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J. Phys. A: Math. Gen. 37 (2004) 7895-7907

PII: S0305-4470(04)76260-5

# The HVT technique and the 'uncertainty' relation for central potentials

# M E Grypeos, C G Koutroulos, K J Oyewumi<sup>1</sup> and Th Petridou

Department of Theoretical Physics, Aristotle University of Thessaloniki, Greece

Received 13 February 2004, in final form 16 June 2004 Published 28 July 2004 Online at stacks.iop.org/JPhysA/37/7895 doi:10.1088/0305-4470/37/32/005

#### Abstract

The quantum mechanical hypervirial theorems (HVT) technique is used to treat the so-called 'uncertainty' relation for quite a general class of central potential wells, including the (reduced) Poeschl–Teller and the Gaussian one. It is shown that this technique is quite suitable in deriving an approximate analytic expression in the form of a truncated power series expansion for the dimensionless product  $P_{nl} \equiv \langle r^2 \rangle_{nl} \langle p^2 \rangle_{nl} / \hbar^2$ , for every (deeply) bound state of a particle moving non-relativistically in the well, provided that a (dimensionless) parameter *s* is sufficiently small. Attention is also paid to a number of cases, among the limited existing ones, in which exact analytic or semi-analytic expressions for  $P_{nl}$  can be derived. Finally, numerical results are given and discussed.

PACS numbers: 02.60.-x, 03.65.-w, 21.80.+a

### 1. Introduction

The quantum mechanical hypervirial theorems (HVT) technique [1, 2] is a very useful technique in dealing with various problems encountered in physics and chemistry. Its main advantage is that one can calculate expectation values of interesting quantities, avoiding the use of the wavefunction and thus achieving considerable simplification. Particular attention was paid in obtaining energy eigenvalues for a particle moving in a potential and a lot of work has been done in this direction for various types of potentials [3].

The case of a general class of even-power series central potentials and in particular those of the form  $V(r) = -V_0 f(\frac{r}{R})$  was studied in [4, 5]. In that procedure, one obtains in a unified way the general expressions of the (lower) bound state energy eigenvalues and of the expectation values of certain other physical quantities with respect to the eigenstates of the single particle Hamiltonian. Application of these expressions to specific potentials

0305-4470/04/327895+13\$30.00 © 2004 IOP Publishing Ltd Printed in the UK

<sup>&</sup>lt;sup>1</sup> Permanent address: Physics Department, University of Ilorin, Nigeria.

of the class leads immediately to the corresponding expressions for the particular potential considered. These expressions are of the form of expansions in powers of a small parameter and the first terms of the expansions are expected to provide a reasonable approximation of the calculated quantities, as long as the parameter is sufficiently small. For potentials of the form  $V(r) = -V_0 f\left(\frac{r}{R}\right)$ , the expressions are power-series of the dimensionless parameter  $s = \left(\frac{\hbar^2}{2\mu V_0 R^2}\right)^{1/2}$  and the structure of the first terms of the expansions is fairly simple. The successive terms of each expansion are obtained by means of suitable recurrence relations on the basis of Swenson and Danforth hypervirial relations [6] and the Hellmann–Feynman theorem [7]. See also Killingbeck [2].

In a recent paper [8] another useful application of the HVT technique was considered, namely the study of inequalities of physical interest. Two basic inequalities were studied, relating the lowest energy level spacing  $\Delta E$  of a particle in its ground state, moving nonrelativistically in a central well, to the mean-square radius of its orbit and the expectation value of its kinetic energy, respectively, with the aim of investigating their (approximate) 'saturation', that is whether they become equalities approximately (e.g. within a few per cent) [9].

The aim of this paper is to discuss another inequality which is important to physics. It has been pointed out (see [10] and section 2 of [11]) that for a particle moving non-relativistically in a central potential V(r), the following 'uncertainty' relation holds:

$$\langle r^2 \rangle \langle p^2 \rangle / \hbar^2 \geqslant \frac{9}{4}. \tag{1}$$

It was pointed out that the inequality becomes equality for the ground state of the harmonic oscillator (HO) potential. In all other cases the above relation is an inequality and it would be of interest to provide analytic ways of calculating the dimensionless product  $P_{nl} \equiv \langle r^2 \rangle \langle p^2 \rangle / \hbar^2 \ge \frac{9}{4}$ , where the expectation values are calculated with respect to the Hamiltonian single-particle eigenstates. This would provide the means to investigate to what extent the inequality is saturated, depending on the potential shape considered and on the specific state. We may recall that the usual uncertainty relation for the position and its conjugate momentum:  $\Delta \hat{x} \Delta \hat{p} \ge \hbar/2$  and its generalizations have been the subject of detailed investigations since the publication of Heisenberg's original paper [12] until recently (see, e.g., [13] and references therein). We refer for detail in this respect to the very informative review article [14]. Among the topics of interest have been the analytic calculations of the uncertainty product  $(\Delta \hat{x})(\Delta \hat{p})$  for various types of one-dimensional potentials (see, e.g., [14]).

Before proceeding to the main topic of this paper (in the third section), attention is paid (in the following section and in the appendix) to certain typical cases in which the product  $P_{nl}$  can be given exactly analytically or semi-analytically. The final section is devoted to numerical results and to discussion.

# 2. Exact analytic results for the dimensionless product $P_{nl}$ for a number of potentials

Among the various central potentials, only a few have the property to lead to an exact analytic expression for the dimensionless product  $P_{nl} \equiv \langle r^2 \rangle_{nl} \langle p^2 \rangle_{nl} / \hbar^2$  for any bound eigenstate  $|nl\rangle$  of the Hamiltonian. It should be clear that not only should the energy eigenvalues be given analytically, but also the integrations in  $\langle r^2 \rangle_{nl}$  should be performed analytically and the result be given by a closed-form analytic expression. Typical examples of central potentials having these desired properties are the isotropic harmonic oscillator, the Coulomb (C) potential and the spherically symmetric rectangular well with infinite walls (IW). In this section the

corresponding expressions for the dimensionless products  $P_{nl}$  are given and discussed. These expressions are also useful for comparisons.

(a) For the HO potential.  $V^{\text{HO}}(r) = \frac{1}{2}\mu\omega^2 r^2$ , the energy eigenvalues  $E_{nl} = \langle \hat{T} \rangle_{nl} + \langle \hat{V} \rangle_{nl}$ , where by  $\hat{T}$  and  $\hat{V}$  we denote the kinetic and potential energy operators, respectively, are given by the well-known expression [15]

$$E_{nl}^{\rm HO} = \left(2n + l + \frac{3}{2}\right)\hbar\omega = \left(N + \frac{3}{2}\right)\hbar\omega \qquad \text{with} \quad n, l = 0, 1, 2, 3, \dots$$
(2)

where N = 2n + l is the HO quantum number. In addition, application of the virial theorem, to the case of the HO potential leads to the following relations:

$$\langle \widehat{T} \rangle_{nl}^{\rm HO} = \langle \widehat{V} \rangle_{nl}^{\rm HO} = \frac{E_{nl}^{\rm HO}}{2}.$$
(3)

Multiplying  $\langle \hat{T} \rangle_{nl}^{\text{HO}}$  and  $\langle \hat{V} \rangle_{nl}^{\text{HO}}$ , the following very simple expression for  $P_{nl}^{\text{HO}}$  results:

$$P_{nl}^{\rm HO} = \langle r^2 \rangle_{nl}^{\rm HO} \langle p^2 \rangle_{nl}^{\rm HO} / \hbar^2 = \left(2n + l + \frac{3}{2}\right)^2. \tag{4}$$

It is apparent from (4) that the dimensionless product  $P_{nl}^{\text{HO}}$  increases as the quantum numbers (nl) of the state increase, that is as the state becomes more excited. Furthermore, states with fixed N have the same dimensionless product. In addition,  $P_{nl}^{\text{HO}}$  is in accordance with (in)equality  $\langle r^2 \rangle_{nl} \langle p^2 \rangle_{nl} \ge \frac{9}{4}$  and attains its minimum value 9/4 for n = 0, l = 0, that is for the HO ground state.

(b) For the Coulomb potential (in the case of a hydrogen-like atom).  $V^{C}(r) = -\frac{Ze^{2}}{r}$ , the well-known expression of the energy eigenvalues is

$$E_n^C = -\frac{\hbar^2 (a_Z^2 \mu)}{2n^2}$$
 where  $a_Z = \frac{\hbar^2}{\mu e^2} \frac{1}{Z} = \frac{a}{Z}$  (5)

and *a* is the atomic unit of length (the first Bohr radius:  $a = \frac{\hbar^2}{\mu e^2} = 0.5292$  Å). Application of the virial theorem in this case leads to the relation [15]

$$\langle \widehat{T} \rangle_n^C = -\frac{1}{2} \langle \widehat{V} \rangle_n^C = -E_n^C.$$
(6)

Therefore  $\langle p^2 \rangle_{nl}^C = \langle p^2 \rangle_n^C = \frac{\hbar^2}{a_z^2 n^2}.$ 

Furthermore, application of Kramer's relation (see, e.g., [15]) with s = 2 leads to

$$\langle r^2 \rangle_{nl}^C = \frac{n^2 a_Z^2}{2} [5n^2 + 1 - 3l(l+1)].$$
<sup>(7)</sup>

Thus, the analytic expression for the dimensionless product in this case is

$$P_{nl}^{C} = \frac{1}{2} [5n^{2} + 1 - 3l(l+1)].$$
(8)

It should be recalled that here *n* is the principal quantum number: n = 1, 2, 3, ... and l = 0, 1, 2, ... (n - 1).

It is seen that  $P_{nl}^C$  attains its minimum value of 3 for the ground state (n = 1, l = 0). This minimum value is larger than the corresponding one of  $P_{nl}^{HO}$  that is 9/4, which 'saturates the inequality'. It is also seen that for fixed *n*, the minimum value of  $P_{nl}^C$  corresponds to the maximum possible value of l: l = n - 1.

(c) Finally, for the spherically symmetric rectangular infinite potential well

$$V^{\rm IW}(r) = \begin{cases} 0 & \text{if } r \leqslant R\\ \infty & \text{if } r > R \end{cases}$$
(9)

the energy eigenvalues reckoned from the 'bottom' of the well are given by [16]

$$E_{nl}^{\rm IW} = \frac{\hbar^2 X_{nl}^2}{2\mu R^2}$$
(10)

where  $X_{nl}$  are the roots of the *l*th-order spherical Bessel function and n = 1, 2, 3, ... is the principal quantum number, that is the number of the root in order of increasing magnitude.

From the above expression of  $\langle \hat{T} \rangle_{nl}$ , the expression of  $\langle p^2 \rangle_{nl}$  follows immediately. On the other hand, the  $\langle r^2 \rangle_{nl}$  can be obtained analytically as well, in terms of  $X_{nl}$  [17]. The result is

$$\langle r^2 \rangle_{nl}^{\text{IW}} = \frac{R^2}{3} \left[ 1 + \frac{(2l+3)(2l-1)}{2X_{nl}^2} \right].$$
 (11)

Therefore, the expression for  $P_{nl}^{IW}$  is

$$P_{nl}^{\rm IW} = \frac{1}{3} \left[ X_{nl}^2 + \frac{1}{2} (2l+3)(2l-1) \right].$$
(12)

It is seen that for the ground state (n = 1, l = 0), the dimensionless product attains its minimum value and becomes  $P_{10}^{IW} = \left[\frac{\pi^2}{3} - \frac{1}{2}\right] \simeq 2.79$ . This value is in accordance with inequality (1). It is, however, larger than the corresponding HO minimum value  $P_{00}^{HO} = 2.25$ , but smaller than the corresponding dimensionless product for the Coulomb potential  $P_{10}^{C} = 3$ .

We also see that the expression of  $P_{nl}^{\text{IW}}$  becomes very simple for any s state (l = 0). Thus,

$$P_{n0}^{\rm IW} = \left[\frac{n^2 \pi^2}{3} - \frac{1}{2}\right].$$
 (13)

Finally, it is worth mentioning that there are potentials for which the dimensionless product can be given 'semi-analytically', for certain states, when for example, an integral involved has to be calculated numerically. This is the case of the s states of the (reduced) Poeschl–Teller (PT) potential. The corresponding semi-analytic expressions for  $P_{n0}^{PT}$  which may be derived are given in the appendix and the values obtained with them are useful in comparing them with the HVT values (see section 4).

#### 3. The formalism and the expression for the dimensionless product $P_{nl}$

In this section the s-series expansions, mentioned in the introduction, are used, which were derived by means of the HVT technique [4, 5].

The class of two-parameter potential wells of the general form

$$V(r) = -V_0 f(r/R) \qquad 0 \leqslant r < \infty \tag{14}$$

is considered and a particle of mass  $\mu$  is assumed to move (non-relativistically) in a well of this form. In the above expression,  $V_0 > 0$  is the potential depth, R > 0 its 'radius' and f(f(0) = 1) the 'potential form factor' which determines its shape. The function f is assumed to be an appropriate analytic function of even powers of x = r/R with  $d^2 f/dx^2|_{x=0} > 0$ . Such potentials behave like a harmonic oscillator potential near the origin and therefore the terminology 'oscillator-like' potentials has been used. The results of this paper corroborate the suitability in using such terminology (see section 4). Apart from the above mentioned resemblance, their shape is quite different from that of the harmonic oscillator.

Typical potentials of the class are

(a) The Gaussian potential

$$V_G(r) = -V_0 e^{-r^2/R^2}$$
.

(b) The (reduced) PT potential

$$V_{\rm PT}(r) = -V_0 \cosh^{-2}(r/R)$$

but there are many others belonging to the same class.

In order to obtain the dimensionless product  $P_{nl}$  it is convenient to use for the energy eigenvalues and the expectation values of the kinetic energies and the mean square radii of the particle orbits the dimensionless expressions of their *s*-expansions of [5] which are denoted by a tilde on the top of the corresponding symbol. In the pertinent formulae, displayed below, it was found appropriate to rearrange somehow the terms in the coefficient of powers greater than 2, so that there is a more convenient way of factorizing the two sorts of contributions, that is those originating from the quantum numbers n, l of the state and those from the numbers  $d_k$ , determined by the potential shape, which are related to the derivatives of the potential form factor f

$$d_k = \frac{1}{(2k)!} \frac{d^{2k}}{dx^{2k}} f(x)|_{x=0} \qquad k = 0, 1, 2, \dots, \quad d_1 < 0.$$
(15)

The above rearrangements of terms in the coefficients of the *s* powers will facilitate their use in the following.

We also note that it would be desirable to consider in addition a renormalized hypervirial perturbation theory [2, 18] which is a very efficient one and has been used in treating various problems [19, 20]. This matter is under investigation and requires further work in order that the method is adjusted to our purposes. Among the recent work in connection with the HVT perturbation theory, we mention in particular the paper by Killingbeck *et al* (2001). In that paper, the advantages which stem from an appropriate choice of the unperturbed potential and of the origin at which the energy expansion is carried out, are discussed.

The expression of the expansion for the energy eigenvalues is as follows:

$$\widetilde{E}_{nl} = \frac{E_{nl}}{V_0} = \sum_{k=0}^{\infty} e_k s^k \tag{16}$$

where

$$e_0 = -1 \tag{17}$$

$$e_1 = 2a_{nl}(-d_1)^{1/2}$$
  $a_{nl} = \left(2n + l + \frac{3}{2}\right)$  (18)

$$e_2 = \frac{d_2}{8d_1} \left( 12a_{nl}^2 - 4l(l+1) + 3 \right) \tag{19}$$

$$e_{3} = -\frac{a_{nl}(-d_{1})^{1/2}}{32d_{1}^{3}} \left\{ 4d_{1}d_{3} \left[ 20a_{nl}^{2} - 12l(l+1) + 25 \right] + d_{2}^{2} \left[ -68a_{nl}^{2} + 36l(l+1) - 67 \right] \right\}$$
(20)

$$e_{4} = \frac{1}{1024d_{1}^{4}} \{ 12d_{1}d_{2}d_{3} [880a_{nl}^{4} - 8a_{nl}^{2} [84l(l+1) - 295] + 3[4l(l+1) - 3][4l(l+1) - 35]] \\ + d_{2}^{3} [-6000a_{nl}^{4} + 24a_{nl}^{2} [172l(l+1) - 569] \\ - [4l(l+1) - 3][44l(l+1) - 513]] \\ + 8d_{1}^{2}d_{4} [-560a_{nl}^{4} + 40a_{nl}^{2} [12l(l+1) - 49] \\ - 3[4l(l+1) - 3][4l(l+1) - 35]] \}.$$
(21)

For the mean-square radii of the particle orbits we have

$$\langle \widetilde{r^2} \rangle_{nl} \equiv \frac{\langle r^2 \rangle_{nl}}{R^2} = \sum_{k=0}^{\infty} r_k s^k \tag{22}$$

where

$$r_0 = 0 \tag{23}$$

$$r_1 = \frac{a_{nl}}{(-d_1)^{1/2}} \tag{24}$$

$$r_2 = \frac{d_2}{8d_1^2} \left( 12a_{nl}^2 - 4l(l+1) + 3 \right)$$
<sup>(25)</sup>

$$r_{3} = -\frac{a_{nl}(-d_{1})^{1/2}}{64d_{1}^{4}} \left\{ 12d_{1}d_{3} \left( 20a_{nl}^{2} - 12l(l+1) + 25 \right) + 5d_{2}^{2} \left[ -68a_{nl}^{2} + 36l(l+1) - 67 \right] \right\}$$
(26)

$$r_{4} = -\frac{1}{256d_{1}^{5}} \left\{ 9d_{1}d_{2}d_{3} \left[ -880a_{nl}^{4} + 8a_{nl}^{2} \left[ 84l(l+1) - 295 \right] - 3\left[ 4l(l+1) - 3 \right] \left[ 4l(l+1) - 35 \right] \right] \right. \\ \left. + d_{2}^{3} \left[ 6000a_{nl}^{4} - 24a_{nl}^{2} \left[ 172l(l+1) - 569 \right] + \left[ 4l(l+1) - 3 \right] \left[ 44l(l+1) - 513 \right] \right] \right. \\ \left. + 4d_{1}^{2}d_{4} \left[ 560a_{nl}^{4} - 40a_{nl}^{2} \left[ 12l(l+1) - 49 \right] + 3\left[ 4l(l+1) - 3 \right] \left[ 4l(l+1) - 35 \right] \right] \right\}.$$

$$(27)$$

Finally, for the expectation value of the kinetic energy operator in the various energy eigenstates we have

$$\langle \widetilde{T} \rangle_{nl} \equiv \frac{T_{nl}}{V_0} = \sum_{k=0}^{\infty} t_k s^k \tag{28}$$

where

$$t_k = \frac{k}{2}e_k \qquad k = 0, 1, 2....$$
 (29)

For the product  $\langle r^2 \rangle_{nl} \langle p^2 \rangle_{nl}$  we may write  $\langle r^2 \rangle_{nl} \langle p^2 \rangle_{nl} = 2\mu V_0 R^2 \langle \widetilde{r^2} \rangle_{nl} \langle \widetilde{T} \rangle_{nl}$ 

$${}^{2}\rangle_{nl} \langle p^{2}\rangle_{nl} = 2\mu V_{0} R^{2} \langle \tilde{r}^{2}\rangle_{nl} \langle \tilde{T}\rangle_{nl}$$

$$= \frac{\hbar^{2}}{s^{2}} \langle \tilde{r}^{2}\rangle_{nl} \langle \tilde{T}\rangle_{nl}$$

$$= \frac{\hbar^{2}}{s^{2}} \left(\sum_{k=0}^{\infty} r_{k} s^{k}\right) \left(\sum_{k=0}^{\infty} t_{k} s^{k}\right)$$

$$= \frac{\hbar^{2}}{s^{2}} \left(\sum_{k=0}^{\infty} \gamma_{k} s^{k}\right)$$
(30)

where

$$\gamma_k = \sum_{\rho=0}^k r_\rho t_{k-\rho}.$$
(31)

The expressions of  $\gamma_k$ , k = 0, 1, 2... follow easily from the expressions of  $r_k$  and  $t_k$ . We find

$$\begin{aligned} \gamma_{0} &= \gamma_{1} = 0 \qquad \gamma_{2} = r_{1}t_{1} = a_{nl}^{2} \qquad \gamma_{3} = r_{1}t_{2} + r_{2}t_{1} = 0 \\ \gamma_{4} &= r_{1}t_{3} + r_{2}t_{2} + r_{3}t_{1} = \frac{1}{64d_{1}^{3}} \Big\{ d_{1}d_{3} \Big[ 12a_{nl}(a_{nl} - 1) \Big( 20a_{nl}^{2} + 25 - 12l(l+1) \Big) \Big] \\ &+ d_{2}^{2} \Big[ \Big( 12a_{nl}^{2} - 4l(l+1) + 3 \Big)^{2} + a_{nl}(5a_{nl} - 3) \Big( -68a_{nl}^{2} + 36l(l+1) - 67 \Big) \Big] \Big\} \end{aligned}$$

$$(32)$$

and

$$\gamma_5 = r_1 t_4 + r_2 t_3 + r_3 t_2 + r_4 t_1 = -\frac{(-d_1)^{1/2}}{8^3 d_1^5} \left\{ 6d_1 d_2 d_3 \left[ q_{nl}^{(1)} + q_{nl}^{(2)} + q_{nl}^{(3)} \right] + d_2^3 \left[ q_{nl}^{(4)} + q_{nl}^{(5)} \right] \right\}$$
(33)

where

$$\begin{aligned} q_{nl}^{(1)} &= -8a_{nl}^{3} \left[ 110a_{nl}^{2} - 84l(l+1) + 295 \right] \\ q_{nl}^{(2)} &= -3a_{nl} \left[ 4l(l+1) - 3 \right] \left[ 4l(l+1) - 35 \right] \\ q_{nl}^{(3)} &= 2(1+a_{nl}) \left[ 12a_{nl}^{2} - 4l(l+1) + 3 \right] \left[ 20a_{nl}^{2} - 12l(l+1) + 25 \right] \\ q_{nl}^{(4)} &= 24a_{nl}^{3} \left[ 250a_{nl}^{2} - 172l(l+1) + 569 \right] \\ q_{nl}^{(5)} &= a_{nl} \left[ 4l(l+1) - 3 \right] \left[ 44l(l+1) - 513 \right] \\ &+ (3+5a_{nl}) \left[ 12a_{nl}^{2} - 4l(l+1) + 3 \right] \left[ -68a_{nl}^{2} + 36l(l+1) - 67 \right]. \end{aligned}$$
(34)

Therefore, the result for the dimensionless product  $P_{nl}$  is

$$P_{nl} \equiv \frac{\langle r^2 \rangle_{nl} \langle p^2 \rangle_{nl}}{\hbar^2} = \left(2n + l + \frac{3}{2}\right)^2 + \gamma_4 s^2 + \gamma_5 s^3 + \vartheta \left(s^4\right) \equiv P_{nl}^{(0)} + P_{nl}^{(2)} + P_{nl}^{(3)} + \vartheta \left(s^4\right).$$
(35)

It is seen that the structure of the dimensionless product is fairly simple, but the coefficients  $\gamma_k$  become progressively more complicated as the power of *s* increases. It is further seen that there is no contribution of terms proportional to the small dimensionless quantity *s* but of terms of  $s^2$  and higher.

### 4. Numerical values of the dimensionless product $P_{nl}$ and discussion

In this section we report the numerical results obtained with the derived expression (35) of the dimensionless product  $P_{nl}$  for the first bound states and the various values of the small quantity *s*. Each contribution to  $P_{nl}$ :  $P_{nl}^{(0)}$ ,  $P_{nl}^{(2)}$  and  $P_{nl}^{(3)}$  is also given in each case. The detailed results obtained with the PT potential are given in tables 1–4, while those with the Gaussian potential are displayed in tables 5–8, respectively.

It is clear from the results obtained in all tables that the main contribution to  $P_{nl}$ , for each bound state, comes from the corresponding zeroth-order term  $P_{nl}^{(0)}$  (see expression (35)). This is more pronounced for the ground state (n = 0, l = 0) and the smaller values of s, as is expected. It is also noted that the (absolute) values of  $P_{nl}^{(3)}$  are smaller than the corresponding ones of  $P_{nl}^{(2)}$  and often the difference between the two values is quite substantial.

On the basis of the above observations, it is therefore seen that the values of the dimensionless product  $P_{nl}$  are quite close to the corresponding values of the harmonic oscillator potential  $P_{nl}^{(HO)} = P_{nl}^{(0)}$ . This fact corroborates the suitability of the terminology of the potentials of this class as 'oscillator-like' potentials. Pertaining to other types of potentials,

**Table 1.** Numerical values of the dimensionless product  $P_{nl}$  and the partial contributions  $P_{nl}^{(s)}$  to it for the states nl = 00 for the various values of *s*. The reduced PT potential was used.

S	$P_{00}^{(0)}$	$P_{00}^{(2)}$	$P_{00}^{(3)}$	$P_{00}$
0.00	2.250	0	0	2.2500
0.02	2.250	0.00014	0.00001	2.2501
0.04	2.250	0.000 55	0.00004	2.2506
0.06	2.250	0.001 24	0.000 14	2.2514
0.08	2.250	0.002 20	0.000 33	2.2525
0.10	2.250	0.003 44	0.000 64	2.2541
0.12	2.250	0.00495	0.001 10	2.2561

**Table 2.** Numerical values of the dimensionless product  $P_{nl}$  and the partial contributions  $P_{nl}^{(s)}$  to it for the states nl = 10 for the various values of *s*. The reduced PT potential was used.

S	$P_{10}^{(0)}$	$P_{10}^{(2)}$	$P_{10}^{(3)}$	$P_{10}$
0.00	12.250	0	0	12.2500
0.02	12.250	-0.00256	-0.00021	12.2472
0.04	12.250	-0.01025	-0.00167	12.2381
0.06	12.250	-0.02306	-0.00565	12.2213
0.08	12.250	-0.04100	-0.01339	12.1956
0.10	12.250	-0.06462	-0.02616	12.1598
0.12	12.250	-0.09225	-0.04520	12.1126

**Table 3.** Numerical values of the dimensionless product  $P_{nl}$  and the partial contributions  $P_{nl}^{(s)}$  to it for the states nl = 01 for the various values of *s*. The reduced PT potential was used.

S	$P_{01}^{(0)}$	$P_{01}^{(2)}$	$P_{01}^{(3)}$	$P_{01}$
0.00	6.250	0	0	6.2500
0.02	6.250	0.00071	0.00005	6.2508
0.04	6.250	0.00284	0.000 37	6.2532
0.06	6.250	0.00639	0.001 26	6.2577
0.08	6.250	0.01136	0.002 99	6.2644
0.10	6.250	0.01774	0.005 84	6.2736
0.12	6.250	0.025 55	0.010 09	6.2856

**Table 4.** Numerical values of the dimensionless product  $P_{nl}$  and the partial contributions  $P_{nl}^{(s)}$  to it for the states nl = 02 for the various values of *s*. The reduced PT potential was used.

s	$P_{02}^{(0)}$	$P_{02}^{(2)}$	$P_{02}^{(3)}$	P <sub>02</sub>
0.00	12.250	0	0	12.2500
0.02	12.250	0.003 24	0.000 26	12.2535
0.04	12.250	0.01295	0.00206	12.2650
0.06	12.250	0.029 14	0.00697	12.2861
0.08	12.250	0.05180	0.016 51	12.3183
0.10	12.250	0.08094	0.032 24	12.3632
0.12	12.250	0.11655	0.05572	12.4223

such as the Coulomb and the infinite spherical well discussed in section 2, the values of  $P_{nl}$ , are quite different, as is clear, at least for the ground state, from the values quoted there.

**Table 5.** Numerical values of the dimensionless product  $P_{nl}$  and the partial contributions  $P_{nl}^{(s)}$  to it for the states nl = 00 for various values of *s*. The Gaussian potential was used.

S	$P_{00}^{(0)}$	$P_{00}^{(2)}$	$P_{00}^{(3)}$	$P_{00}$
0.00	2.250	0	0	2.2500
0.02	2.250	0.00026	0.00001	2.2503
0.04	2.250	0.001 03	0.00010	2.2511
0.06	2.250	0.00232	0.000 33	2.2527
0.08	2.250	0.00413	0.00077	2.2549
0.10	2.250	0.00645	0.001 51	2.2580
0.12	2.250	0.009 28	0.002 61	2.2619

**Table 6.** Numerical values of the dimensionless product  $P_{nl}$  and the partial contributions  $P_{nl}^{(s)}$  to it for the states nl = 10 for various values of *s*. The Gaussian potential was used.

s	$P_{10}^{(0)}$	$P_{10}^{(2)}$	$P_{10}^{(3)}$	$P_{10}$
0.00	12.250	0	0	12.2500
0.02	12.250	0.00668	0.000 34	12.2570
0.04	12.250	0.02672	0.00273	12.2794
0.06	12.250	0.06012	0.009 22	12.3193
0.08	12.250	0.10688	0.021 85	12.3787
0.10	12.250	0.16699	0.042 67	12.4597
0.12	12.250	0.24047	0.07374	12.5642

**Table 7.** Numerical values of the dimensionless product  $P_{nl}$  and the partial contributions  $P_{nl}^{(s)}$  to it for the states nl = 01 for various values of *s*. The Gaussian potential was used.

S	$P_{01}^{(0)}$	$P_{01}^{(2)}$	$P_{01}^{(3)}$	$P_{01}$
0.00	6.250	0	0	6.2500
0.02	6.250	0.00202	0.000 10	6.2521
0.04	6.250	0.008 09	0.000 83	6.2589
0.06	6.250	0.018 21	0.002 80	6.2710
0.08	6.250	0.03238	0.006 63	6.2890
0.10	6.250	0.050 59	0.012 95	6.3135
0.12	6.250	0.07284	0.022 39	6.3452

**Table 8.** Numerical values of the dimensionless product  $P_{nl}$  and the partial contributions  $P_{nl}^{(s)}$  to it for the states nl = 02 for various values of *s*. The Gaussian potential was used.

S	$P_{02}^{(0)}$	$P_{02}^{(2)}$	$P_{02}^{(3)}$	$P_{02}$
0.00	12.250	0	0	12.2500
0.02	12.250	0.00778	0.00046	12.2582
0.04	12.250	0.03111	0.003 68	12.2848
0.06	12.250	0.06999	0.01243	12.3324
0.08	12.250	0.12443	0.029 45	12.4039
0.10	12.250	0.19441	0.05752	12.5019
0.12	12.250	0.279 90	0.099 50	12.6294

We would also like to point out that the  $P_{nl}$  values obtained with the Gaussian potential are quite close to the corresponding ones resulted with the PT potential. However due to the difference in their shape, small but marked differences are observed. We may recall [4]



**Figure 1.** The dimensionless product  $P_{nl} = \langle r^2 \rangle_{nl} \langle p^2 \rangle_{nl} / \hbar^2$  as a function of *s*  $(s = [\hbar^2/(2\mu V_0 R^2)]^{1/2})$  for the PT potential for the 00 state (n = 0, l = 0) with the HVT technique (solid line) and with the semianalytic formula of the appendix (dashed line).



**Figure 2.** The dimensionless product  $P_{nl} = \langle r^2 \rangle_{nl} \langle p^2 \rangle_{nl} / \hbar^2$  as a function of *s*  $(s = [\hbar^2/(2\mu V_0 R^2)]^{1/2})$  for the PT potential for the 10 state (n = 1, l = 0) with the HVT technique (solid line) and with the semianalytic formula of the appendix (dashed line).

that the numbers  $d_k$  which are determined by the potential shape are for the PT potential  $d_0 = 1, d_1 = -1, d_2 = 2/3, d_3 = -17/45, d_4 = 62/315$ , while those for the Gaussian potential are given by  $d_k = \frac{(-1)^k}{(k)!}$ . Due to the difference in these values, the values of the dimensionless product  $P_{nl}$  differ a little. Our numerical results show that the values of  $P_{nl}$  obtained with the Gaussian potential are a little larger than the corresponding ones obtained with the PT potential.

In figures 1 and 2, the variation of  $P_{nl}$  with s is shown for the states n = 0, l = 0 and n = 1, l = 0 using the PT potential. In the same figures, the corresponding results obtained with the semi-analytic expression (44) of the appendix are also shown (dashed lines). It is seen that there is a fairly good agreement with the HVT results, as long as s is sufficiently small. We should also point out that in those cases of small s the agreement is also satisfactory with the corresponding results for the  $P_{nl}$  values obtained with the more laborious numerical

solution of the Schrödinger eigenvalue problem and the further numerical integration of the two integrals involved.

It is clear, since  $s = \left(\frac{\hbar^2}{2\mu V_0 R^2}\right)^{1/2}$ , that small values of *s* imply deep (large  $V_0$ ) and wide (large *R*) potential wells. An interesting physical system corresponding to the situation of a wide well, (for which certain energy eigenvalues are known experimentally) is a rather heavy  $\Lambda$ -hypernucleus. The self-consistent field felt by the  $\Lambda$ -particle in the hypernucleus is very complicated, but suitable single-particle potentials can be used often very satisfactorily. Two-parameter central potentials of the type used here may be considered as possible candidates for a rough representation of a more realistic single-particle potential. These potentials are in their turn, more realistic than the well-known harmonic oscillator potential, which because of its considerable analytic advantages has been very popular in nuclear physics problems for purposes of rough estimates. The use of the HVT technique has shown that potentials of the class considered can be useful in a number of cases for these purposes [21, 22]. To guarantee rather small values of *s* one should consider, however, hypernuclei with fairly large mass numbers.

In conclusion, this paper shows that the HVT technique provides for sufficiently small values of *s*, a rather simple and handy way to estimate the dimensionless product  $P_{nl}$  for any (deeply) bound eigenstate of a wide class of central single particle Hamiltonians, treating them in a unified way.

#### Acknowledgments

The authors would like to thank Professor S Massen and Dr K Ypsilantis for useful technical advice and assistance. One of the authors (KJO) is grateful to the Aristotle University of Thessaloniki for a scholarship which made possible for him a short term visit to the School of Physics of this University.

# Appendix. The semi-analytic expression for $P_{n0}$ in the case of the (reduced) Poeschl–Teller potential

The (reduced) PT central potential has the advantage that its energy-eigenvalues and eigenfunctions can be given analytically not only for the ground-single particle state but also for any bound single particle s-state [22–24, 4].

The energy eigenvalues  $E_{n0}$  are given in terms of the dimensionless parameter *s* by the very simple expression

$$E_{n0} = -V_0 \left\{ s \left[ 2n + \frac{3}{2} - \sqrt{s^{-2} + 4^{-1}} \right] \right\}^2 \qquad n = 0, 1, 2, \dots$$
(36)

Application of the Hellmann–Feynman theorem leads to an analytic expression of the expectation value of the kinetic energy operator  $\langle \hat{T} \rangle_{n0}$  from which the expectation value of the square of the momentum follows. The result is

$$\langle p^2 \rangle_{n0} = \frac{\hbar^2}{R^2} A_{n0}(s)$$
 (37)

where

$$A_{n0}(s) = \left\{ -\left(2n + \frac{3}{2}\right)s^{-2}(s^{-2} + 4^{-1})^{-1/2} + s^{-2} - \left[\left(2n + \frac{3}{2}\right) - (s^{-2} + 4^{-1})^{-1/2}\right]^2 \right\}.$$
 (38)

The corresponding normalized eigenfunctions are given in terms of the hypergeometric function  $_2F_1$ , by the formula

$$\Psi_{n0}(r) = \left[2^{3} \frac{\Gamma(n+3/2)\Gamma(2\lambda-n+1/2)(2\lambda-2n-1)}{R\Gamma(n+1)\Gamma(2\lambda-n)}\right]^{1/2} \left(\operatorname{ch}\frac{r}{R}\right)^{-2\lambda} \operatorname{sh}\frac{r}{R} \times {}_{2}F_{1}\left(-n,n-2\lambda+1;\frac{3}{2};-\operatorname{sh}^{2}\frac{r}{R}\right)$$
(39)

where  $\lambda = \frac{1}{2} \left[ \sqrt{s^{-2} + 4^{-1}} - \frac{1}{2} \right]$ , and hence  $s^2 = \frac{1}{2\lambda(2\lambda+1)}$ . For the mean square radius of the particle-orbit we have

$$\langle r^2 \rangle_{n0} = \frac{C_{n0}^2(s)}{R} \int_0^\infty r^2 \operatorname{ch}^{-4\lambda} \frac{r}{R} \operatorname{sh}^2 \frac{r}{R^2} F_1^2 \left( -n, n-2\lambda+1; \frac{3}{2}; -\operatorname{sh}^2 \frac{r}{R} \right) \mathrm{d}r \tag{40}$$

where

$$C_{n0}^{2}(s) = \left[\frac{2^{3}\Gamma(n+3/2)\Gamma(2\lambda-n+1/2)(2\lambda-2n-1)}{\pi\Gamma(n+1)\Gamma(2\lambda-n)}\right].$$
(41)

By making the transformation x = r/R we get for  $\langle r^2 \rangle_{n0}$ 

$$\langle r^2 \rangle_{n0} = C_{n0}^2(s) R^2 I_{n0}(s) \tag{42}$$

where the one-dimensional integral  $I_{n0}(s)$  is given by

$$I_{n0}(s) = \int_0^\infty x^2 \operatorname{ch}^{-4\lambda} x \operatorname{sh}^2 x_2 F_1^2 \left( -n, n - 2\lambda + 1; \frac{3}{2}; -\operatorname{sh}^2 x \right) \mathrm{d}x.$$
(43)

Multiplying (37) with (42) we obtain the final result for the dimensionless product  $P_{n0}$  in the case of the PT potential

$$P_{n0}^{\text{PT}}(s) \equiv \langle r^2 \rangle_{n0} \langle p^2 \rangle_{n0} / \hbar^2 = C_{n0}^2(s) I_{n0}(s) A_{n0}(s).$$
(44)

This is a semi-analytic expression for  $P_{n0}(s)$ , since the integral  $I_{n0}(s)$  has to be computed numerically by using an appropriate subroutine.

The above expression (44) was used for the semi-analytic results shown in figures 1 and 2.

# References

- [1] Hirschfelder J O 1960 J. Chem. Phys. 33 1462
  McRae S M and Vrscay E R 1992 J. Math. Phys. 33 3004
  Fernandez F M and Castro E A 1987 Hypervirial Theorems (Lecture Notes in Chemistry vol 43) (Berlin: Springer)
- Killingbeck J 1978 Phys. Lett. A 65 87
   Killingbeck J 1983 Microcomputer Quantum Mechanics (Bristol: Hilger) chapter 9 and references therein
- [3] Grant M and Lai C S 1979 *Phys. Rev.* A 20 718
   Lai C S 1981 *Phys. Rev.* A 23 455
   Lai C S and Lin H E 1982 *J. Phys. A: Math. Gen.* 15 1495
- [4] Liolios Th E and Grypeos M E 1997 Int. J. Theor. Phys. 2051
   Liolios Th E 1997 Comput. Phys. Commun. 105 254
   Liolios Th E 1997 PhD Thesis University of Thessaloniki
- [5] Grypeos M E and Liolios Th 1999 Phys. Lett. A 252 125
- [6] Swenson R J and Danforth S H 1972 J. Chem. Phys. 57 1734
- [7] Feynman R P 1930 *Phys. Rev.* 56 340 Hellmann H 1937 *Einfuhrung in die Quantenchemie* (Vienna: Deuticke)
  [8] Grypeos M E, Koutroulos C G and Petridou Th A 2002 *J. Phys. A: Math. Gen.* 35 2223
- [9] Lombard R J, Marcos S and Mares J 1994 *Phys. Rev.* C **50** 2900
- [10] Thirring W 1979 A Course in Mathematical Physics 3. Quantum Mechanics of Atoms and Molecules (New York: Springer)
  - Wokky A M 1974 Am. J. Phys. 42 760
- [11] Bertlmann R A and Martin A 1980 Nucl. Phys. B 168 111

7906

- [12] Heisenberg W 1927 Z. Phys. 43 172
- [13] Hall M J W 2001 Phys. Rev. A 64 052103 and references therein
- [14] Dodonov V V and Man'ko V I 1989 Generalization of the uncertainty relations in quantum mechanics *Proc. Lebedev Science Institute* vol 183 (New York: Nova Science) Nieto M M 1979 *Phys. Rev.* A 20 700
- [15] Messiah A 1972 Quantum Mechanics vol 1 (Amsterdam: North-Holland) Constantinesku F and Magyari E 1971 Problems in Quantum Mechanics (Oxford: Pergamon)
- [16] Durand E 1970 Mechanique Quantique vol 1 (Paris: Masson) Hornyak W F 1975 Nuclear Structure (New York: Academic)
- [17] Levy A 1969 C.R. Acad. Sci., Paris 269 227
- [18] Killingbeck J 1981 J. Phys. A: Math. Gen. 14 1005 Killingbeck J 1987 J. Phys. A: Math. Gen. 20 601
- [19] Witwit M R M 1991 J. Phys. A: Math. Gen. 24 3041 Witwit M R M 1991 J. Phys. A: Math. Gen. 24 3053 Witwit M R M 1991 J. Phys. A: Math. Gen. 24 4535
- [20] Killingbeck J and Jolicard G 1998 Chem. Phys. Lett. 284 359
   Killingbeck J, Grosjean A and Zucconi J M 1999 Phys. Lett. A 261 169
   Killingbeck J, Grosjean A and Jolicard G 2001 J. Phys. A: Math. Gen. 34 8309
- [21] Liolios Th E 1999 Eur. Lett. 49 329
- [22] Grypeos M E, Koutroulos C G and Petridou Th A 2001 Int. J. Mod. Phys. E 10 393
- [23] Bessis N, Bessis G and Joulakian B 1982 J. Phys. A: Math. Gen. 15 3679
- [24] Lalazissis G 1989 PhD Thesis University of Thessaloniki Lalazissis G 1993 Phys. Rev. C 48 198