most popular theoretical laboratories for examining the validity of various approximation techniques and represents a non-trivial physics. Interest in this model Hamiltonian arises in quantum field theories and molecular physics [16].

(i) *Ground state* ( $n = 0$ )

For the first-order correction, substituting  $\phi_{0l,0}(r) = 1$  in eq. (34) and solving it, we get the first-order correction for the ground state wave function as

$$\phi_{0l,1} = -\frac{\lambda}{16\alpha}r^4 - \frac{\lambda(2l+5)}{32\alpha^2}r^2 \quad (43)$$

and the corresponding correction of energy as

$$E_{01} = \frac{\lambda(2l+3)(2l+5)}{16\alpha^2}. \quad (44)$$

Now, substituting the values of  $\phi_{0l,1}(r)$  and  $E_{01}$  in eq. (35) and solving, we obtain the second-order correction for the ground state eigenfunction as

$$\begin{aligned} \phi_{0l,2}(r) = & \frac{\lambda^2}{512\alpha^2}r^8 + \frac{\lambda^2(6l+19)}{1536\alpha^3}r^6 \\ & + \frac{\lambda^2[(6l+19)(2l+7) - (2l+5)(2l+3)]}{4096\alpha^4}r^4 \\ & + \frac{\lambda^2(4l+11)(2l+5)}{1024\alpha^5}r^2 \end{aligned} \quad (45)$$

and the corresponding correction of energy as

$$E_{02} = -\frac{\lambda^2(4l+11)(2l+5)(2l+3)}{512\alpha^5}. \quad (46)$$

(ii) *First excited state* ( $n = 1$ )

Now, by putting the value of the first excited state,  $\phi_{10} = 1 - (4\alpha r^2/(2l+3))$ , in eq. (34) and solving it, we obtain the first-order correction of the eigenfunction as

$$\phi_{1l,1}(r) = \frac{\lambda}{4(2l+3)}r^6 + \frac{\lambda(2l+15)}{16\alpha(2l+3)}r^4 - \frac{\lambda(2l+15)(2l+5)}{32\alpha^2(2l+3)}r^2 \quad (47)$$

and the correction of energy as

$$E_{11} = \frac{\lambda(2l+15)(2l+5)}{16\alpha^2}. \quad (48)$$

Similarly, solving eq. (35), we get the second-order correction of eigenfunction as

$$\begin{aligned} \phi_{1l,2}(r) = & -\frac{\lambda^2}{128\alpha(2l+3)}r^{10} - \lambda^2 \frac{(18l+115)}{1536\alpha^2(2l+3)}r^8 - \lambda^2 \frac{(4l+45)}{384\alpha^3(2l+3)}r^6 \\ & + \lambda^2 \frac{((22l+93)(2l+15)(2l+5) - (18l+115)(2l+9)(2l+7))}{4096\alpha^4(2l+3)}r^4 \\ & + \frac{1575\lambda^2}{1024(2l+3)\alpha^5}r^2 \end{aligned} \quad (49)$$

and the corresponding correction of energy

$$E_{12} = -\frac{\lambda^2(4l+45)(2l+7)(2l+5)}{512\alpha^5}. \quad (50)$$

It is seen that our technique does lead to the explicit perturbation expansion in powers of the small parameter  $\lambda (< 1)$ . Our obtained expression for the energy eigenvalues coincide with the results given in [17].

### 3.2 *Perturbed Coulomb interaction*

The perturbed Coulomb potentials represent simplified models of many situations found in atomic, molecular, condensed matter and particle physics. There has been much interest in obtaining analytical solutions of such potentials in arbitrary dimensions. These

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problems have been studied for years and a general solution has not yet been found. Such a class of potentials is

$$V(r) = -\frac{1}{r} + ar + br^2 + cr^4. \quad (51)$$

As the exact form of such interactions are unknown to a great extent, it is desirable to study the general analytical properties of a large class of potentials in eq. (51). In connection with this, the analyticity of the energy levels for these kinds of potentials was investigated rigorously by many authors using different theories [18] in relation to their potential applications in spectroscopic problems.

Here we introduce our approach for an algebraic solution of the Schrödinger equation for Coulomb plus non-singular and the perturbed Coulomb potentials. To describe this technique, we also restore the exact result for the wave functions and eigenvalues of the radial Coulomb wave functions as

$$R_{nl}(r) = N_{nl}r^{l+1}e^{-\gamma_n r} {}_1F_1(-n_r; 2l+2; 2\gamma_n r), \quad (52)$$

where  $\gamma_n = 1/2n$ , and with the normalization constant

$$N_{nl} = \frac{1}{(2l+1)!} \sqrt{\frac{(n+l)!}{2n(n-l-1)!}} (2\gamma_n)^{l+\frac{3}{2}}, \quad n = n_r + l + 1. \quad (53)$$

Substituting  $\alpha = \gamma_n$ ,  $f(r) = r$  in eqs (34) and (35), one can obtain the differential equations for the first- and second-order corrections of energy and wave functions as

$$\begin{aligned} \phi''_{nl,1}(r) + \left(\frac{2(l+1)}{r} - 2\gamma_n\right)\phi'_{nl,1}(r) + \left(\frac{n-(l+1)}{nr}\right)\phi_{nl,1} \\ = (V_p - E_{n1})\phi_{nl,0}(r) \end{aligned} \quad (54)$$

and

$$\begin{aligned} \phi''_{nl,2}(r) + \left(\frac{2(l+1)}{r} - 2\gamma_n\right)\phi'_{nl,2}(r) + \left(\frac{n-(l+1)}{nr}\right)\phi_{nl,2} \\ = -E_{n2}\phi_{nl,0}(r) + (V_p - E_{n1})\phi_{nl,1}(r). \end{aligned} \quad (55)$$

**3.2.1 Coulomb plus non-singular interaction.** For the perturbed Coulomb interactions (eq. (51)), for the ground state (1s) ( $n = 1, l = 0, \phi_{10,0}(r) = 1$ ), the solution of eq. (54) gives the first-order corrections of wave function as

$$\phi_{10,1}(r) = -\frac{c}{5}r^5 - \frac{3}{2}cr^4 - \left(\frac{b}{3} + 10c\right)r^3 - \left(2b + \frac{a}{2}\right)r^2 - 60cr^2$$

and the first correction of energy like

$$E_{10,1} = 3a + 12b + 360c$$

and eq. (55) gives the second order correction of energy as

$$E_{10,2} = -12a^2 - 216ab - 169920bc - 8886240c^2 - 1032b^2 - 9720ac.$$

For the 2s state ( $n = 2, l = 0, \phi_{20,0} = 1 - \gamma_2 r$ ), as before, solving eqs (54) and (55) by iterative way, we obtain first-order correction of wave function as

$$\begin{aligned} \phi_{20,1}(r) = & \frac{c}{10}r^6 + \frac{8c}{5}r^5 + \left(\frac{b}{6} + 32c\right)r^4 \\ & + \left(\frac{7b}{3} + \frac{a}{4} + 640c\right)r^3 - (2a + 28b + 7680c)r^2 \end{aligned}$$

and the corresponding first-order and second-order corrections of energies as

$$E_{20,1} = 12a + 168b + 46080c$$

and

$$\begin{aligned} E_{20,2} = & -(473088b^2 + 528a^2 + 31104ab + 30597120ac + 542638080bc \\ & + 248405114880c^2), \end{aligned}$$

respectively.

For 3s state ( $n = 3, l = 0, \phi_{30,0} = 1 - 2\gamma_3 r + \frac{2}{3}\gamma_3^2 r^2$ ) solving eqs (54) and (55) we get the first- and second-order corrections of wave functions as

$$\begin{aligned} \phi_{30,1}(r) = & -\frac{c}{90}r^7 - \frac{13c}{60}r^6 - \left(\frac{b}{54} + \frac{101c}{10}\right)r^5 \\ & - \left(\frac{b}{3} + \frac{a}{36} + \frac{909c}{2}\right)r^4 + \left(\frac{5a}{6} + 23b + 27270c\right)r^3 \\ & - \left(\frac{9a}{2} + 138b + 163620c\right)r^2 \end{aligned}$$

and the corresponding first-order correction of energy as  $E_{30,1} = 27a + 828b + 981720c$ . Similarly, by solving eq. (55), one can generate the second-order correction of wave function and energy for this state.

**3.2.2 Perturbed Coulomb interactions limit.** Now we consider the perturbed Coulomb interactions as

$$V(r) = -\frac{1}{r} + ar + br^2 \tag{56}$$

which are possible candidates for the quarkonium potential as has been indicated by the quarkonium spectroscopy [19]. In the special case of  $b = 0$  and  $a > 0$  such potentials reduce to the well-known charmonium potential. Apart from its relevance in heavy quarkonium spectroscopy, this class of potentials with  $b = 0$  has important applications

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in atomic physics. The Stark effect in a hydrogen atom in one dimension is given exactly by the charmonium-like potential ( $a$  being the electric field parameter). The more general class of these potentials with  $b > 0$  is also relevant in atomic physics. This could be interpreted as the potential seen by an electron of an atom exposed to a suitable admixture of electric and magnetic fields. In addition, nuclei in the presence of an electron background form a system which is important for condensed matter physics and for laboratory and stellar plasmas. The potential between two nuclei embedded in such a plasma is approximately Coulomb plus harmonic oscillator, which corresponds to  $a = 0$  in eq. (56). The potential in eq. (56) behaves like a perturbed harmonic oscillator for large values of the parameter  $b$  with respect to the parameter  $a$ .

For 1s state (ground state) ( $n = 1, l = 0, \phi_{10,0} = 1$ ), solving eqs (54) and (55) by iterative way we get the first- and second-order corrections of wave functions as

$$\phi_{10,1}(r) = -\frac{b}{3}r^3 - \left(2b + \frac{a}{2}\right)r^2$$

and

$$\begin{aligned} \phi_{10,2}(r) = & \frac{b^2}{18}r^6 + \left(\frac{ab}{6} + \frac{13b^2}{15}\right)r^5 + \left(\frac{a^2}{8} + \frac{3}{2}ab + \frac{11}{2}b^2\right)r^4 \\ & + \left(\frac{a^2}{3} + 6ab + \frac{86}{3}b^2\right)r^3 + \left(2a^2 + 36ab + 172b^2\right)r^2. \end{aligned}$$

Subsequently we get the corresponding energy corrections as  $E_{10,1} = 3a + 12b$  and  $E_{10,2} = -(1032b^2 + 12a^2 + 216ab)$ .

For 2s state ( $n = 2, l = 0, \phi_{20,0} = 1 - \gamma_2 r$ ), as before, solving (54) and (55) by iterative way, we obtain first- and second-order corrections of wave functions as

$$\phi_{20,1}(r) = \frac{b}{6}r^4 + \left(\frac{7b}{3} + \frac{a}{4}\right)r^3 - (28b + 2a)r^2$$

and

$$\begin{aligned} \phi_{20,2}(r) = & -\frac{b^2}{18}r^7 - \left(\frac{ab}{6} + \frac{98b^2}{45}\right)r^6 - \left(\frac{a^2}{8} + \frac{8}{3}ab + \frac{266}{15}b^2\right)r^5 \\ & + \left(\frac{5a^2}{6} + 12ab - \frac{280}{3}b^2\right)r^4 - \left(\frac{22a^2}{3} + 432ab + \frac{19712b^2}{3}\right)r^3 \\ & + (88a^2 + 5184ab + 78848b^2)r^2 \end{aligned}$$

and the corresponding first- and second-order corrections of energies as  $E_{20,1} = 12a + 168b$  and  $E_{20,2} = -(473088b^2 + 528a^2 + 31104ab)$ , respectively.

For 2p state ( $n = 2, l = 1, \phi_{21,0} = 1$ ) solving eqs (54) and (55) we get the first- and second-order corrections of wave functions as

$$\phi_{21,1}(r) = -\frac{2b}{3}r^3 - (12b + a)r^2$$

and

$$\begin{aligned}\phi_{21,2}(r) = & \frac{2b^2}{9}r^6 + \left(\frac{2ab}{3} + \frac{48b^2}{5}\right)r^5 + \left(\frac{a^2}{2} + 16ab + 152b^2\right)r^4 \\ & + \left(\frac{8a^2}{3} + \frac{416}{3}ab + \frac{5632}{3}b^2\right)r^3 + (48a^2 + 2496ab + 33792b^2)r^2\end{aligned}$$

and the corresponding first- and second-order corrections of energies as  $E_{21,1} = 10a + 120b$  and  $E_{21,2} = -(480a^2 + 337920b^2 + 24960ab)$ , respectively.

For 3s state ( $n = 3, l = 0, \phi_{30,0} = 1 - 2\gamma_3 r + \frac{2}{3}\gamma_3^2 r^2$ ) similarly, we get first- and second-order corrections of wave functions as

$$\phi_{30,1}(r) = -\frac{b}{54}r^5 - \left(\frac{b}{3} + \frac{a}{36}\right)r^4 + \left(23b + \frac{5a}{6}\right)r^3 - \left(\frac{9a}{2} + 138b\right)r^2$$

and

$$\begin{aligned}\phi_{30,2}(r) = & \frac{b^2}{108}r^8 + \left(\frac{ab}{36} + \frac{3b^2}{5}\right)r^7 + \left(\frac{a^2}{48} + \frac{5}{12}ab - \frac{71}{20}b^2\right)r^6 \\ & - \left(\frac{17a^2}{24} + 33ab + \frac{2871}{10}b^2\right)r^5 + \left(\frac{69a^2}{8} + \frac{1377ab}{2} + \frac{31293}{2}b^2\right)r^4 \\ & - (153a^2 + 18954ab + 595998b^2)r^3 \\ & + (918a^2 + 113724ab + 3575988b^2)r^2\end{aligned}$$

and the corresponding first- and second-order corrections of energies as  $E_{30,1} = 27a + 828b$  and  $E_{30,2} = -(21455928b^2 + 5508a^2 + 682344ab)$ , respectively.

For 3p state ( $n = 3, l = 1, \phi_{31,0} = 1 - \frac{1}{2}\gamma_3 r$ ), the solution of eqs (54) and (55) give the first- and second-order corrections of wave functions as

$$\phi_{31,1}(r) = \frac{b}{12}r^4 + \left(2b + \frac{a}{8}\right)r^3 - \left(72b + \frac{5a}{2}\right)r^2$$

and

$$\begin{aligned}\phi_{31,2}(r) = & -\frac{b^2}{24}r^7 - \left(\frac{ab}{8} + \frac{59b^2}{20}\right)r^6 - \left(\frac{3a^2}{32} + \frac{25}{8}ab + \frac{819}{40}b^2\right)r^5 \\ & + \left(\frac{15a^2}{8} + 87ab + 621b^2\right)r^4 - (15a^2 + 1746ab + 51678b^2)r^3 \\ & + (540a^2 + 62856ab + 1860408b^2)r^2\end{aligned}$$

and the corresponding first- and second-order corrections of energies as  $E_{31,1} = 25a + 720b$  and  $E_{31,2} = -(18604080b^2 + 5400a^2 + 628560ab)$ , respectively.



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For 3d state ( $n = 3, l = 2, \phi_{30,0} = 1$ ), the solutions of eqs (54) and (55) give the first- and second-order corrections of wave functions as

$$\phi_{32,1}(r) = -br^3 - \left(36b + \frac{3a}{2}\right)r^2$$

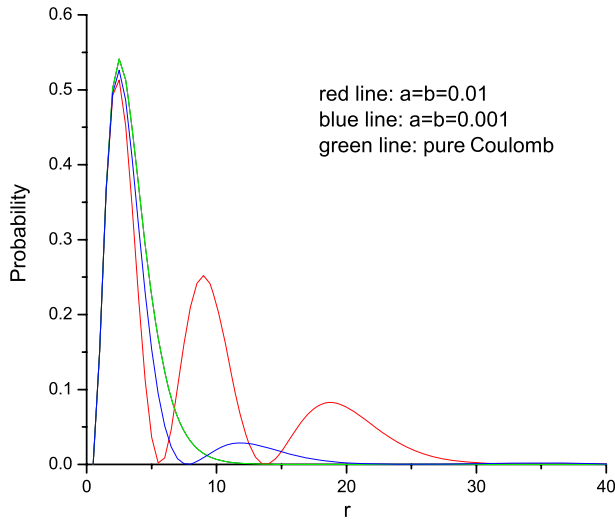
and

$$\begin{aligned} \phi_{32,2}(r) = & \frac{b^2}{2}r^6 + \left(\frac{3ab}{2} + \frac{207b^2}{5}\right)r^5 - \left(\frac{3a^2}{8} + \frac{135}{2}ab + \frac{2349}{2}b^2\right)r^4 \\ & + (9a^2 + 918ab + 24138b^2)r^3 \\ & + (324a^2 + 33048ab + 868968b^2)r^2 \end{aligned}$$

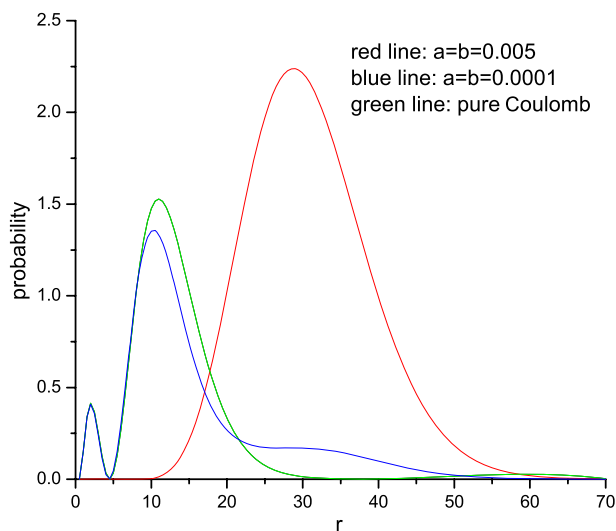
and the corresponding first- and second-order corrections of energies as  $E_{32,1} = 21a + 504b$  and  $E_{32,2} = -(12165552b^2 + 4536a^2 + 462672ab)$ , respectively.

Charge distributions between pure Coulomb and perturbed Coulomb interactions are shown in figures 1–3.

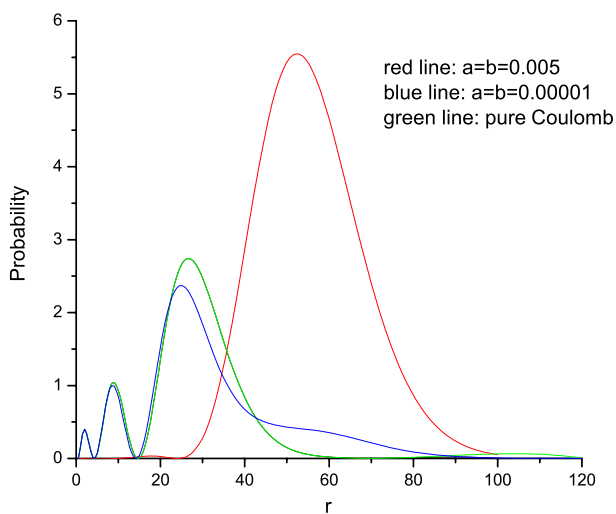
Here, we have plotted the charge distributions of the 1s, 2s and 3s states for pure Coulomb and perturbed Coulomb interactions upto the second-order corrections of the wave function. It is well known that with increasing principal quantum number  $n$ , the maximum of the charge distribution shifts away from the nucleus; the electron is less tightly bound. According to the radial quantum number  $n_r$ , there are several maxima, a principal maximum and some supplementary maxima. It is observed that similar nature also occurs in perturbed Coulomb system for the values of parameters ( $a, b$ ) within the interval  $0 < a \leq 0.0001$  and  $0 < b \leq 0.0001$ . It has been checked that as  $a \rightarrow 0$  and



**Figure 1.** The probability of charge distribution of 1s state for pure Coulomb (green line) and perturbed Coulomb for the parameters  $a = b = 0.01$  (red line) and  $a = b = 0.001$  (blue line).



**Figure 2.** The probability of charge distribution of 2s state for pure Coulomb (green line) and perturbed Coulomb for the parameters  $a = b = 0.005$  (red line) and  $a = b = 0.0001$  (blue line).



**Figure 3.** The probability of charge distribution of 3s state for pure Coulomb (green line) and perturbed Coulomb for the parameters  $a = b = 0.005$  (red line) and  $a = b = 0.00001$  (blue line).

$b \rightarrow 0$ , the probability of charge distribution for the perturbed Coulomb system tends to coincide with the charge distribution of the pure Coulomb. But for  $a, b > 0.0001$  we also observe that, the charge distributions for all states are very large with respect to the unperturbed Coulomb system.

#### 4. Conclusion

In this work, an iterative technique within the framework of LDE techniques has been developed for deriving the wave functions and eigenvalues of quartic, sextic and octic anharmonic oscillators in one dimension and spherical anharmonic oscillator and perturbed Coulomb potential in three dimensions. We would like to stress that, although we have displayed the results up to a few orders in the perturbative expansion, it is very easy to push the calculation to any order, as the method only requires the solution of algebraic equations order by order. Apart from the theoretical interest, this simple technique can be used to look for and to obtain polynomial solutions to eigenvalue problems of Schrödinger type and similarly for polynomial solution of quasi-exactly solvable models in quantum mechanics [20]. The study of the quartic, sextic and octic anharmonic potentials in one dimension have applications in nonlinear mechanics, molecular physics, quantum optics, nuclear physics and field theory [21].

Unfortunately, the study of these anharmonic potentials have not been carried out further. This approach may be used to analyse disorder system [22], to study the slow role potential inflationary model [23] and the Bose–Einstein condensation problems [24]. The present formalism can also be generalized to all the polynomial forces of the form

$$V_m(r) = Ar^{2m} + Br^{2m-1} + \dots + \frac{F}{r} + \frac{G}{r^2},$$

as an alternative treatment to the works in [25] and the references therein. We conclude by noting that the LDE technique can be used for non-perturbative as well as perturbative systems to find approximate solutions of eigenvalue problems and this technique is equivalent to modified homotopy perturbation method [26] upto a few order.

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