# **Application of the Quantum Mechanical Hypervirial Theorems to Even-Power Series Potentials**

Th. E. Liolios<sup>1</sup> and M. E. Grypeos<sup>1</sup>

Received March 4, 1997

The class of the even-power series potentials,  $V(r) = -D + \sum_{k=0}^{\infty} V_k \lambda^k r^{2k+2}$ ,  $V_0 = \omega^2 > 0$ , is studied with the aim of obtaining approximate analytic expressions for the nonrelativistic energy eigenvalues, the expectation values for the potential and kinetic energy operators, and the mean square radii of the orbits of a particle in its ground and excited states. We use the hypervirial theorems (HVT) in conjunction with the Hellmann-Feynman theorem (HFT), which provide a very powerful scheme for the treatment of the above and other types of potentials, as previous studies have shown. The formalism is reviewed and the expressions of the above-mentioned quantities are subsequently given in a convenient way in terms of the potential parameters, the mass of the particle, and the corresponding quantum numbers, and are then applied to the case of the Gaussian potential and to the potential  $V(r) = -D/\cosh^2(r/R)$ . These expressions are given in the form of series expansions, the first terms of which yield, in quite a number of cases, values of very satisfactory accuracy.

### 1. INTRODUCTION

Various approaches can be employed in an effort to obtain approximate expressions for the energy eigenvalues and other quantities of interest for a particle moving in a certain potential. Unfortunately, the majority entail cumbersome calculations of matrix elements or the ingenious deduction of a trial function. These obstacles can be overcome by using the hypervirial theorem (Hirschfelder, 1960) in conjunction with the Hellmann–Feynman theorem, the HVT-HFT method, which could have been labeled as classical, had it not been for the peculiarities of the potential we select each time.

2051

<sup>&</sup>lt;sup>1</sup>Department of Theoretical Physics, University of Thessaloniki, Thessaloniki 54006, Greece.

Consequently, this method constitutes a very effective alternative to a pure perturbation or variational treatment.

A number of authors have applied variations of this method to several potentials (see, e.g., Marc and McMillan, 1985; Fernandez and Castro, 1987; McRae and Vrscay, 1992; Swenson and Danforth, 1972; Killingbeck, 1978, 1985a,b; Grant and Lai, 1979; Lai, 1981, 1982, 1983; Lai and Lin, 1982; Mateo *et al.*, 1990; Witwit, 1991a–d; and references therein). The results vary each time, according to the properties of the potential in question. The scheme makes use of a perturbation parameter  $\lambda$  which enables us to expand the potential as well as the total energy and the moments in a  $\lambda$ -series. The first nontrivial term of our expanded potential is then adopted as the unperturbed term of our problem. The energy of the unperturbed Schrödinger equation will serve as a parameter in terms of which the other terms of the series will be calculated.

In the present work we consider a wide class of potentials of the form

$$V(r) = -D + \sum_{k=0}^{\infty} V_k \lambda^k r^{2k+2}, \qquad V_0 = \omega^2 > 0$$

The general formalism for such a class of potentials is thoroughly reviewed in the next section and subsequently a general approximate expression of the energy eigenvalues is derived in terms of the potential parameters, the mass of the particle, and the quantum numbers of the respective eigenstate. In Section 3 the corresponding general expressions of the expectation values of the kinetic and the potential energy operators are derived, as are those of the mean square radius of the orbit of a particle in any bound state in the potential.

In Section 4 the derived expressions are applied to the well-known Gaussian potential and to the Poeschl–Teller (PT)-type potential  $V(r) = -D/\cosh^2(r/R)$ , respectively. The final section is devoted to a test of the accuracy of the derived expressions by comparing the values they yield mainly with the corresponding results obtained with a numerical integration of the Schrödinger equation. This is accomplished by taking as an example the nonrelativistic motion of a  $\Lambda$ -particle in a hypernucleus moving in the above-mentioned PT potential.

# 2. DESCRIPTION OF THE HVT-HFT SCHEME FOR EVEN-POWER SERIES POTENTIALS. DERIVATION OF A GENERAL APPROXIMATE EXPRESSION FOR THE ENERGY EIGENVALUES

We consider the class of potentials V(r) mentioned in the introduction, namely

$$V(r) = -D + \sum_{k=0}^{\infty} V_k \lambda^k r^{2k+2}$$
 (1)

where  $V_0 = \omega^2 > 0$ . It is obvious that certain anharmonic oscillators, such as the  $V(r) = \frac{1}{2}kr^2 + k_1r^m$ , which was studied in Swenson and Danforth (1972; see also p. 339 of Marc and McMillan, 1985, and references therein) belong in that class. Furthermore, there also belongs in that class a number of potentials encountered in applications. Those potentials are of the form

$$V(r) = -Df\left(\frac{r}{R}\right), \qquad 0 \le r < \infty$$
(2)

where D > 0 is the potential depth, R > 0 is the potential radius, and the "potential form factor" f, f(0) = 1, is an even analytic function of x = r/R, namely

$$f(x) = \sum_{k=0}^{\infty} d_k x^{2k} \tag{3}$$

where  $d_k$  are the numbers

$$d_k = \frac{1}{(2k)!} \frac{d^{2k}}{dx^{2k}} f(x)|_{x=0}, \qquad k = 0, 1, 2, \dots, \qquad d_1 < 0 \tag{4}$$

The radial Schrödinger equation for the radial wave function  $u_{nl} = rR_{nl}(r)$  then reads

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}+\sum_{k=0}^{\infty}V_k\lambda^k r^{2k+2}\right]u_{nl}=\tilde{E}_{nl}u_{nl}$$
(5)

where  $\tilde{E}_{nl}$  is the shifted energy eigenvalue  $E_{nl}$ . That is,

$$\tilde{E}_{nl} = E_{nl} + D \tag{6}$$

Setting

$$\tilde{V}(r) = \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2} + \sum_{k=0}^{\infty} V_k \lambda^k r^{2k+2}$$
(7)

we find that the Hamiltonian becomes

$$\tilde{H} = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \tilde{V}(r) \tag{8}$$

As a result the Schrödinger equation can now be written as

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\tilde{V}(r)\right]u_{nl}=\tilde{E}_{nl}u_{nl}$$
(9)

The Hamiltonian  $\tilde{H}$  is now identical to the one used by Swenson and Danforth (1972), which means that we can make full use of the hypervirial relation that they obtained, namely (Swenson and Danforth, 1972; Lai, 1983)

$$\tilde{E}_{nl} \langle r^{N} \rangle_{nl} = \frac{1}{2} \left( N + 1 \right)^{-1} \left\langle r^{N+1} \frac{d\tilde{V}}{dr} \right\rangle_{nl} + \left\langle r^{N} \tilde{V} \right\rangle_{nl} - \frac{\hbar^{2}}{8\mu} N(N-1) \left\langle r^{N-2} \right\rangle_{nl}$$
(10)

If we expand the energy  $\tilde{E}_{nl}$  and the moments  $\langle r^N \rangle$  in  $\lambda$ -series, we have, respectively,

$$\tilde{E}_{nl} = \sum_{k=0}^{\infty} E^{(k)} \lambda^k \tag{11}$$

$$\langle r^N \rangle_{nl} = \sum_{k=0}^{\infty} C_N^{(k)} \lambda^k$$
 (12)

Note that the indices (nl) on  $E^{(k)}$  and  $C^{(k)}_{N+2}$  have been suppressed for the sake of simplicity. According to the above definitions the unperturbed term of our potential is

$$\tilde{V}^{(0)}(r) = \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2} + \omega^2 r^2$$
(13)

and the corresponding energy eigenvalue is

$$E^{(0)} = 2\omega a_{nl} \sqrt{\frac{\hbar^2}{2\mu}}$$
(14)

which is, in fact, the energy of the Harmonic oscillator. In the interest of simplicity we have adopted the following notation:

$$a_{nl} = (2n + l + \frac{3}{2}) \tag{15}$$

n = 0, 1, 2, 3, ... (principal quantum number) and l = 0, 1, 2, 3, ... (orbital angular momentum quantum number).

Applying the Hellmann–Feynman theorem (HFT) (Hellmann, 1937; Feynman, 1939; Bertlmann and Martin, 1980) to our Hamiltonian, we get

$$\frac{\partial \tilde{E}_{nl}}{\partial \lambda} = \left\langle \frac{\partial \tilde{H}}{\partial \lambda} \right\rangle \tag{16}$$

After some trivial calculations we obtain

$$E^{(k)} = \frac{1}{k} \sum_{m=0}^{k} m V_m C_{2m+2}^{(k-m)}, \qquad k \neq 0$$
(17)

Substituting (11), (12), and (17) into (10), we get the familiar recurrence relation (Lai, 1983)

$$C_{N+2}^{(k)} = \frac{N+1}{(N+2)V_0} \left\{ \sum_{q=0}^{k} E^{(q)} C_N^{(k-q)} - \left[ \frac{Nl(l+1)}{N+1} - \frac{N(N-1)}{4} \right] \frac{\hbar^2}{2\mu} C_{N-2}^{(k)} - \frac{N+3}{N+1} V_1 C_{N+4}^{(k-1)} - \frac{N+4}{N+1} V_2 C_{N+6}^{(k-2)} - \dots - \frac{N+k+2}{N+1} V_k C_{N+2k+2}^{(0)} \right\}$$
(18)

where  $C_0^{(k)} = \delta_{0k}$ .

The recurrence relation (18) is used to evaluate the coefficients  $E^{(k)}$  used in (11). In fact what we need to do is evaluate the coefficients  $C_N^{(k)}$  used in (12) and (17). We perform this calculation in a hierarchical manner (Lai, 1982), i.e., to obtain  $E^{(1)}$  in (11), we resort to (17), which readily yields

$$E^{(1)} = V_1 C_4^{(0)} \tag{19}$$

We still need to calculate the  $C_4^{(0)}$  coefficient, which will be extracted from (18). Indeed, (18) gives

$$C_4^{(0)} = \frac{3}{4\omega^2} \left[ E^{(0)} C_2^{(0)} - \left( \frac{2l(l+1)}{3} - \frac{1}{2} \right) \frac{\hbar^2}{2_{\mu}} \right]$$
(20)

To calculate  $C_2^{(0)}$ , we need to resort to (18) once more, so that we get

$$C_2^{(0)} = \frac{E^{(0)}}{2\omega^2} \tag{21}$$

 $E^{(1)}$  can be obtained by virtue of (19)–(21).

The same pattern of calculations is adhered to for each coefficient (either  $E^{(k)}$  or  $C_N^{(k)}$ ). Applying this method to the class of potentials given by (1), we arrive at the following general expression (where  $b = \hbar^2/2\mu$ ):

$$E_{nl} = -D + E^{(0)} + E^{(1)}\lambda + E^{(2)}\lambda^{2} + E^{(3)}\lambda^{3} + E^{(4)}\lambda^{4} + \cdots$$
(22)  
$$= -D + 2\omega a_{nl}b^{1/2} + \frac{V_{1}}{8\omega^{2}} [12a_{nl}^{2} - 4l(l+1) + 3]b\lambda$$
  
$$- \frac{a_{nl}}{32\omega^{5}} [4a_{nl}^{2}(17V_{1}^{2} - 20V_{2}\omega^{2}) + 12l(l+1)(4V_{2}\omega^{2} - 3V_{1}^{2}) + 67V_{1}^{2} - 100V_{2}\omega^{2}]b^{3/2}\lambda^{2}$$
  
$$+ \frac{1}{1024\omega^{8}} \{80a_{nl}^{4}(75V_{1}^{3} - 132V_{1}V_{2}\omega^{2} + 56V_{3}\omega^{4})$$

$$- 8a_{nl}^{2}[12l(l + 1)(43V_{1}^{3} - 84V_{1}V_{2}\omega^{2} + 40V_{3}\omega^{4}) - 1707V_{1}^{3} + 20\omega^{2}(177V_{1}V_{2} - 98V_{3}\omega^{2})] + [4l(l + 1)(11V_{1}^{3} - 36V_{1}V_{2}\omega^{2} + 24V_{3}\omega^{4}) - 3(171V_{1}^{3} - 420V_{1}V_{2}\omega^{2} + 280V_{3}\omega^{4})] \times [4l(l + 1) - 3]\}b^{2}\lambda^{3} - \frac{a_{nl}}{8192\omega^{11}} \{48a_{nl}^{4}[3563V_{1}^{4} - 8344V_{1}^{2}V_{2}\omega^{2} + 4032V_{1}V_{3}\omega^{4} + 16\omega^{4}(131V_{2}^{2} - 84V_{4}\omega^{2})] - 40a_{nl}^{2}[4l(l + 1)(891V_{1}^{4} - 2280V_{1}^{2}V_{2}\omega^{2} + 1216V_{1}V_{3}\omega^{4} + 624V_{2}^{2}\omega^{4} - 448V_{4}\omega^{6}) - 17833V_{1}^{4} + 47288V_{1}^{2}V_{2}\omega^{2} - 28224V_{1}V_{3}\omega^{4} - 13264V_{2}^{2}\omega^{4} + 12096V_{4}\omega^{6}] + 48[l(l + 1)]^{2}[303V_{1}^{4} - 1048V_{1}^{2}V_{2}\omega^{2} + 704V_{1}V_{3}\omega^{4} + 16\omega^{4}(23V_{2}^{2} - 20V_{4}\omega^{2})] - 8l(l + 1)(28647V_{1}^{4} - 85656V_{1}^{2}V_{2}\omega^{2} + 58048V_{1}V_{3}\omega^{4} + 27120V_{2}^{2}\omega^{4} - 28480V_{4}\omega^{6}) + 305141V_{1}^{4} - 938248V_{1}^{2}V_{2}\omega^{2} + 673344V_{1}V_{3}\omega^{4} + 16\omega^{4}(19277V_{2}^{2} - 22428V_{4}\omega^{2})\}b^{5/2}\lambda^{4} + \cdots$$
 (23)

For potentials of the general form (2), the above expression may be rewritten in terms of the depth and radius parameters. The relation which links the coefficients  $V_k \lambda^k$  with the potential parameters D and R and the coefficients  $d_k$  is the following:

$$V_k \lambda^k = -\frac{D}{R^{2k+2}} d_{k+1}, \qquad k = 0, 1, 2, 3, \dots$$
 (24)

Thus, in that case, the expansion for the energy eigenvalue becomes:

$$E_{nl} = -D + \frac{2a_{nl}(-Dd_1)^{1/2}}{R}b^{1/2} + \frac{d_2}{8d_1R^2}[12a_{nl}^2 - 4l(l+1) + 3]b$$
$$-\frac{a_{nl}(-Dd_1)^{1/2}}{32Dd_1^3R^3} \left\{4a_{nl}^2(20d_1d_3 - 17d_2^2)\right\}$$

$$+ 4d_{1}d_{3}[25 - 12l(l + 1)] + d_{2}^{2}[36l(l + 1) - 67]\}b^{3/2}$$

$$- \frac{1}{1024Dd_{1}^{4}R^{4}} \{80a_{nl}^{4}(56d_{1}^{2}d_{4} - 132d_{1}d_{2}d_{3} + 75d_{2}^{3})$$

$$- 8a_{nl}^{2}\{40d_{1}^{2}d_{4}[12l(l + 1) - 49]$$

$$+ 12d_{1}d_{2}d_{3}[295 - 84l(l + 1)] + 3d_{2}^{3}[172l(l + 1) - 569]\}$$

$$+ [4l(l + 1) - 3]$$

$$\times \{24d_{1}^{2}d_{4}[4l(l + 1) - 35] + 36d_{1}d_{2}d_{3} [35 - 4l(l + 1)]$$

$$+ d_{3}^{3}[44l(l + 1) - 513]\}b^{2} + \cdots$$
(25)

It is of interest that equation (25) coincides with the corresponding result of Sharma *et al.* (1980) [once correction of a few misprints or minor errors is made (B. Kotsos, private communication)], in which, however, a perturbation approach is used and not the HVT-HFT one. That coincidence corroborates the validity of the above expressions for  $E_{nl}$ .

Equation (25) is suitable for investigating the conditions under which the first few terms are sufficient to provide a good approximation to the energy eigenvalues. By considering the ratio of successive terms, we easily realize that the above condition is satisfied when the parameter  $s = (\hbar^2/2\mu DR^2)^{1/2}$  is small, that is, when the potential well is quite deep and wide, as well as when the particle mass large.

# 3. APPROXIMATE EXPRESSIONS FOR THE $\langle V \rangle_{nl}$ , $\langle T \rangle_{nl}$ , AND $\langle r^2 \rangle_{nl}$

A number of authors have applied the hypervirial relations to specific potentials only to obtain an asymptotic series for the energy eigenvalue, the general expression of which has been derived in the previous section for the class of potentials considered. Nevertheless, the matter of the expectation values (with respect to the energy eigenfunctions) of the kinetic energy operator  $\langle T \rangle_{nl} = \langle T \rangle$  and of the potential energy operator  $\langle V \rangle_{nl} = \langle V \rangle$ , and mainly of the mean square radius of the orbit of a particle in a given energy eigenstate  $\langle r^2 \rangle_{nl} = \langle r^2 \rangle$ , remain to be settled. Below we extract general expressions for these quantities.

As for the expectation value of the kinetic and potential energy operators, the application of the Hellmann–Feynman theorem (Hellmann, 1937; Feynman, 1939; Bertlmann and Martin, 1980), according to which

$$\frac{\langle T \rangle}{\mu} = -\frac{\partial E}{\partial \mu} \tag{26}$$

yields  $\lambda$ -series of the form

 $\langle T \rangle = \sum_{k=0}^{\infty} T^{(k)} \lambda^k$  (27)

and

$$\langle V \rangle = -D + \sum_{k=0}^{\infty} V^{(k)} \lambda^k$$
(28)

The relations between  $T^{(k)}$ ,  $V^{(k)}$ , and  $E^{(k)}$  can be easily extracted and are as follows:

$$T^{(k)} = \left(\frac{k+1}{2}\right) E^{(k)}$$
(29)

and

$$V^{(k)} = \left(\frac{1-k}{2}\right) E^{(k)} \tag{30}$$

By using relations (17) and (18) we can extract the coefficients  $C_N^{(k)}$  used in (12) in order to evaluate the orbital mean square radii. The  $\lambda$ -series for  $\langle r^2 \rangle$  is

$$\langle r^2 \rangle_{nl} = C_2^{(0)} + C_2^{(1)} \lambda + C_2^{(2)} \lambda^2 + C_2^{(3)} \lambda^3 + \cdots$$

$$= \frac{a_{nl}}{\omega} b^{1/2} - \frac{V_1}{8\omega^4} [12a_{nl}^2 - 4l(l+1) + 3]b\lambda$$

$$+ \frac{a_{nl}}{64\omega^7} [20a_{nl}^2(17V_1^2 - 12V_2\omega^2)$$

$$+ 36l(l+1)(4V_2\omega^2 - 5V_1^2) + 335V_1^2 - 300V_2\omega^2]b^{3/2}\lambda^2$$

$$- \frac{1}{256\omega^{10}} \{80a_{nl}^4(75V_1^3 - 99V_1V_2\omega^2 + 28V_3\omega^4)$$

$$- 8a_{nl}^2(12l(l+1)(43V_1^3 - 63V_1V_2\omega^2 + 28V_3\omega^4)$$

$$+ (4l(l+1))^2(11V_1^3 - 27V_1V_2\omega^2 + 12V_3\omega^4)$$

$$+ (171V_1^3 - 315V_1V_2\omega^2 + 140V_3\omega^4)\}b^2\lambda^3 + \cdots$$

$$(31)$$

2058

For potentials of the form (2),  $\langle r^2 \rangle_{nl}$  is expressed in terms of the depth and radius as follows:

$$\langle r^2 \rangle_{nl} = \frac{a_{nl}R}{(-Dd_1)^{1/2}} b^{1/2} + \frac{d_2}{8Dd_1^2} [12a_{nl}^2 - 4l(l+1) + 3]b - \frac{a_{nl}(-Dd_1)^{1/2}}{64D^2d_1^4R} \{20a_{nl}^2(12d_1d_3 - 17d_2^2) + 12d_1d_3[25 - 12l(l+1)] + 5d_2^2[36l(l+1) - 67]\}b^{3/2} - \frac{1}{256D^2d_1^5R^2} \{80a_{nl}^4(28d_1^2d_4 - 99d_1d_2d_3 + 75d_2^3) - 8a_{nl}^2\{20d_1^2d_4[12l(l+1) - 49] + 9d_1d_2d_3[295 - 84l(l+1)] + 3d_2^3[172l(l+1) - 569]\} + [4l(l+1) - 3] \times \{12d_1^2d_4[4l(l+1) - 35] + 27d_1d_2d_3[35 - 4l(l+1)] + d_2^3[44l(l+1) - 513]\}\}b^2 + \cdots$$
(32)

In the same way we can obtain moments of higher order.

## 4. APPLICATION OF THE DERIVED FORMULAS

Typical members of the potential class in question are the Gaussian potential, which is given by

$$V(r) = -De^{-r^2/R^2}, \quad 0 \le r < \infty$$
 (33)

and the well-known Poeschl-Teller-type potential, given by

$$V(r) = \frac{-D}{\cosh^2(r/R)}, \qquad 0 \le r < \infty$$
(34)

where D is the potential depth and R its radius. Such potentials may be considered, for example, a first approximation to the self-consistent potential for a nucleon in light nuclei, or for a  $\Lambda$ -hyperon in light hypernuclei in nonrelativistic quantum mechanics. In such a case the potential radius R is expressed (in the framework of the rigid-core model) in terms of the mass number of the core nucleus by means of the relation  $R = r_0 A_c^{1/3}$ , where  $A_c$  is the mass number of the core nucleus ( $A_c = A - 1$ ). The expression for  $d_k$  for the Gaussian potential is

$$d_k = \frac{(-1)^k}{k!}$$
(35)

The energy  $\lambda$ -series (where  $\lambda = 1/R^2$ ,  $\omega^2 = D/R^2$ ) for the Gaussian potential has already been obtained by Lai (1983) up to  $\lambda^3$  (see also Sharma *et al.*, 1980).

In our study of the above potentials, we derive the ms radii of the particle orbits  $\langle r^2 \rangle_{nl}$ , while the expectation values of the potential and the kinetic energy follow readily from (29) and (30). For the Gaussian potential the expression for  $\langle r^2 \rangle_{nl}$  is

$$\langle r^{2} \rangle_{nl} = \frac{a_{nl}}{\omega} b^{1/2} + \frac{1}{16\omega^{2}} [12a_{nl}^{2} - 4l(l+1) + 3]b\lambda$$
  
+  $\frac{3a_{nl}}{256\omega^{3}} [60a_{nl}^{2} - 28l(l+1) + 45]b^{3/2}\lambda^{2}$   
+  $\frac{1}{6144\omega^{4}} \{4400a_{nl}^{4} + 8a_{nl}^{2}[791 - 276l(l+1)]$   
+  $3[3 - 4l(l+1)][12l(l+1) + 23]\}b^{2}\lambda^{3} + \cdots$  (36)

An interesting feature of the potential (34) is that the corresponding Schrödinger eigenvalue problem can be solved exactly for the *s*-states. That potential has been used rather extensively in studies of hypernuclei (Lalazissis *et al.*, 1988; Lalazissis, 1989, 1993). The exact analytic expression for the *s*-state energy eigenvalues is (Lalazissis *et al.*, 1988; Lalazissis, 1989, 1993; Bessis *et al.*, 1982)

$$E_{n0} = -\frac{\hbar^2}{2\mu R^2} \left[ 2n + \frac{3}{2} - \frac{1}{2} \sqrt{\frac{8\mu DR^2}{\hbar^2} + 1} \right]^2$$
(37)

Note that for the energy eigenvalues

$$n = 0, 1, 2, ..., n_{\text{max}}, \qquad n_{\text{max}} < \frac{1}{4} \left[ \left( 1 + \frac{8\mu DR^2}{\hbar^2} \right)^{1/2} - 3 \right]$$

For the same states exact analytic results are also available, through the application of the Hellmann–Feynman theorem, for  $\langle T \rangle$  and  $\langle V \rangle$ , and thus one can test safely whether the first terms of the corresponding expansions constitute a good approximation to the relevant quantities. The expressions (Lalazissis *et al.*, 1988; Lalazissis, 1989, 1993, 1994) for  $\langle T \rangle_{n0}$  and  $\langle V \rangle_{n0}$  can be written, respectively, as

$$\langle T \rangle_{n0} = E_{n0} + D - \frac{2D(2n+3/2)}{\sqrt{8\mu DR^2/\hbar^2 + 1}}, \qquad n = 0, 1, 2, \dots, n_{\text{max}}$$
 (38)

$$\langle V \rangle_{n0} = -D + \frac{2D(2n+3/2)}{\sqrt{8\mu DR^2/\hbar^2 + 1}}, \qquad n = 0, 1, 2, \dots, n_{\max}$$
 (39)

The expressions for the coefficients  $d_k$  are

$$d_0 = 1 \tag{40}$$

$$d_1 = -1 \tag{41}$$

$$d_2 = 2/3$$
 (42)

$$d_3 = -17/45 \tag{43}$$

$$d_4 = 62/315 \tag{44}$$

$$d_5 = -1382/14175 \tag{45}$$

According to the analysis of Section 2, we have the following HVT energy series (again here  $\lambda = 1/R^2$  and  $\omega^2 = D/R^2$ ):

$$E_{nl} = -D + 2\omega a_{nl} b^{1/2} - \frac{1}{12} [12a_{nl}^2 - 4l(l+1) + 3]b\lambda$$
  
+  $\frac{a_{nl}}{60\omega} [15 - 4l(l+1)]b^{3/2}\lambda^2$   
-  $\frac{4}{945\omega^2} l(l+1)[12a_{nl}^2 - 4l(l+1) + 3]b^2\lambda^2$   
-  $\frac{a_{nl}}{907200\omega^3} \{33280a_{nl}^2l(l+1)$   
-  $12816[l(l+1)]^2 + 25[440l(l+1) + 567]\}b^{5/2}\lambda^3$   
-  $\frac{1}{1247400\omega^4} l(l+1)\{32720a_{nl}^4$   
+  $8a_{nl}^2[1445 - 828l(l+1)]$   
+  $[3 - 4l(l+1)][1084l(l+1) - 2445]\}b^3\lambda^4 + \cdots$  (46)

If we set l = 0 in the above expression, the ensuing expansion is summed up, leading to a closed-form result which is identical to relation (37).

According to relations (29) and (30), we can readily derive the expectation value of the both the kinetic and the potential energy in the form of a  $\lambda$ -series. Moreover, using (32) we can obtain the corresponding  $\langle r^2 \rangle \lambda$ -series for the PT potential:

$$\langle r^{2} \rangle_{nl} = \frac{a_{nl}}{\omega} b^{1/2} + \frac{1}{12\omega^{2}} [12a_{nl}^{2} - 4l(l+1) + 3]b\lambda$$
  
+  $\frac{a_{nl}}{90\omega^{3}} [85a_{nl}^{2} - 36l(l+1) + 50]b^{3/2}\lambda^{2}$   
+  $\frac{1}{120960\omega^{4}} \{105840a_{nl}^{4} + 24a_{nl}^{2}[4725 - 1532l(l+1)]$   
-  $8912[l(l+1)]^{2} + 12984l(l+1) - 4725\}b^{2}\lambda^{3} + \cdots$  (47)

### 5. NUMERICAL RESULTS, COMMENTS, AND SUMMARY

In this section we give numerical results for the Poeschl–Teller-type potential (34). The potential parameters we use here for purposes of illustration were obtained by a least squares fitting procedure to experimental 1*s*-state energies of a  $\Lambda$ -particle in hypernuclei and are as follows (Lalazissis *et al.*, 1988; Lalazissis, 1989, 1993):

$$D = 38.9 \text{ MeV}$$
  $r_0 = 0.986 \text{ fm}$ 

The results are displayed in the tables that follow by using the following notation:

 $A_c$ : The mass number of the host nucleus.

 $E_{\rm hvt}$ : The total energy value obtained through the HVT-HFT scheme using the terms given in the table.

 $E_{an}$ : The total energy value from the analytic solution (only s-states).

 $E_p$ : The total energy value from a perturbation method (Lalazissis, 1993) (only for the n = 0 states).

 $E_{int}$ : The total energy value obtained through numerical integration.

 $\langle r^2 \rangle_{hvt}^{1/2}$ : The root-mean-square radius of the orbit of the particle obtained through the HVT-HFT scheme.

 $\langle r^2 \rangle_{int}^{1/2}$ : The root-mean-square radius obtained through numerical integration.

The energy and  $\langle r^2 \rangle$  series obtained through the present scheme are provided on a term-by-term basis so that the accuracy for various hypernuclei can be observed. The first few terms of the HVT series for the *s*-state energies as well as for the corresponding radii are seen, in the whole range of  $A_c$  values studied, to practically coincide with the ones extracted through numerical integration, or calculated by means of the corresponding exact expression in the case of the *s*-states of the PT-type potential (34).

For the lower excited states the accuracy of the HVT energy values is in general quite satisfactory, in particular for the heavier elements. We should also keep in mind that the computation of various quantities through numerical integration is also subject to certain inaccuracies, which are expected, however, to be usually very small. We also observe that the HVT energy eigenvalues with n = 0, for the PT-type potential (34) are also in quite good agreement with the values  $E_p$  (see Table I) obtained with the perturbation method of Lalazissis (1993). The HVT values are in fact a little closer to those obtained by numerical integration in comparison to the  $E_p$  ones. The remarks previously made regarding the accuracy of the HVT energy quantities also hold to some extent for the orbital radii (Table II), although in that case the accuracy is less satisfactory, mainly for certain states and in particular for the lighter elements.

We note that the formulas derived in this paper for the extraction of both  $\langle T \rangle$  and  $\langle V \rangle$  can be linked directly to the previous papers which have calculated the energy series for a great number of potentials. Thus, one may obtain  $\langle T \rangle$  as well as  $\langle V \rangle$  by modifying the HVT energy coefficients in a way analogous to that followed in the present paper.

We finally observe that the HVT values of both the energy quantities and the orbital radii are, for a given state, more accurate for the heavier elements than for the lighter ones. This is in accordance with our expectations, since, as observed in Section 2, in the former case the parameter s is smaller. Furthermore, the accuracy of the results depends on the state (being more satisfactory for the lower states).

In conclusion, we summarize the main results of the present investigation:

1. The HVT-HFT scheme is applied to a wide class of potentials, namely of the type (1) or of the form (2). So far as we know, such a procedure has never been followed before in such a unified way in connection with the HVT-HFT scheme. The energy eigenvalues are expressed in terms of the potential parameters, the mass of the particle, and the corresponding quantum numbers, in the form of an expansion which is suitable to be applied to specific examples. In a number of cases, the first terms of this expansion yield values of very satisfactory accuracy.

2. The HVT-HFT scheme is extended (for the first time, to our knowledge) to obtain analogous expansions for other interesting quantities, such as the expectation values, of the kinetic and potential energy operators [by using the Hellman–Feynman theorem, as done in other studies for the same purpose, such as in Bertlmann and Martin (1980)] and of the mean-square radius of the orbit of a particle.

3. The accuracy of the first terms of the expansion depends on the state as well as on the potential parameters and the particle mass. The lower the

$ \begin{array}{rclcrcrc} E^{(0)} - D & E^{(1)}\lambda & E^{(2)}\lambda^2 & E^{(3)}\lambda^3 & E^{(4)}\lambda^4 & E^{(5)}\lambda^5 \\ \hline 8.84 & -16.27 & 0.99 & 0 & -0.01 & 0 \\ 1.64 & -111.73 & 0.61 & 0 & -0.004 & 0 \\ 1.64 & -110.05 & 0.48 & 0 & -0.001 & 0 \\ 1.6.75 & -18.57 & 0.26 & -0.15 & -0.081 & -0.043 \\ -13.18 & -4.72 & 0.15 & 0 & 0.0001 & 0 \\ 3.95 & -11.01 & 0.14 & -0.05 & -0.02 & -0.003 \\ -20.36 & -2.45 & 0.05 & 0 & 0.00005 & 0 \\ -8.01 & -5.72 & 0.04 & 0.01 & -0.004 & -0.001 \\ 4.34 & -10.30 & -0.08 & -0.07 & -0.03 & 0 \\ 16.69 & -19.45 & 0.08 & -0.07 & -0.03 & 0 \\ -8.01 & -5.72 & 0.04 & 0.01 & -0.004 & -0.013 \\ 4.34 & -12.26 & 0.13 & 0 & 0.0004 & 0 \\ 16.69 & -19.45 & 0.08 & -0.07 & -0.03 & 0 \\ -11.98 & -4.34 & 0.03 & 0 & -0.004 & 0 \\ -11.21 & -7.82 & -0.054 & -0.045 & -0.005 \\ -1.21 & -7.82 & -0.054 & -0.045 & -0.005 \\ -1.21 & -7.82 & -0.054 & -0.045 & -0.005 \\ -1.21 & -7.82 & -0.054 & -0.045 & -0.005 \\ -1.21 & -7.82 & -0.054 & -0.045 & -0.005 \\ -1.21 & -7.82 & -0.054 & -0.045 & -0.005 \\ -1.21 & -7.82 & -0.054 & -0.045 & -0.005 \\ -1.21 & -7.82 & -0.054 & -0.045 & -0.005 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.045 & -0.005 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.062 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.052 & -0.035 \\ -1.21 & -7.82 & -0.054 & -0.052 & -0.035 \\ -1.21 $					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$E^{(5)}\lambda^5$ E	E <sub>hvt</sub> E	$E_{ m an}$	$E_{ m p}$	$E_{ m int}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0		-6.44	-6.44	-6.44
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0		-9.48	-9.48	-9.48
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0 -1	I	10.95	-10.95	-10.95
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0 -1	ı	-13.13	-13.13	-13.13
$\begin{array}{cccccccccccccccccccccccccccccccccccc$				- 1.81	-1.91
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		·	-17.75	-17.75	-17.75
$\begin{array}{cccccccccccccccccccccccccccccccccccc$				-7.01	-7.03
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			-22.76	-22.76	-22.76
$\begin{array}{cccccccccccccccccccccccccccccccccccc$				-13.70	-13.71
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		-6.16		-6.14	-6.17
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			-7.78		-7.78
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		-2.76			-2.78
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	•	ł	-24.57	-24.57	-24.57
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		6.30		-16.30	-16.31
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		-9.159		-9.14	-9.16
		-3.22		-3.19	-3.27
	-	1	-10.43		- 10.44
-14.77 0.05 $-0.028$ $-0.013$		-5.218			-5.22

2064

$\overline{A_c}$	n	l	$C_{2}^{(0)}$	$C_2^{(1)}\lambda$	$C_2^{(2)}\lambda^2$	$C_2^{(3)}\lambda^3$	$C_2^{(4)}\lambda^4$	$C_{2}^{(5)}\lambda^{5}$	$\sqrt{\langle r^2 \rangle_{\rm hvt}}$	$\sqrt{\langle r^2 \rangle_{\rm int}}$
6	0	0	1.97	1.34	0.88	0.58	0.38	0.25	2.32	2.43
9	0	0	2.19	1.26	0.70	0.39	0.22	0.12	2.21	2.25
11	0	0	2.32	1.24	0.64	0.33	0.174	0.09	2.19	2.21
15	0	0	2.53	1.21	0.55	0.257	0.11	0.055	2.17	2.18
15	0	1	4.22	2.82	1.95	1.43	1.08	.84	3.51	4.04
31	0	0	3.17	1.16	0.41	0.14	0.05	0.01	2.22	2.22
31	0	1	5.28	2.71	1.45	0.81	0.47	0.28	3.32	3.39
80	0	0	4.30	1.14	0.29	0.07	0.02	0.005	2.41	2.41
80	0	1	7.17	2.66	1.02	0.415	0.175	0.076	3.39	3.39
80	0	2	10.03	4.78	2.46	1.36	0.79	0.47	4.46	4.55
80	1	0	10.03	5.69	3.07	1.64	0.88	0.48	4.67	4.72
80	1	1	12.90	9.03	6.14	4.19	2.90	2.04	6.10	6.53
120	0	0	4.91	1.13	0.25	0.056	0.013	0.003	2.52	2.52
120	0	1	8.18	2.64	0.89	0.31	0.12	0.04	3.49	3.49
120	0	2	11.46	4.76	2.13	1.03	0.52	0.27	4.49	4.52
120	0	3	14.73	7.47	4.20	2.55	1.65	0.71	5.60	5.87
120	1	0	11.46	5.66	2.66	1.24	0.58	0.27	4.68	4.70
120	1	1	14.73	8.98	5.33	3.17	1.91	1.17	5.94	6.10

Table 2. The Orbital Radius for the Poeschl-Teller Potential.

state and the smaller the value of the parameter  $s = (\hbar^2/2\mu DR^2)^{1/2}$ , that is, the deeper and wider the potential and the larger the particle mass, the fewer are the terms needed for the achievement of a satisfactory accuracy of the above-mentioned quantities.

4. The procedure discussed is applied to two typical two-parameter potentials, the Gaussian (33) and the Poeschl–Teller (PT) type (34). Extensive numerical calculations are performed in a number of cases. The accuracy of our HVT values is assessed by comparing them with those obtained either by solving the Schrödinger equation numerically or, whenever possible, using exact analytic expressions. The accuracy of the approximate analytic expressions of the quantities considered is discussed in connection with a problem of physical interest, namely that of the motion of a  $\Lambda$ -particle in hypernuclei.

#### ACKNOWLEDGMENTS

Partial financial support from the Greek Ministry of Industry, Energy and Technology (through project PENED 360/91) is kindly acknowledged.

### REFERENCES

Bertlmann, R. A., and Martin, A. (1980). Nuclear Physics B, 168, 111.

Bessis, N., Bessis, G., and Joulakian, B. (1982). Journal of Physics A: Mathematical and General, 15, 3679.

- Fernandez, F. M., and Castro, E. A. (1987). *Hypervirial Theorems*, Springer-Verlag, Berlin. Feynman, R. P. (1930). *Physical Review*, **56**, 340.
- Grant, M., and Lai, C. S. (1979). Physical Review A, 20, 718.
- Hellmann, H. (1937). Einfuhrung in die Quantenchemie, Deuticke, Vienna.
- Hirschfelder, J. O. (1960). Journal of Chemical Physics, 33, 1462.
- Killingbeck, J. (1978). Physics Letters, 65A, 87.
- Killingbeck, J. (1985a). Journal of Physics A: Mathematical and General, 18, L1925.
- Killingbeck, J. (1985b). Journal of Physics A: Mathematical and General, 18, 245.
- Lai, C. S. (1981). Physical Review A, 23, 455.
- Lai, C. S. (1982). Physical Review A, 26, 2245.
- Lai, C. S. (1983). Journal of Physics A: Mathematical and General, 16, L181.
- Lai, C. S., and Lin, H. E. (1982). Journal of Physics A: Mathematical and General, 15, 1495.
- Lalazissis, G. A. (1989). Ph.D. thesis, Aristotle University of Thessaloniki.
- Lalazissis, G. A. (1993). Physical Review C, 48, 198.
- Lalazissis, G. A. (1994). Physical Review C, 49, 1412.
- Lalazissis, G. A., Grypeos, M. E., and Massen, S. E. (1988). Physical Review C, 37, 2098.
- Marc, G., and McMillan, W. G. (1985). Advances in Chemical Physics, 58, 209.
- Mateo, F. G., et al. (1990). Journal of Physics B, 23, 2771.
- McRae, S. M., and Vrscay, E. R. (1992). Journal of Mathematical Physics, 33, 3004.
- Sharma, L. K., Choubey, Jyoti, and Muller-Kirsten, H. J. W. (1980). Journal of Mathematical Physics, 21, 1533.
- Swenson, R. J., and Danforth, S. H. (1972). Journal of Chemical Physics, 57, 1734.
- Witwit, M. R. M. (1991a). Journal of Physics A: Mathematical and General, 24, 5291.
- Witwit, M. R. M. (1991b). Journal of Physics A: Mathematical and General, 24, 4535.
- Witwit, M. R. M. (1991c). Journal of Physics A: Mathematical and General, 24, 3053.
- Witwit, M. R. M. (1991d). Journal of Physics A: Mathematical and General, 24, 3041.