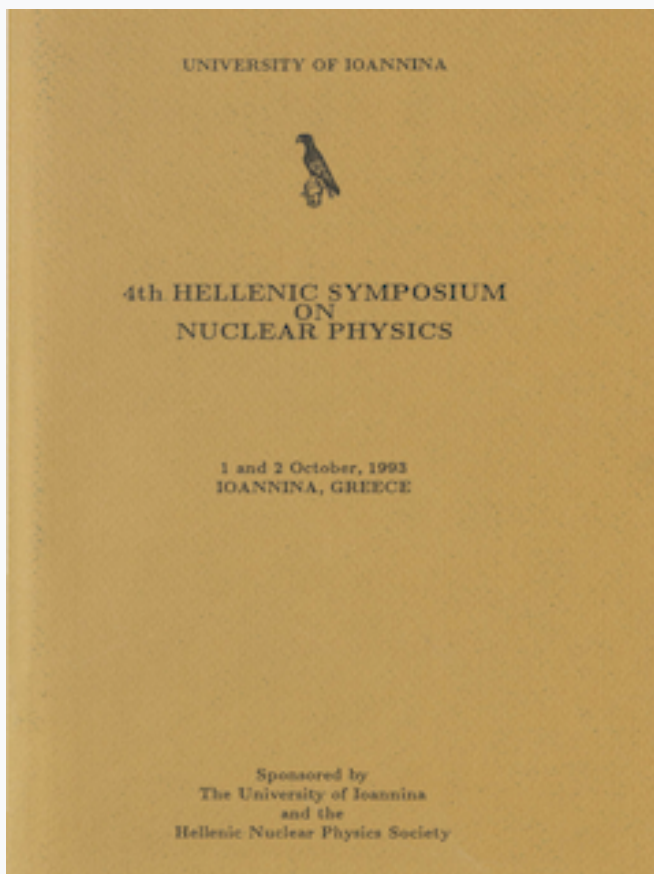


Annual Symposium of the Hellenic Nuclear Physics Society

Τόμ. 4 (1993)

HNPS1993



Application of the hypervirial theorem scheme to the potential $-D/\cosh^2(r/R)$

T. Liolios, M. Grypeos

doi: [10.12681/hnps.2874](https://doi.org/10.12681/hnps.2874)

Βιβλιογραφική αναφορά:

Liolios, T., & Grypeos, M. (2020). Application of the hypervirial theorem scheme to the potential $-D/\cosh^2(r/R)$. *Annual Symposium of the Hellenic Nuclear Physics Society*, 4, 51–58. <https://doi.org/10.12681/hnps.2874>

**APPLICATION OF THE HYPERVIRIAL-THEOREMS
SCHEME TO THE POTENTIAL $\frac{-D}{\cosh^2(\frac{r}{R})}$**

Theodore Liolios, Michael Grypeos
Theoretical Physics Department
Aristotle University of Thessaloniki
GR-54006 Thessaloniki, Greece

Abstract

The well known potential $-D\cosh^{-2}(\frac{r}{R})$ is studied with the aim of obtaining approximate analytic expressions mainly for the energies of the excited states with $l \neq 0$. Use is made of the Hypervirial Theorems (HVT) in conjunction with the Hellmann-Feynman Theorem (HFT) which provide a very powerful scheme especially for the treatment of 'Oscillator-like' potentials, as previous studies have shown. The energy eigenvalues are calculated in the form of an expansion, the first terms of which, in many cases, yield very satisfactory results.

1. Introduction

Various approaches can be employed in an effort to obtain the energy eigenvalues of the Schroedinger eigenvalue problem for a certain potential. Unfortunately the majority entails cumbersome calculations of matrix elements or the ingenious deduction of a trial function. The previous obstacles can be overcome by using the Hypervirial Theorems, ref[1,2], in conjunction with the Hellmann-Feynman Theorem, ref[3]. This (HVT-HFT) method could have been labeled as classical, had it not been for the peculiarities of the potential we select each time. Consequently, this method constitutes a very handsome alternative to a pure perturbational or variational treatment. A multitude of authors has applied variations of this very method to a good number of potentials Ref[3-10] and references therein. The results vary each

time, according to the susceptibility of the potential in question. The scheme makes use of a small parameter λ , which enables one to expand the potential as well as the energy and the moments in an appropriate λ -series. We traditionally adopt the first non trivial term of our expanded potential as the unperturbed term of our problem. The energy of the unperturbed Schroedinger equation serves as a quantity by means of which the other energy terms are calculated.

The content of this contribution is a preliminary part of a work related to the application of the Hypervirial Theorems. In the next section the relevant formalism is reviewed, see ref[9,10], while in section 3, that formalism is applied to the potential $\frac{-D}{\cosh^2(\frac{r}{R})}$. In the final section numerical results are given and discussed.

2. Description of the (HVT-HFT) scheme.

We consider a potential $V(r)$ which can be written in the form

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

where $V_0 = \omega^2 > 0$. The radial Schroedinger equation, for $u_{nl} = r R_{nl}(r)$ then reads:

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

Note that

$$\tilde{E}_{nl} = E_{nl} + D \quad (3)$$

Setting

$$\tilde{V}(r) = \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2} + \sum_{k=0}^{\infty} V_k \lambda^k r^{2k+2} \quad (4)$$

the Hamiltonian operator becomes

$$\tilde{H} = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \tilde{V}(r) \quad (5)$$

As a result, the radial Schroedinger equation can now be written as:

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \tilde{V}(r) \right] u_{nl} = \tilde{E}_{nl} u_{nl} \quad (6)$$

The Hamiltonian \tilde{H} is now identical to the one used by Swenson and Danford ref[3], which means that use can be made of the Hypervirial relation that they obtained. Namely:

$$\tilde{E}_{nl} \langle r^N \rangle = \frac{1}{2}(N+1)^{-1} \langle r^{N+1} \frac{d\tilde{V}}{dr} \rangle + \langle r^N \tilde{V} \rangle - \frac{\hbar^2}{8\mu} N(N-1) \langle r^{N-2} \rangle \quad (7)$$

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

$$\tilde{E}_{nl} = \sum_{k=0}^{\infty} E^{(k)} \lambda^k \quad (8)$$

$$\langle r^N \rangle = \sum_{k=0}^{\infty} C_N^{(k)} \lambda^k \quad (9)$$

According to the above definitions the unperturbed term of our potential is

$$\tilde{V}_0(r) = \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2} + \omega^2 r^2 \quad (10)$$

and the corresponding energy eigenvalue is

$$E^{(0)} = 2\omega a \sqrt{\frac{\hbar^2}{2\mu}} \quad (11)$$

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

$$j = 2n + l + 1 \quad (12)$$

$$a = j + \frac{1}{2} \quad (13)$$

where

$n = 0, 1, 2, 3, \dots$ (principal quantum number)

$l = 0, 1, 2, 3, \dots$ (orbital angular momentum quantum number)
 Applying the Hellmann-Feynman theorem (HFT) to our Hamiltonian
 we get:

$$\frac{\partial \tilde{E}_{nl}}{\partial \lambda} = \left\langle \frac{\partial \tilde{H}}{\partial \lambda} \right\rangle \quad (14)$$

After some algebra one obtains:

$$E^{(k)} = \frac{1}{k} \sum_{m=0}^k m V_k C_{2m+2}^{(k-m)} \quad (15)$$

Substituting (8) and (9) into (7) we get the familiar recurrence relation:

$$C_{N+2}^{(k)} = \frac{N+1}{(N+2)\omega^2} \left\{ \sum_{q=0}^k E^{(q)} C_N^{(k-q)} - \left[\frac{Nl(l+1)}{N+1} - \frac{N(N-1)}{4} \right] \frac{\hbar^2}{2\mu} C_{N-2}^{(k)} - \right. \\ \left. - \frac{N+3}{N+3} V_1 C_{N+4}^{(k-1)} - \frac{N+4}{N+1} V_2 C_{N+6}^{(k-2)} - \dots - \frac{N+k+2}{N+1} V_k C_{N+k+2}^{(0)} \right\} \quad (16)$$

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

The recurrence relation (16) is used to evaluate the coefficients $E^{(k)}$ used by (8). In fact what we need to do is evaluate the coefficients $C_N^{(k)}$ used by (15) and (16). We perform this calculation in a hierarchical manner (ref. [8]) i.e.:

To obtain $E^{(1)}$ in (8) we resort to (15) which readily yields

$$E^{(1)} = V_1 C_4^{(0)} \quad (17)$$

We still need to calculate the $C_4^{(0)}$ coefficient which will be extracted from (16). Indeed, (16) gives

$$C_4^{(0)} = E^{(0)} C_2^{(0)} \quad (18)$$

To calculate $C_2^{(0)}$ we need to resort to (16) once more so that we get

$$C_2^{(0)} = \frac{E^{(0)}}{2\omega^2} \quad (19)$$

Eventually $E^{(1)}$ can be obtained by virtue of (17), (18) and (19).

The same pattern of calculations is adhered to, for each coefficient (either $E^{(k)}$ or $C_N^{(k)}$)

3. Application of the (HVT-HFT) scheme to the potential: $\frac{-D}{\cosh^2(\frac{r}{R})}$

A well known member of the family (1) is the potential given by the formula:

$$V(r) = \frac{-D}{\cosh^2(\frac{r}{R})} \quad (20)$$

where D is the potential depth, and R its radius. R is the distance from the origin at which the value of the potential becomes: $V(R) = -0.4199D$.

This potential has been used, in ref[11], as a convenient simple approximation of the self-consistent Λ -nucleus potential (for the ground or the low lying excited states in relatively light hypernuclei). In that case, the radius R may be simply expressed in terms of the mass number of the core nucleus $A_c = A - 1$, by means of the relation

$$R = r_0 A_c^{\frac{1}{3}}. \quad (21)$$

In the present case, we choose as parameter λ the following:

$$\lambda = \frac{1}{R^2} < 1 \quad (22)$$

By expanding our potential in the form (1), we obtain the following coefficients:

$$V_0 = \omega^2 \quad (23a)$$

$$V_1 = -\frac{2}{3}\omega^2 \quad (23b)$$

$$V_2 = \frac{17}{45}\omega^2 \quad (23c)$$

$$V_3 = -\frac{62}{315}\omega^2 \quad (23d)$$

$$V_4 = \frac{1328}{14175}\omega^2 \quad (23e)$$

$$V_5 = -\frac{21844}{467775}\omega^2 \quad (23f)$$

where $\omega^2 = \lambda D$

According to the previous analysis we have the following terms for the energy series (setting $b = \frac{\hbar^2}{2\mu}$):

$$E^{(0)} = 2wa\sqrt{b} \quad (24a)$$

$$E^{(1)} = -\frac{1}{12} [12a^2 - 4l(l+1) + 3] b \quad (24b)$$

$$E^{(2)} = \frac{a}{60\omega} [15 - 4l(l+1)] b^{\frac{3}{2}} \quad (24c)$$

$$E^{(3)} = -\frac{4}{945\omega^2} l(l+1) [12a^2 - 4l(l+1) + 3] b^2 \quad (24d)$$

$$E^{(4)} = -\frac{a}{907200\omega^3} \left\{ 33280a^2l(l+1) - 12816 [l(l+1)]^2 + \right. \\ \left. + 25 [440l(l+1) + 567] \right\} b^{\frac{5}{2}} \quad (24e)$$

$$E^{(5)} = -\frac{1}{1247400\omega^4} l(l+1) \left\{ 32720a^4 + 8a^2 [1445 - 828l(l+1)] + \right. \\ \left. + [3 - 4l(l+1)] [1084l(l+1) - 2445] \right\} b^3 \quad (24f)$$

A rather interesting feature of this potential is that in the case of the s-states, the energy series may be summed up leading to the following closed form:

$$E_{n0} = -\frac{\hbar^2}{2\mu R^2} \left[\frac{1}{2} \sqrt{\frac{8\mu D R^2}{\hbar^2} + 1} - (2n+1) - \frac{1}{2} \right]^2 \quad (25)$$

$$n = 0, 1, 2, \dots$$

This expression coincides, as expected, with the well known expression, refs[11,12], of the s-state energy eigenvalues for this potential, which is obtained by direct solution, in the usual way, of the corresponding Schroedinger eigenvalue problem. The exact analytic expression for the s-states appears to be quite useful because it offers in this case a way of checking safely both, the accuracy of

the numerical solution and also the adequacy of the first terms in the series of the energy eigenvalues obtained through the technique of the Hypervirial Theorems

4. Numerical results and comments

In this section we give numerical results for a number of energy eigenvalues, by using for the potential parameters the values ($r_0 = 0.986$, $D = 38.9$), which correspond to the Λ -nucleus potential, and were determined by a least squares fitting procedure to experimental $1s$ -state eigenvalues in ref[11]. The results are displayed in the table that follows by using the notation:

A_c : the mass number of the host nucleus

E_{hvt} : the energy value obtained through the (HVT-HFT) scheme using the terms given in the table.

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

E_p : the energy value from a perturbation method ref[11c]

E_{int} : the energy value obtained through numerical integration.

1. NUMERICAL RESULTS FOR THE ENERGY EIGENVALUES (see text)												
A_c	n	l	$E^{(0)} - D$	$E^{(1)}\lambda$	$E^{(2)}\lambda^2$	$E^{(3)}\lambda^3$	$E^{(4)}\lambda^4$	$E^{(5)}\lambda^5$	E_{hvt}	E_{an}	E_p	E_{int}
6	0	0	8.84	-16.27	0.99	0	-0.01	0	-6.44	-6.44	-6.44	-6.44
9	0	0	1.64	-11.73	0.61	0	-0.004	0	-9.48	-9.48	-9.48	-9.48
11	0	0	1.64	-10.05	0.48	0	-0.003	0	-10.95	-10.95	-10.95	-10.95
15	0	0	-5.50	-7.96	0.34	0	-0.001	0	-13.13	-13.13	-13.13	-13.13
15	0	1	16.75	-18.57	0.26	-0.15	-0.081	-0.043	-1.84		-1.81	-1.91
31	0	0	-13.18	-4.72	0.15	0	0.0001	0	-17.75	-17.75	-17.75	-17.75
31	0	1	3.95	-11.01	0.14	-0.05	-0.02	-0.009	-7.02		-7.01	-7.03
80	0	0	-20.36	-2.45	0.05	0	0.00005	0	-22.76	-22.76	-22.76	-22.76
80	0	1	-8.01	-5.72	0.04	-0.01	-0.004	-0.001	-13.70		-13.70	-13.71
80	0	2	4.34	-10.30	-0.08	-0.07	-0.03	-0.013	-6.16		-6.14	-6.17
80	1	0	4.34	-12.26	0.13	0	0.0004	0	-7.78	-7.78		-7.78
80	1	1	16.69	-19.45	0.08	-0.049	-0.025	-0.013	-2.76			-2.78
120	0	0	-22.74	-1.86	0.038	0	-0.0004	0	-24.57	-24.57	-24.57	-24.57
120	0	1	-11.98	-4.34	0.03	-0.008	-0.002	-0.0005	-16.30		-16.30	-16.31
120	0	2	-1.21	-7.82	-0.054	-0.045	-0.015	-0.005	-9.159		-9.14	-9.16
120	0	3	9.55	-12.29	-0.255	-0.143	-0.062	-0.03	-3.22		-3.19	-3.27
120	1	0	-1.21	-9.31	0.090	0	-0.0001	0	-10.43	-10.43		-10.44
120	1	1	9.55	-14.77	0.05	-0.028	-0.013	-0.005	-5.218			-5.22

The energy series obtained through the present scheme is provided on a term-by-term basis, so that the accuracy, for various hypernuclei, can be observed. Apparently, the first few terms of the HVT-series for the s -state energies, in the whole range of A_c values studied, practically coincide with the ones given by the analytic exact expression. Moreover, for relatively heavy hypernuclei, the energy of the lower excited states is also very satisfactory as one can readily observe by comparing the HVT-energy with the one obtained through numerical integration. From the same table it is also observed that the agreement between E_{hvt} and E_{int} is somehow less satisfactory for the excited states when the absolute value of the energy is rather small.

References

- [1] Hirschfelder J.D 1960 J.Chem.Phys.33,1462
- [2] F.M.Fernandez,E.A.Castro Hypervirial Theorems (Springer-Verlag) (1987) M.S.Rae,E.R.Vrscay(1992),J.Math.Phys.33,9
- [3] Swenson R.J and Danforth S.H(1972) J.Chem.Phys.57,1734
- [4] J.Killingbeck (1978) Phys.Letters 65A,87
- [5] M.Grant C.S.Lai(1979) Phys.Rev.A20, 718
- [6] Lai C.S (1983) J.Phys.A:Math.Gen.16, L181-L185
- [7] Lai C.S (1981) Phys.Rev.A,23,455
- [8] Lai C.S (1982) Phys.Rev.A26,2245
- [9] Lai C.S and Lin H.E (1982) J.Phys.A:Math.Gen.15,1495
- [10] Witwit M.R.M(1991) J.Phys.A:Math.Gen.24,5291
- [11] a) G. A. Lalazissis, M. E. Grypeos, S. E. Massen (1988) Phys. Rev. C 37, 2098, b) G. A. Lalazissis, (1989) Ph.D thesis, Aristotle University of Thessaloniki, c) G.A.Lalazissis (preprint) (1992), accepted for publication in Phys. Rev. C
- [12] N Bessis,G Bessis and B Joulakian,(1982) J.PhysA:Math.Gen.15, 3679