

# A perturbative treatment for the bound states of the Hellmann potential

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## Abstract

A new approximation formalism is applied to study the bound states of the Hellmann potential, which represents the superposition of the attractive Coulomb potential  $-a/r$  and the Yukawa potential  $b \exp(-\delta r)/r$  of arbitrary strength  $b$  and screening parameter  $\delta$ . Although the analytic expressions for the energy eigenvalues  $E_{n,\ell}$  yield quite accurate results for a wide range of  $n, \ell$  in the limit of very weak screening, the results become gradually worse as the strength  $b$  and the screening coefficient  $\delta$  increase. This is because that the expansion parameter is not sufficiently small enough to guarantee the convergence of the expansion series for the energy levels.

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## I. INTRODUCTION

Adamowski [1] has presented a study of the systematics of the energy eigenvalues of the two-particles interacting via the superposition of the Coulomb and Yukawa potential (SCYP):

$$V(r) = -a/r + b \exp(-\delta r)/r, \quad (1)$$

where  $a$  and  $b$  are the strengths of the Coulomb and the Yukawa potentials, respectively, and  $\delta$  is the screening parameter. It is assumed that  $a$  and  $\delta$  are positive whereas  $b$  can be positive or negative. The potential in (1) with  $b$  positive was first suggested by Hellmann [2,3] many years ago and henceforth this potential will be referred to as the Hellmann potential irrespectively of the sign of  $b$ . The Hellmann potential has been used by various authors to represent the electron-core [4,5] or the electron-ion [6,7] interaction. Varshni and Shukla [8] used this model potential for alkali hydride molecules. Das and Chakravarty [9] have proposed that such a potential is suitable for the study of inner-shell ionization problems.

The bound-state energies of the Hellmann potential for various sets of values of  $b$  and  $\delta$  have been studied elaborately by Adamowski in a variational framework using ten variational parameters. The energy eigenvalues have been predicted very accurately but the calculations involve extensive computational time and effort. Moreover, compact analytic expressions for the energy eigenvalues are not obtainable. On the other hand, Dutt *et al* [10] have also been investigated the bound-state energies as well as the wave functions of this potential using the large- $N$  expansion technique.

In this paper, we study the bound-state properties by applying a new methodology [11] based on the decompose of the radial Schrödinger equation into two pieces having an exactly solvable part and an additional piece leading to either a closed analytical solution or an approximate treatment depending on the nature of the additional perturbed potential. The application [12,13] of this novel treatment to the different problems in both, bound and continuum regions, have been proven the success of the formalism. We demonstrate here how such interaction potential can be simply treated within the framework of the present formalism.

One of the prime motivations of the present study is to explore the regions of validity of this approximation formalism for the superposition of potentials such as the one in (1) which manifests different structures for various range of values of  $b$  and  $\delta$ . Our calculations reveal that the degree of accuracy of the predicted eigenvalues varies appreciably for different range of values of  $b$  and  $\delta$  and for different quantum states. These observations have relevance in the context of applications of this novel treatment to realistic problems of atomic physics. The other motivation is that potential (1) with  $a = 0$  and  $b = -\alpha Z$  can be reduced into the static screened Coulomb potential (SSCP) of the simple form:

$$V(r) = -(\alpha Z) \exp(-\delta r)/r, \quad (2)$$

where  $a = (137.037)^{-1}$  is the fine-structure constant and  $Z$  is the atomic number, is often used to compute bound-state normalizations and energy levels of neutral atoms [14,15,16,17] which have been studied over the past years. It is known that SSCP yields reasonable results only for the innermost states when  $Z$  is large. However, for the outermost and middle atomic states, it gives rather poor results. Although the bound-state energies for the SSCP with  $Z = 1$  have been studied [18] in the light of the shifted large- $N$  method. Recently, we have also investigated that this novel treatment is useful in predicting bound-state energy levels of light to heavy neutral atoms [17].

The contents of this paper is as follows. In section II we briefly outline the method with all necessary formulae to perform the current calculations. In section III we apply the approach to the Schrödinger equation with Hellmann potential and present the results obtained analytically for the bound-state energy values upto third perturbation energy shift. Section IV contains the numerical results. Finally, in section V we give our conclusions.

## II. THE METHOD

For the consideration of spherically symmetric potentials, the corresponding Schrödinger equation, in the bound state domain, for the radial wave function reads

$$\frac{\hbar^2}{2m} \frac{\psi_n''(r)}{\psi_n(r)} = V(r) - E_n, \quad (3)$$

with

$$V(r) = \left[ V_0(r) + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} \right] + \Delta V(r), \quad (4)$$

where  $\Delta V(r)$  is a perturbing potential and  $\psi_n(r) = \chi_n(r)u_n(r)$  is the full radial wave function, in which  $\chi_n(r)$  is the known normalized eigenfunction of the unperturbed Schrödinger equation whereas  $u_n(r)$  is a moderating function corresponding to the perturbing potential. Following the prescription of Refs. [11,12,13], we may rewrite (3) in the form:

$$\frac{\hbar^2}{2m} \left( \frac{\chi_n''(r)}{\chi_n(r)} + \frac{u_n''(r)}{u_n(r)} + 2 \frac{\chi_n'(r)u_n'(r)}{\chi_n(r)u_n(r)} \right) = V(r) - E_n. \quad (5)$$

The logarithmic derivatives of the unperturbed  $\chi_n(r)$  and perturbed  $u_n(r)$  wave functions are given by

$$W_n(r) = -\frac{\hbar}{\sqrt{2m}} \frac{\chi_n'(r)}{\chi_n(r)} \quad \text{and} \quad \Delta W_n = -\frac{\hbar}{\sqrt{2m}} \frac{u_n'(r)}{u_n(r)}, \quad (6)$$

which leads to

$$\frac{\hbar^2}{2m} \frac{\chi_n''(r)}{\chi_n(r)} = W_n^2(r) - \frac{\hbar}{\sqrt{2m}} W_n'(r) = \left[ V_0(r) + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} \right] - \varepsilon_n, \quad (7)$$

where  $\varepsilon_n$  is the eigenvalue for the exactly solvable potential of interest, and

$$\frac{\hbar^2}{2m} \left( \frac{u_n''(r)}{u_n(r)} + 2 \frac{\chi_n'(r)u_n'(r)}{\chi_n(r)u_n(r)} \right) = \Delta W_n^2(r) - \frac{\hbar}{\sqrt{2m}} \Delta W_n'(r) + 2W_n(r)\Delta W_n(r) = \Delta V(r) - \Delta\varepsilon_n, \quad (8)$$

in which  $\Delta\varepsilon_n = E_n^{(1)} + E_n^{(2)} + E_n^{(3)} + \dots$  is the correction term to the energy due to  $\Delta V(r)$  and  $E_n = \varepsilon_n + \Delta\varepsilon_n$ . If Eq. (8), which is the most significant piece of the present formalism, can be solved analytically as in (7), then the whole problem, in Eq. (3) is

$$[W_n(r) + \Delta W_n(r)]^2 - \frac{\hbar}{\sqrt{2m}} [W_n(r) + \Delta W_n(r)]' = V(r) - E_n, \quad (9)$$

which is a well known treatment within the frame of supersymmetric quantum theory (SSQT) [19]. Thus, if the whole spectrum and corresponding eigenfunctions of the unperturbed interaction potential are known, then one can easily calculate the required superpotential  $W_n(r)$  for any state of interest leading to direct computation of related corrections to the unperturbed energy and wave function.

For the perturbation technique, we can split the given potential (3) into two parts. The main part corresponds to a shape invariant potential, Eq. (7), for which the superpotential is known analytically and the remaining part is treated as a perturbation, Eq. (8). Therefore, it is obvious that Hellmann potential can be treated using this prescription. In this case, the zeroth-order term corresponds to the Coulomb potential while higher-order terms constitute the perturbation. However, the perturbation term in its present form cannot be solved exactly through Eq. (8). Thus, one should expand the functions related to the perturbation in terms of the perturbation parameter  $\lambda$ ,

$$\Delta V(r; \lambda) = \sum_{i=1}^{\infty} \lambda_i V_i(r), \quad \Delta W_n(r; \lambda) = \sum_{i=1}^{\infty} \lambda_i W_n^{(i)}(r), \quad E_n(\lambda) = \sum_{i=1}^{\infty} \lambda_i E_n^{(i)}, \quad (10)$$

where  $i$  denotes the perturbation order. Substitution of the above expansions into Eq. (8) and equating terms with the same power of  $\lambda$  on both sides up to  $O(\lambda^4)$  gives

$$2W_n(r)W_n^{(1)}(r) - \frac{\hbar}{\sqrt{2m}} \frac{dW_n^{(1)}(r)}{dr} = V_1(r) - E_n^{(1)}, \quad (11)$$

$$W_n^{(1)}(r)W_n^{(1)}(r) + 2W_n(r)W_n^{(2)}(r) - \frac{\hbar}{\sqrt{2m}} \frac{dW_n^{(2)}(r)}{dr} = V_2(r) - E_n^{(2)}, \quad (12)$$

$$2 \left[ W_n(r)W_n^{(3)}(r) + W_n^{(1)}(r)W_n^{(2)}(r) \right] - \frac{\hbar}{\sqrt{2m}} \frac{dW_n^{(3)}(r)}{dr} = V_3(r) - E_n^{(3)}, \quad (13)$$

$$2 \left[ W_n(r)W_n^{(4)}(r) + W_n^{(1)}(r)W_n^{(3)}(r) \right] + W_n^{(2)}(r)W_n^{(2)}(r) - \frac{\hbar}{\sqrt{2m}} \frac{dW_n^{(4)}(r)}{dr} = V_4(r) - E_n^{(4)}. \quad (14)$$

Hence, unlike the other perturbation theories, Eq. (8) and its expansion, Eqs. (11)-(14), give a flexibility for the easy calculations of the perturbative corrections to energy and

wave functions for the  $n$ th state of interest through an appropriately chosen perturbed superpotential.

### III. APPLICATION TO THE HELLMANN POTENTIAL

Considering the recent interest in various power-law potentials in the literature, we work through the article within the frame of low screening parameter. In this case, the Hellmann potential can be expanded in power series of the screening parameter  $\delta$  as [13,17,20]

$$V(r) = -\frac{a}{r} + \frac{b}{r} \exp(-\delta r) = -\frac{a}{r} + \frac{b}{r} \sum_{i=0}^{\infty} V_i(\delta r)^i, \quad (15)$$

where the perturbation coefficients  $V_i$  are given by

$$V_1 = +1, \quad V_2 = -1/2, \quad V_3 = 1/6, \quad V_4 = -1/24, \quad \dots \quad (16)$$

We now apply this approximation method to the Hellmann potential with the angular momentum barrier

$$V(r) = -\frac{a}{r} + \frac{b}{r} \exp(-\delta r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2} = \left[ V_0(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2} \right] + \Delta V(r), \quad (17)$$

where the first piece is the shape invariant zeroth-order which is an exactly solvable piece corresponding to the unperturbed Coulomb potential with  $V_0(r) = -(a-b)/r$  while  $\Delta V(r) = -b\delta + (b\delta^2/2)r - (b\delta^3/6)r^2 + (b\delta^4/24)r^3 - \dots$  is the perturbation term. The literature is rich with examples of particular solutions for such power-law potentials employed in different fields of physics, for recent applications see Refs. [21,22]. At this stage one may wonder why the series expansion is truncated at a lower order. This can be understood as follows. It is widely appreciated that convergence is not an important or even desirable property for series approximations in physical problems. Specifically, a slowly convergent approximation which requires many terms to achieve reasonable accuracy is much less valuable than the divergent series which gives accurate answers in a few terms. This is clearly the case for the Hellmann problem [23]. However, it is worthwhile to note that the main contributions come from the first three terms. Thereby, the present calculations are performed up to the

third-order involving only these additional potential terms, which suprisingly provide highly accurate results for small screening parameter  $\delta$ .

### A. Ground State Calculations ( $n = 0$ )

In the light of Eq. (7), the zeroth-order calculations leading to exact solutions can be carried out readily by setting the ground-state superpotential and the unperturbed exact energy as

$$W_{n=0}(r) = -\frac{\hbar}{\sqrt{2m}} \frac{\ell+1}{r} + \sqrt{\frac{m}{2}} \frac{(a-b)}{(\ell+1)\hbar}, \quad E_n^{(0)} = -\frac{m(a-b)^2}{2\hbar^2(n+\ell+1)^2}, \quad n = 0, 1, 2, \dots \quad (18)$$

and from the literature, the corresponding normalized Coulomb bound-state wave function [13,17,24]

$$\chi_n^{(C)}(r) = N_{n,l}^{(C)} r^{\ell+1} \exp[-\beta r] \times L_n^{2\ell+1}[2\beta r], \quad (19)$$

in which  $N_{n,l}^{(C)} = \left[ \frac{2m(a-b)}{(n+\ell+1)\hbar^2} \right]^{\ell+1} \frac{1}{(n+\ell+1)} \sqrt{\frac{m(a-b)n!}{\hbar^2(n+2\ell+1)!}}$  is a normalized constant,  $\beta = \frac{m(a-b)}{(n+\ell+1)\hbar^2}$  and  $L_n^k(x) = \sum_{m=0}^n (-1)^m \frac{(n+k)!}{(n-m)!(m+k)!m!} x^m$  is an associate Laguarre polynomial function [25].

For the calculation of corrections to the zeroth-order energy and wavefunction, one needs to consider the expressions leading to the first to the third-order perturbation given by Eqs. (11)–(14). Multiplication of each term in these equations by  $\chi_n^2(r)$ , and bearing in mind the superpotentials given in Eq. (6), one can obtain the straightforward expressions for the first-order correction to the energy and its superpotential:

$$E_n^{(1)} = \int_{-\infty}^{\infty} \chi_n^2(r) \left( \frac{b\delta^2}{2} r \right) dr, \quad W_n^{(1)}(r) = \frac{\sqrt{2m}}{\hbar} \frac{1}{X_n^2(r)} \int^r \chi_n^2(x) \left[ E_n^{(1)} - \frac{b\delta^2}{2} x \right] dx, \quad (20)$$

and for the second-order correction and its superpotential:

$$E_n^{(2)} = \int_{-\infty}^{\infty} \chi_n^2(r) \left[ -\frac{b\delta^3}{6} r^2 - W_n^{(1)}(r) W_n^{(1)}(r) \right] dr, \quad (21)$$

$$W_n^{(2)}(r) = \frac{\sqrt{2m}}{\hbar} \frac{1}{X_n^2(r)} \int^r \chi_n^2(x) \left[ E_n^{(2)} + W_n^{(1)}(r) W_n^{(1)}(x) + \frac{b\delta^3}{6} x^2 \right] dx,$$

and for the third-order correction and its superpotential:

$$E_n^{(3)} = \int_{-\infty}^{\infty} \chi_n^2(r) \left[ \frac{b\delta^4}{24} r^3 - W_n^{(1)}(r) W_n^{(2)}(r) \right] dr,$$

$$W_n^{(3)}(r) = \frac{\sqrt{2m}}{\hbar} \frac{1}{X_n^2(r)} \int^r \chi_n^2(x) \left[ E_n^{(3)} + W_n^{(1)}(x) W_n^{(2)}(x) - \frac{b\delta^4}{24} x^3 \right] dx, \quad (22)$$

for any state of interest. The above expressions calculate  $W_n^{(1)}(r)$ ,  $W_n^{(2)}(r)$  and  $W_n^{(3)}(r)$  explicitly from the energy corrections  $E_n^{(1)}$ ,  $E_n^{(2)}$  and  $E_n^{(3)}$  respectively, which are in turn used to calculate the moderating wave function  $u_n(r)$ .

Thus, using Eqs. (20)-(22), one finds the zeroth order energy shift and their moderating superpotentials, for  $a \neq b$ , as

$$E_0^{(1)} = \frac{\hbar^2 b (3N_0^2 - L)}{4(a-b)m} \delta^2, \quad W_0^{(1)}(r) = \frac{\hbar b N_0 \delta^2}{2\sqrt{2m}(a-b)} r,$$

$$E_0^{(2)} = -\frac{\hbar^4 b N_0^2 (5N_0^2 - 3L + 1)}{12(a-b)^2 m^2} \delta^3 - \frac{\hbar^6 b^2 N_0^4 (5N_0^2 - 3L + 1)}{16(a-b)^4 m^3} \delta^4,$$

$$W_0^{(2)}(r) = -\frac{\hbar N_0 [(a-b)mr + \hbar^2 N_0 N_1] [3\hbar^2 b^2 N_0^2 \delta + 4mb(a-b)^2] \delta^3}{24\sqrt{2m} m^2 (a-b)^4} r,$$

$$E_0^{(3)} = \frac{\hbar^6 b N_0^2 (5N_0^2 - 3L) (5N_0^2 - 3L + 1)}{96(a-b)^3 m^3} \delta^4 + \frac{\hbar^8 b^2 N_0^4 (5N_0^2 - 3L + 1) (9N_0^2 - 5L)}{48(a-b)^5 m^4} \delta^5$$

$$+ \frac{\hbar^{10} b^3 N_0^6 (5N_0^2 - 3L + 1) (9N_0^2 - 5L)}{64(a-b)^7 m^5} \delta^6, \quad (23)$$

where  $N_0 = (\ell + 1)$ ,  $N_1 = (\ell + 2)$  and  $L = \ell(\ell + 1)$ . Therefore, the analytical expressions for the lowest energy and full radial wave function of the Hellmann potential are then given by

$$E_{n=0,\ell} = E_{n=0}^{(0)} - b\delta + E_0^{(1)} + E_0^{(2)} + E_0^{(3)} + \dots, \quad \psi_{n=0,\ell}(r) \approx \chi_{n=0,\ell}^{(C)}(r) u_{n=0,\ell}(r),$$

$$u_{n=0,\ell}(r) \approx \exp\left(-\frac{\sqrt{2m}}{\hbar} \int^r (W_0^{(1)}(x) + W_0^{(2)}(x)) dx\right). \quad (24)$$

Hence, the explicit form of the full wave function in (24) for the ground state is



$$\psi_{n=0,\ell}(r) = \left[ \frac{2m(a-b)}{(\ell+1)\hbar^2} \right]^{\ell+1} \frac{1}{(\ell+1)} \sqrt{\frac{(a-b)m}{\hbar^2(2\ell+1)!}} r^{\ell+1} \exp(P(r)), \quad (25)$$

with  $P(r) = \sum_{i=2}^3 p_i r^i$  is a polynomial of third order having the following coefficients:

$$p_2 = \frac{bN_0\delta^2}{4(a-b)} \left[ \frac{N_1\hbar^2 c}{m} - 1 \right], \quad p_3 = \frac{1}{6} bc\delta^2, \quad (26)$$

in which

$$c = \frac{N_0\delta}{12m(a-b)^3} \left[ 3\hbar^2 b N_0^2 \delta + 4m(a-b)^2 \right]. \quad (27)$$

### B. Excited state calculations ( $n \geq 1$ )

The procedures applied in the calculations of the ground states becomes extremely cumbersome in the description of radial excitations when nodes of wavefunctions are taken into account, in particular during the higher order calculations. Although several attempts have been made to bypass this difficulty and improve calculations in dealing with excited states, (cf. e.g. [26], and the references therein) within the frame of supersymmetric quantum mechanics.

Using Eqs. (6), (18) and (19), the superpotential  $W_n(r)$  which is related to the excited states can be readily calculated by means of Eqs. (20)-(22). Therefore, the energy shifts in the first excited state, with  $a \neq b$ , are:

$$E_1^{(1)} = \frac{\hbar^2 b (3N_1^2 - L)}{4m(a-b)} \delta^2, \quad W_1^{(1)}(r) = \frac{\hbar b N_1 \delta^2}{2\sqrt{2m(a-b)}} r,$$

$$E_1^{(2)} = -\frac{\hbar^4 b N_1^2 (5N_1^2 - 3L + 1)}{12(a-b)^2 m^2} \delta^3 - \frac{\hbar^6 b^2 N_1^4 (5N_1^2 - 3L + 1)}{16(a-b)^4 m^3} \delta^4,$$

$$W_1^{(2)}(r) = -\frac{\hbar N_1 \left[ (a-b)mr + \hbar^2 N_1 N_2 \right] \left[ 3\hbar^2 b^2 N_1^2 \delta + 4mb(a-b)^2 \right] \delta^3}{24\sqrt{2mm^2(a-b)^4}} r,$$

$$E_1^{(3)} = \frac{\hbar^6 b N_1^2 (5N_1^2 - 3L) (5N_1^2 - 3L + 1)}{96(a-b)^3 m^3} \delta^4 + \frac{\hbar^8 b^2 N_1^4 (5N_1^2 - 3L + 1) (9N_1^2 - 5L)}{48(a-b)^5 m^4} \delta^5$$

$$+ \frac{\hbar^{10} N_1^6 (5N_1^2 - 3L + 1) (9N_1^2 - 5L)}{64(a-b)^7 m^5} \delta^6, \quad (28)$$

Therefore, the approximated energy value of the Hellmann potential corresponding to the first excited state is

$$E_{n=1,\ell} = E_1^{(0)} - b\delta + E_1^{(1)} + E_1^{(2)} + E_1^{(3)} + \dots \quad (29)$$

The related radial wavefunction can be expressed in an analytical form in the light of Eqs (20), (21) and (24), if required. The approximation used in this work would not affect considerably the sensitivity of the calculations. On the other hand, it is found analytically that our investigations put forward an interesting hierarchy between  $W_n^{(1)}(r)$  terms of different quantum states in the first order with  $a \neq b$  after circumventing the nodal difficulties elegantly,

$$W_n^{(1)}(r) = \frac{\hbar b N_n \delta^2}{2\sqrt{2m}(a-b)} r, \quad (30)$$

where  $N_n = (n + \ell + 1)$ . Therefore, for the second excited state ( $n = 2$ ) leads to the first-order energy shift and superpotential

$$E_2^{(1)} = \frac{\hbar^2 b (3N_2^2 - L)}{4m(a-b)} \delta^2, \quad W_2^{(1)}(r) = \frac{\hbar b N_2 \delta^2}{2\sqrt{2m}(a-b)} r, \quad (31)$$

where  $N_2 = (\ell + 3)$ . Thus, the use of  $W_2^{(1)}(r)$  in Eq.(21) gives the energy shift and supersymmetric potential in the second-order with  $a \neq b$  as

$$E_2^{(2)} = -\frac{\hbar^4 b N_2^2 (5N_2^2 - 3L + 1)}{12(a-b)^2 m^2} \delta^3 - \frac{\hbar^6 b^2 N_2^4 (5N_2^2 - 3L + 1)}{16(a-b)^4 m^3} \delta^4,$$

$$W_2^{(2)}(r) = -\frac{\hbar N_2 [(a-b)mr + \hbar^2 N_2 N_3] [3\hbar^2 b^2 N_2^2 \delta + 4mb(a-b)^2] \delta^3}{24\sqrt{2m}(a-b)^4 m^2} r. \quad (32)$$

Finally, we obtain the third-order energy shift as

$$E_2^{(3)} = \frac{\hbar^6 b N_2^2 (5N_2^2 - 3L) (5N_2^2 - 3L + 1)}{96(a-b)^3 m^3} \delta^4 + \frac{\hbar^8 b^2 N_2^4 (5N_2^2 - 3L + 1) (9N_2^2 - 5L)}{48(a-b)^5 m^4} \delta^5$$

$$+ \frac{\hbar^{10} b^3 N_2^6 (5N_2^2 - 3L + 1) (9N_2^2 - 5L)}{64(a-b)^7 m^5} \delta^6. \quad (33)$$

Therefore, the approximated energy eigenvalue of the Hellmann potential corresponding to the second excited state is

$$E_{n=2,\ell} = E_2^{(0)} - b\delta + E_2^{(1)} + E_2^{(2)} + E_2^{(3)} + \dots \quad (34)$$

In general, from the supersymmetry, we find out the  $n$ th state energy shifts together with their supersymmetric potentials with  $a \neq b$  as

$$\begin{aligned} E_n^{(1)} &= \frac{\hbar^2 b [3N_n^2 - L]}{4(a-b)m} \delta^2, \quad W_n^{(1)}(r) = \frac{\hbar b N_n \delta^2}{2\sqrt{2m}(a-b)} r, \\ E_n^{(2)} &= -\frac{\hbar^4 b N_n^2 [5N_n^2 - 3L + 1]}{12(a-b)^2 m^2} \delta^3 - \frac{\hbar^6 b^2 N_n^4 [5N_n^2 - 3L + 1]}{16(a-b)^4 m^3} \delta^4, \\ W_n^{(2)}(r) &= -\frac{\hbar N_n [(a-b)mr + \hbar^2 N_n N_{n+1}] [3\hbar^2 b^2 N_n^2 \delta + 4mb(a-b)^2] \delta^3}{24\sqrt{2mm^2}(a-b)^4} r, \\ E_n^{(3)} &= \frac{\hbar^6 b N_n^2 [5N_n^2 - 3L] [5N_n^2 - 3L + 1]}{96(a-b)^3 m^3} \delta^4 + \frac{\hbar^8 b^2 N_n^4 [5N_n^2 - 3L + 1] [9N_n^2 - 5L]}{48(a-b)^5 m^4} \delta^5 \\ &\quad + \frac{\hbar^{10} b^3 N_n^6 (5N_n^2 - 3L + 1) (9N_n^2 - 5L)}{64(a-b)^7 m^5} \delta^6, \end{aligned} \quad (35)$$

where  $N_{n+1} = (n + l + 2)$ . Consequently, the total energy for the  $n$ th state is

$$E_{n,\ell} = E_n^{(0)} - b\delta + E_n^{(1)} + E_n^{(2)} + E_n^{(3)} + \dots \quad (36)$$

#### IV. NUMERICAL RESULTS

For the numerical work, we take  $a = 2$  and thus our  $b$  is to be identified as the corresponding rescaled parameter in Adamowski's paper. Consequently, our energy eigenvalues are like those obtained by Adamowski. In Tables 1 and 2, we compute the binding energies,  $-E_{n,l}$ , of the lowest-lying states (from  $1s$  up to  $4f$ ) for various values of  $b = \pm 1, -2, -4, -10$

as functions of the screening parameter  $\delta$  obtained from the analytic expressions given in Eqs. (18), (35) and (36). The dependance of the energy levels on  $b$  is shown in Table 3 for the states  $1s$  up to  $3d$ . The results for the higher excited states (from  $5s$  up to  $7i$ ) are presented in Table 4. The energy eigenvalues  $1s - 6h$  for the attractive Yukawa potential with  $\delta = 0.1$  as functions of  $b$  are shown in Table 5. The predicted results are then compared with the accurate energy eigenvalues [1] obtained by Adamowski using a high precision variational technique.

Therefore, we display our results in Tables 1 and 2 only for some sets of values of  $b$  and  $\delta$ . Although we do not present here all the energy eigenvalues considered by Adamowski, our calculation reveals certain interesting features of this approximation method.

The present calculations show that the binding spectra of the Hellmann potential possess the following properties.

(i) For low and strong coupling of  $b$  in Yukawa part, the energy eigenvalues obtained from the perturbation method are in good agreement with the variational results for low values of the screening parameter  $\delta$ . Obviously, when  $\delta$  is small the Coulomb field character prevails and the perturbation method has been adjusted, of course, to that. However, the results become gradually worse as the screening parameter  $\delta$  becomes large. Appreciable discrepancy of our results from the variational calculations occurs almost for most states if  $\delta > 0.2$ . We suspect that this happen because the perturbative parts of potential becomes so shallow and its minimum shifts appreciably from the minimum of the true potential. For certain values of  $\delta$ , the perturbation potentials for some states becomes so shallow that the expansion for the energy seies becomes divergent in the sense that higher perturbation terms in Eq.(35) dominate over the unperturbed term in Eq.(18) and cousequently one gets anomalous results.

(ii) For almost most strongly attractive (negative)  $b$  but small  $\delta$ , it is possible to determine the binding energy eigenvalues for  $1s$  up to  $4f$  states.

(iii) For a given  $n$ , the results of the energy eigenvalues,  $E_{n\ell}$  increase with increasing  $\ell$  if the Yukawa potential is attractive ( $b < 0$ ), and  $E_{n\ell}$  decrease with increasing  $\ell$  if the Yukawa

potential is repulsive ( $b > 0$ ); i.e., for  $\ell > \ell'$ ,  $E_{n\ell} - E_{n\ell'} > 0$  or  $E_{n\ell} - E_{n\ell'} < 0$  if  $b < 0$  or  $b > 0$ , respectively. This is found to be consistent with the level ordering theorem of Grosse and Martin [27]. The  $s$  levels are mostly split off from the hydrogenlike levels  $E_n^H$  [Eq.(18)] (downwards for  $b < 0$  and upwards for  $b > 0$ ). The energy eigenvalues  $E_{n\ell}$  approach  $E_n^H$  if  $n$  and  $\ell$  increase. The shift of the energy levels with respect to  $E_n^H$  is due to an influence of the finite range Yukawa potential in Eq.(2).

(iv) For the attractive Yukawa potential there exist some values of  $b$  and  $\delta$  for which the energy levels with larger  $n$  and smaller  $\ell$  become lower than the levels with smaller  $n$  and larger  $\ell$ , i.e.,  $E_{n\ell} \leq E_{n'\ell'}$  if  $n > n' \geq 3$  and  $\ell < \ell'$ .

(v) For the repulsive Yukawa potential there are some values of the strength  $b$  and the screening parameter  $\delta$  for which the energy eigenvalues for larger  $n$  and  $\ell$  become lower than those for smaller  $n$  and  $\ell$ , i.e.,  $E_{n\ell} \leq E_{n'\ell'}$  if  $n > n' \geq 2$  and  $\ell > \ell'$ .

On the other hand, in Tables 6 and 7, we present the ground and excited energies (in units such that  $\hbar^2/2m = 1$ ) for several states  $\ell = 0, 1, 2$  calculated for the potential in Eq.(2) and compare them with other works [28]. One finds that our results are remarkably good for the  $\ell = 0$  ground state. As  $\ell$  increases for a given  $b$ , the error increases. However as  $b$  increases, the relative error decreases rapidly. This is particularly useful when  $b$  is large. For large  $b$ , the calculated energies compare very well with high precision numerical calculation presented by other works [11,12,28].

## V. CONCLUSIONS

The detailed analysis of the results in terms of various domains of parameters  $b$  and  $\delta$  of the Hellmann potential reveals a few important facts concerning the application of the perturbed formalism. In the present study the discrete energy eigenvalues for the Hellmann potential have been calculated as functions of the strength  $b$  and the screening parameter  $\delta$  of the Yukawa potential. For  $b = 0$  the spectrum is given by Eq. (18). The energy eigenvalues  $E_{n\ell}$  for the Hellmann potential are shifted upwards or downwards with respect

to the hydrogenlike levels, Eq. (18), if  $b > 0$  or  $b < 0$ , respectively. The absolute values of deviations of  $E_{n\ell}$  from  $E_n^H$  decrease with increasing quantum number  $\ell$ , which results in the corresponding ordering of the energy levels for a given  $n$ . This is due to the influence of the finite range Yukawa potential (YP), which decreases with increasing  $\ell$ .

The properties of the energy spectrum for the Hellmann potential obtained in the present work have many analogies in atomic, solid-state, and quark physics. Property (i), giving the order of the energy levels  $E_{n\ell}$  with the same  $n$ , dependent on  $\ell$  and on the sign of the YP, has an application to such systems as an exciton and a bound polaron in polar semiconductors and ionic crystals. These systems consist of two oppositely charged particles interacting with themselves through a polarizable medium. The energy levels of both the systems exhibit this case, although the total effective potential is even more complicated than the Hellmann potential, being a linear combination of the Coulomb potential and an additional potential, which is a sum of two Yukawa potentials with different strengths and screening parameters, and an exponential potential. However, the net contribution of the additional potential is negative for the exciton and positive for the bound polaron and one of the Yukawa potentials dominates at small distances [29,30,31].

Another system, having the energy levels ordered similarly to those for the Hellmann potential with  $b > 0$ , is the quarkonium (the bound state of heavy quark-antiquark pair). For each  $n$  the energy levels of the quarkonium system increase with increasing  $\ell$ . This can be explained in the frames of the simple model, assuming that the quark interact via the potential being the superposition of the attractive Coulomb potential and the positive linear potential (Cornell potential) [32].

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TABLES

TABLE I. Energy,  $-E_{nl}$ , of states  $1s - 4f$  for Hellmann potential as a function of screening parameter  $\delta$ . It is expressed in units of  $\mu a^2/2\hbar^2$ , length in units of  $a_0 = \hbar^2/\mu a$ , and  $\mu$  is the reduced mass.

State\δ	0.001	0.005	0.01	0.05	0.001	0.005	0.01	0.05	0.1
	$b = +1$								
					$b = -1$				
1s	0.250999	0.254963	0.259852		2.24900	2.24501	2.24005	2.20122	
2s	0.063494	0.0673535	0.0719279		0.561502	0.55755	0.552697	0.517151	
2p	0.063495	0.0673775	0.0720203		0.561502	0.557541	0.552664	0.516412	
3s	0.0287644	0.0324574	0.0365575		0.249004	0.245111	0.240435	0.209717	
3p	0.0287654	0.0324803	0.0366436		0.249004	0.245103	0.240404	0.209055	
3d	0.0287674	0.0325260	0.0368131		0.249003	0.245086	0.240341	0.207756	
4s	0.0166014	0.0200766	0.0235509		0.139633	0.135819	0.131381	0.106316	
4p	0.0166024	0.0200984	0.0236407		0.139633	0.135811	0.131351	0.105734	
4d	0.0166043	0.0201416	0.0238136		0.139632	0.135796	0.131290	0.104603	
4f	0.0166072	0.0202058	0.0240562		0.139631	0.135772	0.131200	0.102988	
	$b = -2$								
					$b = -4$				
1s	3.99800	3.99002	3.98007	3.90184	8.99600	8.98002	8.96010	8.80247	8.60979
2s	0.99800	0.990075	0.980297	0.907102	2.24600	2.23010	2.2104	2.05964	1.88728
2p	0.998002	0.990062	0.980248	0.90596	2.24600	2.23008	2.21033	2.05807	1.88135
3s	0.442451	0.434611	0.425103	0.359536	0.996009	0.980220	0.960885	0.820847	0.678082
3p	0.442451	0.434599	0.425055	0.358495	0.996008	0.980207	0.960820	0.819381	0.672826
3d	0.442450	0.434574	0.424959	0.356435	0.996007	0.980174	0.960691	0.816464	0.662442
4s	0.248012	0.240294	0.231150	0.174917	0.558516	0.542894	0.524055	0.397745	0.288281
4p	0.248011	0.240281	0.231103	0.173993	0.558515	0.542878	0.523991	0.396397	0.284004
4d	0.248010	0.240257	0.231011	0.172169	0.558514	0.542845	0.523865	0.393717	0.275519
4f	0.248009	0.240221	0.230872	0.169493	0.558512	0.542797	0.523674	0.389737	0.262966

TABLE II. Energy eigenvalues,  $-E_{nl}$ , of states  $1s - 4f$  for Hellmann potential as a function of screening parameter  $\delta$ . Energy eigenvalues are given in units of Table 1.

State\( $\delta$	0.001	0.005	0.01	0.05	0.1	0.2
$b = -10$						
$1s$	35.99	35.95	35.9001	35.5031	35.0124	34.0489
$2s$	8.99	8.95012	8.90050	8.51527	8.0482	7.18656
$2p$	8.99	8.95010	8.90042	8.51025	8.04037	7.15688
$3s$	3.99001	3.95028	3.90112	3.52703	3.10435	2.39157
$3p$	3.99001	3.95026	3.90103	3.52508	3.09701	2.36532
$3d$	3.99001	3.95022	3.90087	3.52120	3.08240	2.31330
$4s$	2.24002	2.2005	2.15197	1.79676	1.42667	0.88467
$4p$	2.24002	2.20048	2.15189	1.79490	1.41993	0.86351
$4d$	2.24002	2.20043	2.15173	1.79119	1.40652	0.82123
$4f$	2.24001	2.20037	2.15148	1.78565	1.38656	0.757901

TABLE III. Energy eigenvalues,  $-E_{n\ell}$ , of states  $1s - 3d$  as function of the strength  $b$  of the Hellmann potential for  $\delta = 0.01$ . Energy eigenvalues are given in units of Table 1.

$b \backslash \text{State}$	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$
1	0.259852	0.071928	0.0720203	0.036557	0.0366436	0.0368131
0.5	0.567450	0.145431	0.145463	0.067079	0.0671090	0.0671683
0.2	0.811983	0.204435	0.204446	0.091858	0.0918682	0.0918884
0	1	0.25	0.25	0.111	0.111	0.111
-0.2	1.20801	0.300553	0.300545	0.132562	0.132553	0.132537
-0.5	1.55753	0.385743	0.385723	0.168871	0.168852	0.168815
-1	2.24005	0.552697	0.552664	0.240435	0.240404	0.240341
-2	3.98007	0.980297	0.980248	0.425103	0.425055	0.424959
-5	12.2	3.01293	3.01286	1.31206	1.31199	1.31185
-10	35.9	8.9005	8.90042	3.90112	3.90103	3.90087
-20	120.8	30.051	30.0505	13.2460	13.2456	13.2454

TABLE IV. Energy eigenvalues,  $-E_{n\ell}$ , of states  $5s - 7i$  as function of the strength  $b$  of the Hellmann potential for  $\delta = 0.01$ . Energy eigenvalues are given in units of Table 1.

State\ $b$	+1	-1	-2	-4	-8	-10
$5s$	0.0165535	0.081148	0.141758	0.322393	0.922921	1.34306
$5p$	0.0166884	0.0811191	0.141713	0.322331	0.922844	1.34298
$5d$	0.0169435	0.0810614	0.141624	0.322208	0.922692	1.34282
$5f$	0.017289	0.0809751	0.141490	0.322023	0.922463	1.34258
$5g$	0.0176805	0.0808607	0.141312	0.321776	0.922158	1.34225
$6s$	0.0100105	0.0540995	0.093579	0.213386	0.618604	0.904359
$6p$	0.0103092	0.054072	0.0935360	0.213326	0.618530	0.904281
$6d$	0.0108763	0.054017	0.0934503	0.213206	0.618380	0.904123
$6f$	0.011651	0.0539351	0.0933218	0.213027	0.618155	0.903887
$6g$	0.0125417	0.0538266	0.0931512	0.212787	0.617856	0.903572
$6h$	0.013427	0.0536924	0.0929390	0.212489	0.617482	0.903178
$7s$	0.0028019	0.0380167	0.0648977	0.148193	0.435796	0.640565
$7p$	0.0020524	0.0379905	0.0648565	0.148135	0.435723	0.640488
$7d$	0.0006123	0.0379383	0.0647744	0.148018	0.435576	0.640333
$7f$	0.0014009	0.0378606	0.0646516	0.147845	0.435356	0.640101
$7g$	0.0038107	0.0377579	0.0644887	0.147613	0.435064	0.639792
$7h$	0.0063819	0.0376312	0.0642864	0.147325	0.434698	0.639405
$7i$	0.0088204	0.0374816	0.0640455	0.146980	0.434260	0.638942

TABLE V. Energy eigenvalues,  $-E_{n\ell}$ , of states  $1s - 6h$  for  $\delta = 0.1$ . Energy eigenvalues are given in units of Table 1.

State\ $b$	-5	-8	-10	-20	-30	-50
$1s$	11.7605	24.2118	35.0124	119.014	253.014	671.014
$2s$	2.60282	5.49595	8.0482	28.3034	61.0555	164.057
$2p$	2.59637	5.48852	8.04037	28.2947	61.0463	164.048
$3s$	0.946371	2.0766	3.10435	11.562	25.5672	70.2385
$3p$	0.94056	2.06971	3.09701	11.5536	25.5583	70.2292
$3d$	0.929052	2.05602	3.0824	11.5367	25.5406	70.2106
$4s$	0.405183	0.92834	1.42667	5.76553	13.2138	37.4734
$4p$	0.400245	0.922129	1.41993	5.75749	13.2052	37.4643
$4d$	0.390444	0.909778	1.40652	5.74145	13.188	37.4461
$4f$	0.37593	0.89143	1.38656	5.71747	13.1624	37.4189
$5s$	0.185308	0.44099	0.700006	3.14653	7.56577	22.3833
$5p$	0.181729	0.43572	0.694047	3.13896	7.55755	22.3745
$5d$	0.174538	0.425204	0.682168	3.12385	7.54112	22.3568
$5f$	0.16367	0.40949	0.664442	3.10128	7.51654	22.3304
$5g$	0.149027	0.38865	0.640982	3.07135	7.48388	22.2952
$6s$	0.099768	0.213846	0.348659	1.78538	4.56702	14.2628
$6p$	0.097267	0.209807	0.343761	1.77836	4.5592	14.2543
$6d$	0.092169	0.201681	0.333949	1.76435	4.54358	14.2372
$6f$	0.084289	0.189376	0.319193	1.74341	4.5202	14.2116
$6g$	0.073342	0.172749	0.299444	1.71562	4.48915	14.17775
$6h$	0.058954	0.151614	0.274642	1.68109	4.45051	14.1351

TABLE VI. Some bound state energies,  $-E_{n\ell}$ , for neutral atoms.

$b = -Ze^2$	State	Present	Calculated [28]	Exact [28]
-4	1s	3.25647	3.219965	3.250536
	2p	0.37172		
	3d	0.003891		
-8	1s	14.4581	14.419973	14.457119
	2s	2.61756		
	2p	2.58365	2.433176	2.583677
	3d	0.54034		
-16	1s	60.8590	60.819285	60.859039
	2s	13.0276	13.027315	13.03259
	2p	12.9910	12.837459	12.991055
	3s	4.39692	4.372037	4.405697
	3p	4.36357	4.348041	4.388576
	3d	4.29724		
-24	1s	139.2590	139.22008	139.259362
	2s	31.4314	31.431281	31.43595
	2p	31.3938	31.238464	31.393815
	3s	11.7014	11.699808	11.70926
	3p	11.6662	11.665284	11.683877
	3d	11.5959	11.245640	11.595949
	4s	5.05037	5.044185	5.0590
	4p	5.01801	5.013466	5.05410
	4d	4.95352	4.951600	5.00855
	5s	2.21653	2.203309	2.22372
	5p	2.18793	2.177040	2.241432
5d	2.13080	2.124124	2.24278	



TABLE VII. Some bound state energies,  $-E_{nl}$ , for neutral atoms.

$b = -Ze^2$	$1s$	$2s$	$2p$	$3s$	$3p$	$4s$	$4p$
-13	39.7088	8.18765	8.15172	2.57025	2.53816	0.82329	0.79663
-36	316.86	74.0341	73.9958	29.3129	29.2763	13.9316	13.897
-79	1544.51	374.5	374.461	158.088	158.05	82.6361	82.599