Application of Hellman-Feynman and Hypervirial theorems to the eigenvalue problem: Coulomb plus linear term and quartic anharmonic oscillator potentials

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Abstract

We use the Hellman-Feynman (HF) and Hypervirial (HV) theorems, to calculate the perturbative coefficients of the eigenergies formal series, in the case of the Coulomb potential with a radial linear term and the radial quartic anharmonic oscillator potential. This calculation method, contrary to the usual Rayleigh-Schrödinger Perturbation Theory (RSPT), does not require the calculation of eigenfunctions coefficients. This method is a fast and efficient tool for the calculation of large order eigenergies coefficients.

1 Introduction

Many physical phenomena encountered in different fields of physics, require the modelization of the interaction through potentials that are believed to account for the physical mechanisms occurring in the system. The construction of these potentials is constrained by physical consideration in their analytical forms and introduces parameters. For instance, the problem of the electron in the field of a nucleus is tackled with a Coulomb potential, since it is known that this is the interaction which is in work. In nuclear physics, the nuclear energy levels are obtained by modelizing the interaction, the nucleon feels through (e.g.) a Woods-Saxon potential. In particle physics, the mesons are described as quark antiquark bound states through a phenomenological model where the potential is given at once.

While bound states problem can be solved analytically [1] for few potentials, among which Coulomb and harmonic oscillator potentials, for most of potentials of physical interest, one has to resort to direct numerical techniques or to approximation methods. Note that, beyond the physical problem itself, these solving techniques have become a field of study in their own.
Perturbation theory is one of the most widely used approximation method to solve eigenvalue problems in theoretical physics [2, 3, 4]. Mathematical aspects of perturbation theory are treated in monographs [5, 6, 7], while applications in various fields are described in books [8, 9, 10].

Rayleigh-Schrödinger Perturbation Theory (RSPT) is designed for systems whose Hamiltonian can be partitioned into a completely solvable part with known eigenvalues and eigenfunctions, and a perturbation part [2, 3, 4, 11]. The formalism of RSPT expresses the eigenenergies and the eigenfunctions as formal series in the chosen perturbation parameter. Accurate results for physical observables have been obtained from this perturbative method. However, one of the shortcomings of the RSPT approach is that it requires, in general, considerable computational time and effort. Indeed, this method uses the eigenfunctions solutions which are time consuming and intermediary results in an eigenvalue problem [4, 11].

For various interactions, a way to bypass the computation of the eigenfunctions is to use Hellman-Feynman (HF) and the Hypervirial (HV) theorems [12, 13] to generate eigenenergies perturbative coefficients [14, 15, 16, 17, 18].

The purpose of the paper is to use these theorems (denoted by HFHV method) to calculate the eigenvalues perturbative coefficients for two potentials of physical interest namely: the Coulomb potential plus radial linear term and the radial quartic anharmonic oscillator potential. The eigenenergies coefficients are computed recursively without the need to calculate the eigenfunctions. Moreover, we show that the application of the HFHV method requires considerable less computational time comparatively to the usual RSPT method and allows a fast and efficient calculation of very large order eigenvalues coefficients.

2 Method of calculation

2.1 Hellman-Feynman and Hypervirial theorems

Let us recall Hellman-Feynman (HF) and Hypervirial (HV) theorems. The HF theorem states that if we consider a system with a Hamiltonian \( H = H(\lambda) \), depending on some parameters \( \lambda \), with normalized eigenvector \( \Psi(\lambda) \) and eigenvalue \( E(\lambda) \), then:

\[
\frac{\partial E}{\partial \lambda} = \langle \Psi(\lambda) \left| \frac{\partial H}{\partial \lambda} \right| \Psi(\lambda) \rangle = \langle \frac{\partial H}{\partial \lambda} \rangle
\]  

Let \( H \) be a time-independant Hamiltonian with a normalized bound state eigenfunction \( \Psi \), and \( \Theta \) a time-independant linear operator. If the expectation value of \( \Theta \) over the stationnary eigenstate \( \Psi \) is not infinite, then the HV theorem states that, for the operator \( \Theta \):

\[
\langle \Psi \left| [\Theta, H] \right| \Psi \rangle = \langle [\Theta, H] \rangle = 0
\]

where \( [\Theta, H] = \Theta H - H \Theta \) is the commutator of \( H \) and \( \Theta \). Physically, this, is just the statement that, for a stationary state, the expectation value of \( \Theta \) is time-independant.
2.2 General formalism

The two-body stationary Schrödinger equation with central potential \( V(r) \), can be written (in \( \hbar = c = 1 \) units) as:

\[
-\frac{1}{2\mu} \frac{d^2}{dr^2} + V(r) + \frac{\ell(\ell + 1)}{2\mu r^2} - E_{n,l} \]

\[ y_{n,l}(r) = 0 \]  

where \( \mu \) is the reduced mass of the system, \( E_{n,l} \) and \( y_{n,l}(r) \) are respectively the eigenvalue and the reduced radial wave function, describing a bound state of radial and orbital angular momentum quantum numbers \( n \) and \( l \) respectively. The wave function obeys the following boundary conditions:

\[ y_{n,l}(0) = y_{n,l}(\infty) = 0 \]

Setting \( x = \lambda r \), the scaling property of the Schrödinger equation allows to write (3) as:

\[ H y_{n,l}(x) = \epsilon_{n,l} y_{n,l}(x) \]

with:

\[ H = -\frac{d^2}{dx^2} + U(x) \]

and:

\[ U(x) = V_0(x) + \frac{\ell(\ell + 1)}{x^2} + g V_1(x) \]

The perturbation is cast in the term \( g V_1(x) \) where \( g \) is the controlling parameter, i.e., the expansion parameter.

In the usual RSPT method, the eigenvalues and eigenfunctions are written as series expansions in the perturbative parameter \( g \):

\[ \epsilon_{n,l} = \sum_{k=0}^{\infty} \epsilon_{n,l}(k) \ g^k \]  

\[ y_{n,l}(x) = \sum_{k=0}^{\infty} y_{n,l}(k, x) \ g^k \]

where \( \epsilon_{n,l}(k) \) and \( y_{n,l}(k, x) \) are, respectively, the eigenenergies and eigenfunctions perturbative coefficients. \( k = 0 \) in the expansion corresponds to the unperturbed system, i.e., \( \epsilon_{n,l}(0) \) and \( y_{n,l}(0, x) \) are the eigenvalues and eigenfunctions for the potential (7) with \( g = 0 \).

With the RSPT method, the calculation of \( \epsilon_{n,l}(k) \) coefficients requires then the knowledge of \( y_{n,l}(i, x) \) where \( i = 0, \cdots k - 1 \) [2, 3, 4, 11]. This is the shortcomings of the method.

It happens that, for various interactions, and thanks to HF and HV theorems, the \( \epsilon_{n,l}(k) \) coefficients can be given by a recursion formula (see below) and thus there is no need to calculate the intermediary eigenfunctions [14, 15, 16, 17, 18].

2.3 The potentials

We consider two central potentials of physical interest, the Coulomb potential with a radial linear term and the quartic anharmonic oscillator potential.
The Coulomb potential with a radial linear term:

\[ V(r) = -\frac{\alpha}{r} + \beta r \quad \alpha, \beta \geq 0 \quad (10) \]

corresponds to a spherical Stark effect in hydrogenic atoms and is, also, a successful phenomenological model for the description of heavy quark antiquark bound states in particle physics [19, 20]. In this case, taking \( \lambda = 2\mu\alpha \), the eigenvalues are given by:

\[ \epsilon_{n,l} = \frac{1}{\alpha^2} \frac{E_{n,l}}{2\mu} \quad (11) \]

and the scaled potential (7) reads:

\[ U(x) = -\frac{1}{x} + \frac{l(l+1)}{x^2} + g \cdot x, \quad g = \frac{\beta}{(2\mu)^2\alpha^3} \quad (12) \]

where \( g \) is the dimensionless parameter used in the expansion. The term \( g \cdot x \) is thus treated as a perturbation, while the unperturbed Hamiltonian is the usual radial Coulomb Hamiltonian whose eigenfunctions and eigenvalues are known [1, 11].

The second potential is the quartic anharmonic oscillator potential:

\[ V(r) = ar^2 + br^4 \quad a, b \geq 0 \quad (13) \]

which has received a great deal of interest because of its importance in the understanding of molecular vibrations [21], in some areas of solid state physics [22, 23] and in Quantum Field Theory [24, 25]. Furthermore, the quartic anharmonic oscillator serves as a testing tool to check various approximative methods in Quantum Mechanics [26, 27]. Setting \( \lambda = (2\mu a)^{1/4} \), the eigenvalues are given by:

\[ \epsilon_{n,l} = \sqrt{\frac{2\mu}{a}} E_{n,l} \quad (14) \]

and the scaled form of this potential (7) reads:

\[ U(x) = x^2 + \frac{l(l+1)}{x^2} + g \cdot x^4, \quad g = \frac{b}{\sqrt{2\mu a^{3/2}}} \quad (15) \]

where \( g \) is the perturbative dimensionless parameter. Here again, the term \( g \cdot x^4 \) is treated as a perturbation, while the unperturbed Hamiltonian is the radial harmonic oscillator Hamiltonian whose eigenfunctions and eigenvalues are known [1, 11].

### 2.4 Recurrence equations on the \( \epsilon_{n,l}(k) \) coefficients

Let us consider the time-independent linear operator \( \Theta \) as \( \Theta = x^{j+1} \frac{d}{dx} \), where \( j \) is an integer such that \( j \geq 0 \) [14, 15, 18, 28, 29]. Taking the Hamiltonian in the form (6), one has:

\[ [x^{j+1} \frac{d}{dx}, H] = 2(j+1) x^j \frac{d^2}{dx^2} + j(j+1)x^{j-1} \frac{d}{dx} + x^{j+1} \frac{dU(x)}{dx} \quad (16) \]
From the definition (5), one can easily show that:

$$\langle x^j \frac{d^2}{dx^2} \rangle = \langle x^j U(x) \rangle - \epsilon_{n,l} \langle x^j \rangle$$  \hspace{1cm} (17)$$

Integration by parts, using the boundary conditions (4) together with the asymptotic behavior $y_{n,l}(x) \sim x^{j+1}$ for small $x$, leads to:

$$\langle x^{j-1} \frac{d}{dx} \rangle = -\frac{1}{2}(j - 1) \langle x^{j-2} \rangle$$  \hspace{1cm} (18)$$

Inserting relations (16-18) into equation (2), the HV theorem provides relationships between $\epsilon_{n,l}$ and the various expectation values $\langle x^j \rangle$ through the following equations [14, 15, 18, 28, 29]:

$$2(j+1) \epsilon_{n,l} \langle x^j \rangle = -\frac{1}{2}j(j^2-1) \langle x^{j-2} \rangle + 2(j+1) \langle x^j U(x) \rangle + \langle x^{j+1} \frac{dU(x)}{dx} \rangle$$ \hspace{1cm} (19)$$

The HF theorem (1) allows to derive a further relation:

$$\frac{\partial \epsilon_{n,l}}{\partial g} = \langle \frac{\partial U(x)}{\partial g} \rangle = \langle V_1(x) \rangle = \left\{ \begin{array}{l} \langle x \rangle \text{ for the potential (12)} \\
\langle x^4 \rangle \text{ for the potential (15)} \end{array} \right\}$$ \hspace{1cm} (20)$$

The essence of the application of the HF and HV theorems (HFHV perturbative method) is to assume, in the spirit of perturbative methods, that the energy and the expectation values of position coordinates can be expanded in power series of the perturbation parameter $g$ as (see eq. (8) for the energy):

$$\langle x^j \rangle = \sum_{k=0}^{\infty} x_{j}^{(k)} g^k$$  \hspace{1cm} (21)$$

By equating like powers of $g$ on both sides of equations (19-20) after substitution of expansions (8) and (21), we find a set of coupled relations involving $\epsilon_{n,l}(k)$ and $x_{j}^{(k)}$.

To be more precise, let us consider the Cornell potential defined by (10) or (12). In this case, equation (19) can be written as:

$$\epsilon_{n,l} \langle x^j \rangle = \alpha_j \langle x^{j-2} \rangle + \beta_j \langle x^{j-1} \rangle + g \gamma_j \langle x^{j+1} \rangle$$ \hspace{1cm} (22)$$

with:

$$\alpha_j = \frac{(2l+1)^2 - j^2}{4j+4}; \hspace{0.5cm} \beta_j = -\frac{2j+1}{2j+2}; \hspace{0.5cm} \gamma_j = \frac{2j+3}{2j+2}$$ \hspace{1cm} (23)$$

Inserting the expansions (8) and (21), in equations (22-20), the identification of the coefficients of powers of $g$ leads to ($j$ integer $\geq 0$):

$$\sum_{p=0}^{k} \epsilon_{n,l}(k-p) x_{j}^{(p)} = \alpha_j x_{j-2}^{(k)} + \beta_j x_{j-1}^{(k)} + \theta(k-1) \gamma_j x_{j+1}^{(k-1)} \hspace{0.5cm} k \geq 0$$ \hspace{1cm} (24)$$

$$\epsilon_{n,l}(k) = \frac{x_{j}^{(k-1)}}{k} \hspace{1cm} k \geq 1$$ \hspace{1cm} (25)$$

\text{1}Throughout this paper, the notation $\langle \xi \rangle$ stands, the quantum number indices $n$ and $l$ being understood, for the expectation value $\langle \xi \rangle = \langle \Psi \mid \xi \mid \Psi \rangle$, where $\Psi$ represents the normalized eigenstate of the hamiltonian $H$ under consideration.
where $\theta(t)$ is the Heaviside Step function. It is clear from the above equations that the starting point is the normalization condition:

$$x^{(0)}_0 = 1 \quad \text{and} \quad x^{(k)}_0 = 0 \quad \text{for} \quad k \geq 1$$  \hspace{1cm} (26)

and the Coulomb eigenvalues:

$$\epsilon_{n,l}(0) = -\frac{1}{4(n+l+1)^2} \hspace{1cm} (27)$$

The set of equations (24-25) together with (26-27) allows one (see below) to calculate all the $\epsilon_{n,l}(k)$ coefficients.

In a similar way for the quartic anharmonic oscillator (13) or (15), taking $j$ even ($j = 2i$), equation (19) reads:

$$\epsilon_{n,l} \langle x^{2i} \rangle = \alpha_i \langle x^{2i-2} \rangle + \beta_i \langle x^{2i+2} \rangle + g \gamma_i \langle x^{2i+4} \rangle \hspace{1cm} (28)$$

with:

$$\alpha_i = i \frac{(2i+1)^2 - 4i^2}{4i+2}; \quad \beta_i = \frac{2i+2}{2i+1}; \quad \gamma_i = \frac{2i+3}{2i+1} \hspace{1cm} (29)$$

By analogy with equations (24-25) and noting $x^{(p)}_{2i} = \hat{x}^{(p)}_i$, one obtains in the quartic anharmonic potential case:

$$\sum_{p=0}^{k} \epsilon_{n,l}(k-p) \hat{x}^{(p)}_i = \alpha_i \hat{x}^{(k-1)}_{i-1} + \beta_i \hat{x}^{(k)}_{i+1} + \theta(k-1) \gamma_i \hat{x}^{(k-1)}_{i+2} \quad k \geq 0 \hspace{1cm} (30)$$

$$\epsilon_{n,l}(k) = \frac{\hat{x}^{(k-1)}_2}{k} \quad k \geq 1 \hspace{1cm} (31)$$

together with the normalization condition:

$$\hat{x}^{(0)}_0 = 1 \quad \text{and} \quad \hat{x}^{(k)}_0 = 0 \quad \text{for} \quad k \geq 1 \hspace{1cm} (32)$$

and the harmonic oscillator eigenvalues:

$$\epsilon_{n,l}(0) = 3 + 4n + 2l \hspace{1cm} (33)$$

### 2.5 Calculation of the $\epsilon_{n,l}(k)$ coefficients

To calculate explicitly the $\epsilon_{n,l}(k)$ coefficients from the equations (24-25) or (30-31), one proceeds in a hierarchical manner by giving to $k$ various integer values starting with $k = 0$. Let us describe this method in details for the case of the Cornell potential. Consider equation (24) for $k = 0$, one obtains:

$$\epsilon_{n,l}(0) x^{(0)}_j = \alpha_j x^{(0)}_{j-2} + \beta_j x^{(0)}_{j-1} \hspace{1cm} (34)$$

which is a recurrence of depth three on the $x^{(0)}_j$ coefficients. One needs two initial conditions to calculate all the $x^{(0)}_j$ coefficients. One condition is given by the normalization (26), namely $x^{(0)}_0 = 1$, the second one is given by taking $j = 0$ in eq. (34) and one has:

$$x^{(0)}_{-1} = -2 \epsilon_{n,l}(0) = \frac{1}{2(n+l+1)^2} \hspace{1cm} (35)$$
The recurrence equation (34) together with the initial conditions (26) and (35) allow to calculate all \( x_j^{(0)} \) coefficients. The next step is to consider equation (24) for \( k \geq 1 \), which can be written, using (25), in the following form:

\[
\epsilon_{n,l}(0) \ x_j^{(k)} = \alpha_j \ x_{j-2}^{(k)} + \beta_j \ x_{j-1}^{(k)} + \delta(j,k) \quad k \geq 1
\]

(36)

where \( \delta(j,k) \) depends only on \( x_j^{(p)} \) terms with \( p < k \) and reads:

\[
\delta(j,k) = - \sum_{p=0}^{k-1} \frac{x_1^{(k-1-p)} x_j^{(p)}}{k-p} + \gamma_j \ x_j^{(k-1)}
\]

(37)

The obtained equation (36) is an inhomogenous recurrence of depth three on the \( x_j^{(k)} \) coefficients \( (k \) kept fixed), \( \delta(j,k) \) being the inhomogenous term. In the same way, one needs two initial conditions to calculate the \( x_j^{(k)} \) coefficients.

One condition is given by the normalization (26), namely \( x_0^{(k)} = 0 \) \((k \geq 1)\), the second one is given by taking \( j = 0 \) in eq. (36) and one has, using (26):

\[
x_{-1}^{(k)} = \left(3 - \frac{2}{k}\right) x_1^{(k-1)} \quad k \geq 1
\]

(38)

One proceeds step by step by giving to \( k \) various integer values in equations (36-38), starting with \( k = 1 \).

Finally, we can, thus, calculate the \( r_0^{th} \) perturbative coefficient \( \epsilon_{n,l}(r_0) \) through the relation (25) from the knowledge of the \( x_j^{(k)} \) with \( 2 \leq k \leq r_0 - 1 \) and \(-1 \leq j \leq r_0 - k \).

For the quartic anharmonic oscillator (15), similarly, one obtains \( k = 0 \):

\[
\beta_i \ x_{i+1}^{(0)} = \epsilon_{n,l}(0) \ x_i^{(0)} - \alpha_i \ x_{i-1}^{(0)}
\]

(39)

\( x_0^{(0)} = 1 \) and \( x_1^{(0)} = \epsilon_{n,l}(0)/2 = 3/2 + 2n + l \)

(40)

and \( k \geq 1 \):

\[
\beta_i \ x_{i+1}^{(k)} = \epsilon_{n,l}(0) \ x_i^{(k)} - \alpha_i \ x_{i-1}^{(k)} + \delta(i,k)
\]

(41)

\[
\delta(i,k) = -\gamma_i \ x_{i+2}^{(k-1)} + \sum_{p=0}^{k-1} \frac{x_2^{(k-1-p)} x_i^{(p)}}{k-p}
\]

(42)

\[
\frac{x_0^{(k)}}{x_1^{(k)}} = 0 \quad \text{and} \quad \frac{x_1^{(k)}}{x_1^{(k)}} = \frac{(-3 + 1/k + 1/2)}{x_2^{(k-1)}}
\]

(43)

Consequently, the \( r_0^{th} \) perturbative coefficient \( \epsilon_{n,l}(r_0) \) is calculated through the relation (31) from the knowledge of the \( x_j^{(k)} \) with \( 3 \leq k \leq r_0 - 1 \) and \( 0 \leq j \leq r_0 - k + 1 \).

\(^2\)For \( j = -1, 0 \), the \( x_j^{(k)} \) are given by the initial conditions (26, 35 and 38) and the recurrences displayed above allow to calculate the \( x_j^{(k)} \) for \( j \geq 1 \).

\(^3\)For \( j = 0, 1 \), the \( x_j^{(k)} \) are given by the initial conditions (40 and 43) and the recurrences displayed above allow to calculate the \( x_j^{(k)} \) for \( j \geq 2 \).
3 Results and discussion

We have implemented the HFHV perturbative method described above for the calculations of $\epsilon_{n,l}(k)$ coefficients, at any order $k$, into a Mathematica routine. The first eight eigenergies coefficients are displayed in Tables 1-2 for both the considered potentials.

Table 1. The coefficients $\epsilon_{n,l}(k)$ in the case of the Cornell potential for few states.

| State | $n = 0, l = 0 (1S)$ | $n = 1, l = 0 (2S)$ | $n = 0, l = 1 (1P)$ |
|-------|-------------------|-------------------|-------------------|
| $k = 0$ | $-\frac{1}{4}$ | $-\frac{1}{16}$ | $-\frac{1}{16}$ |
| $k = 1$ | $3$ | $12$ | $10$ |
| $k = 2$ | $-12$ | $-528$ | $-480$ |
| $k = 3$ | $216$ | $105984$ | $99840$ |
| $k = 4$ | $-6360$ | $-34775040$ | $-33054720$ |
| $k = 5$ | $245952$ | $14770372608$ | $14051573760$ |
| $k = 6$ | $-11433984$ | $-7410570756096$ | $-7038283284480$ |
| $k = 7$ | $610773696$ | $4197622600433664$ | $3976876146032640$ |

Table 2. The coefficients $4^k \epsilon_{n,l}(k)$ in the case of the quartic anharmonic oscillator for few states.

| State | $n = 0, l = 0 (1S)$ | $n = 1, l = 0 (2S)$ | $n = 0, l = 1 (1P)$ |
|-------|-------------------|-------------------|-------------------|
| $k = 0$ | $3$ | $7$ | $5$ |
| $k = 1$ | $15$ | $75$ | $35$ |
| $k = 2$ | $-165$ | $-1575$ | $-525$ |
| $k = 3$ | $3915$ | $66825$ | $16025$ |
| $k = 4$ | $-520485/4$ | $-15184575/4$ | $-2894325/4$ |
| $k = 5$ | $21304485/4$ | $1024977375/4$ | $152440575/4$ |
| $k = 6$ | $-2026946145/8$ | $-155898295875/8$ | $-18353729625/8$ |
| $k = 7$ | $108603230895/8$ | $12977225578125/8$ | $1224596281125/8$ |

Table 3. CPU time (in seconds) for the calculation of $\epsilon_{0,0}(k) (k = 0, r_0)$ coefficients in the case of the Cornell potential for the 1S state.

| $r_0$ | RSPT method | HFHV method |
|-------|-------------|-------------|
| $10$  | $26.2$      | $0.016$     |
| $20$  | $188.7$     | $0.032$     |
| $30$  | $1024.9$    | $0.062$     |
| $40$  | $2626.2$    | $0.16$      |

Table 4. CPU time (in seconds) for the calculation of $\epsilon_{0,0}(k) (k = 0, r_0)$ coefficients in the case of the quartic anharmonic oscillator for the 1S state.

| $r_0$ | RSPT method | HFHV method |
|-------|-------------|-------------|
| $10$  | $43.4$      | $0.016$     |
| $20$  | $277.8$     | $0.047$     |
| $30$  | $1213.6$    | $0.11$      |
| $40$  | $2676.6$    | $0.27$      |

We have also compared the present method to the usual RSPT one\(^4\), in the simple case of the 1S state. For both potentials, the respective CPU times\(^5\) are displayed in Tables 3-4. One can see from the latter tables that the computational time of the HFHV method is reduced by a factor $10^4$ comparatively to the

\(^4\)For the RSPT method, we have implemented, in a Mathematica program, the set of equations displayed in section 7.3 of Ref. [4].

\(^5\)Throughout this paper, the mentioned CPU times correspond to runs on a PIV personal computer with 1.5 Go of RAM memory.
usual RSPT method. In addition, let us note that the ratio of the respective
CPU time (RSPT/HFHV) grows with increasing order.

Furthermore, the HFHV method reveals itself as a fast and efficient tool for
a systematic calculation of large order perturbative coefficients. Indeed, consid-
ering, for example, the 1S state in the Cornell potential case, the necessary CPU
time to calculate the first 1000 perturbative coefficients is less than four (04)
hours\(^6\). Consequently, one can find, in principle, the asymptotic behavior of the
\(\epsilon_{n,l}(k)\) coefficients for large \(k\), which reads, for both the considered potentials:

\[
\epsilon_{n,l}(k) \sim (-1)^{k+1} \Gamma(k + b(n, l)) \ a(n, l)^k \quad \text{for } k \to \infty
\]

(44)

where the notation \(\Gamma\) stands for the Euler Gamma function. For example, for the
1S state, considering the Cornell (resp. quartic anharmonic) interaction, we have
found that \(a(0, 0) \simeq 6\) (resp. \(a(0, 0) \simeq 3/2\)) and \(b(0, 0) \simeq 2\) (resp. \(b(0, 0) \simeq 3/2\))\(^7\). Let us note that, for the quartic anharmonic potential, the asymptotic
behavior (44) together with the numerical values of \(a(0, 0)\) and \(b(0, 0)\) are in
perfect agreement\(^8\) with the one dimensional calculation of Bender and Wu in
the framework of WKB analysis and difference-equation method [24, 30, 31]. In
the Cornell interaction case, the large \(k\) behavior (44) agrees fairly well with
the WKB result [32].

Let us make some comments about the asymptotic behavior (44) of the
\(\epsilon_{n,l}(k)\) coefficients. This large \(k\) behavior means that, for the two potentials un-
der consideration, the expansion (8) has its radius of convergence equal to zero
and is, thus, a divergent serie for all \(g\). The divergence of the perturbative serie
(8) indicates that taking, for the Cornell (resp. quartic anharmonic) potential
the term \(g x\) (resp. \(g x^4\)) as a perturbation leads to a singular perturbation. For
the Cornell (resp. quartic anharmonic) interaction, a simple way to understand
this singular behavior is to compare, \(\exp\left(-\frac{1}{2(n+l+1)}x^2\right)\) (resp. \(\exp\left(-\frac{x^2}{2}\right)\)), the
controlling factor of the large \(x\) behavior\(^9\) of the unpertrurbed \((g = 0)\) eigen-
function with, \(\exp\left(-\frac{2g^{1/2}x^{3/2}}{3}\right)\) (resp. \(\exp\left(-\frac{g^{1/2}x^2}{3}\right)\)), the controlling factor of the large \(x\) behavior for \(g \neq 0\). One can see an abrupt change in the nature of the
eigenfunction when we go, for large \(x\), to the limit \(g \to 0_+\). For the Cornell
(resp. quartic anharmonic) potential, this feature occurs because, for large \(x\),
the perturbation term \(g x\) (resp. \(g x^4\)) is not negligible comparatively to \(-1/x\)
(resp. \(x^2\)).

The other remark deals with the following point. Since the the expansion (8)
is a divergent serie, one may worry about the interest of the \(\epsilon_{n,l}(k)\) coefficients
calculation. In fact, different mathematical methods (like the Padé approxi-
mants) allow to sum divergent series and have been used with some success in
different fields of physics [4, 33, 34, 35, 36, 37, 38, 39, 40, 41]. For the eigenergies
expansion (8) in the case of the considered potentials, the choice of an optimized
summation method is beyond the scope the present work. Anyhow, the interest

\(^6\)For the other states, the CPU time has the same order of magnitude.

\(^7\)These results have been obtained with a satisfactory accuracy from the first 1000 pertur-
bative coefficients. For excited states, one needs more perturbative coefficients.

\(^8\)Up to rescaling of the quantities \(g\) and \(\epsilon_{n,l}\) to match the definitions given by Bender and
Wu.

\(^9\)The notion of controlling factor for large \(x\) comes from the fact that \(x = \infty\) is an irregular
singular point of the dimensionless Schrödinger equation (5) with potentials (12) and (15).
For more details, see Ref. [4].
of the $\epsilon_{n,l}(k)$ coefficients calculation lies in the fact that the accuracy of the approximative sum increases with increasing known terms in the expansion, this feature being independent of the particular choice of the summation method used.

4 Comments and conclusion

Before concluding, some comments are in order. We have shown the usefulness of HFHV method for Coulomb plus linear term and the quartic anharmonic oscillator potentials that interest us for other issues. This method can be applied, mutadis mutandis, to radial interactions of the form $V(r) = -1/r + g r^p$ ($p \geq 2$) or $V(r) = r^2 + g r^p$ ($p \geq 3$).

More generally, the HFHV method has been used, in fact, for many interactions, where the potentials take the form of a power serie (or a finite polynomial), the unperturbed Hamiltonian being the Coulomb one or the harmonic oscillator one (for a general discussion see Ref. [29]). For instance, the method was applied for: the screened Coulomb potential [15], the $N-$dimensional generalized exponential cosine-screened Coulomb potential [42, 43], the potential $V(r) = r^2 + \lambda r^2/(1 + g r^2)$ [44], the Gaussian potential [45, 46], etc. More recently [18], it has been applied to a set of potential like the Gaussian potential, Patil potential, etc. To be complete, let us note that the HFHV method has been also extended to the relativistic case for the Klein-Gordon equation, with a Coulomb potential plus polynomial perturbation, to calculate the eigenvalues perturbative coefficients [17].

The interesting and powerful side of the method stems from the fact that one does not need the eigenfunctions. Indeed, expressing the potential as a power serie (or a finite polynomial) in the coordinates $x$, the HF and HV theorems provide recursion relations that give the eigenenergy coefficients through the knowledge of the expansion coefficients of the moments $\langle x^j \rangle$. The coefficients $x_j^{(k)}$ are computed by column, in a hierarchical manner, beginning with $x_j^{(0)}$.

In conclusion, by applying the HF and HV theorems to the interactions (10) and (13), we have shown that the eigenvalues perturbative coefficients $\epsilon_{n,l}(k)$ can be obtained, at any order $k$, without any wave functions calculations. Thus, the HFHV method provides a remarkably fast and reliable tool to calculate very large order eigenenergies perturbative coefficients.

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10This kind of potential is encountered in many fields of physics like plasma, nuclear and solid state physics.
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