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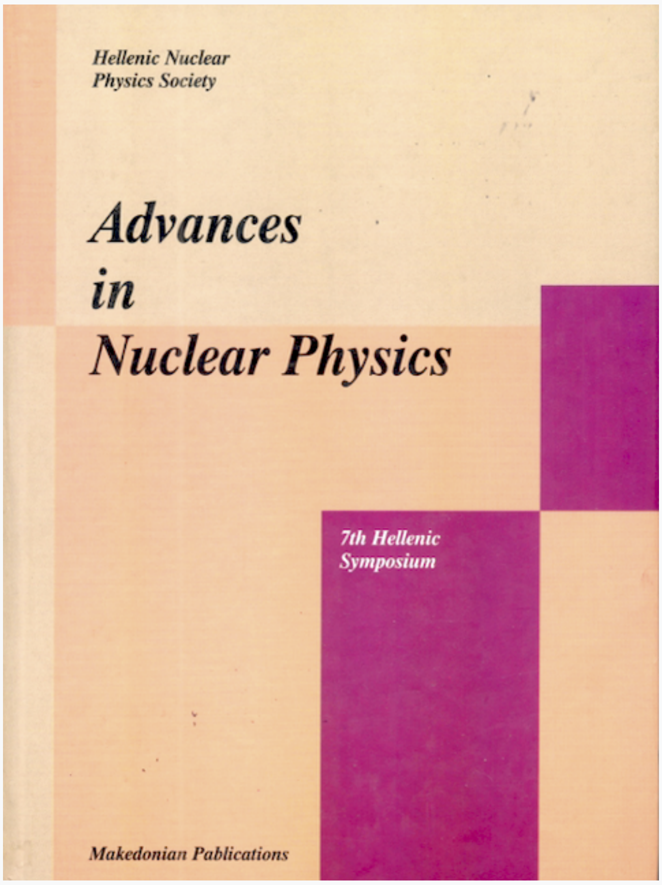

Approximate Determination of the ground-state Schroedinger Eigenfunction by Means of the Hypervirial Theorems Technique

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Approximate Determination of the ground-state Schroedinger Eigenfunction by Means of the Hypervirial Theorems Technique.

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Abstract

The method of the Hypervirial Theorems is used to obtain analytically the ground-state Schroedinger eigenfunction for a wide class of potentials in non-relativistic Quantum Mechanics.The whole scheme, despite its simplicity, yields in many cases a good approximation.

The method of the Hypervirial Theorems (HVT)[1 − 7] is a powerful technique of Perturbation Theory without eigenfunctions. The energy eigenvalues in non-relativistic Quantum Mechanics are obtained in the form of an expansion, the first terms of which are, in many cases, sufficient to achieve a reasonable approximation.

The question arises whether the same technique can be used to obtain the corresponding eigenfunctions in a fair approximation. Here we address this question for quite a general class of potentials of the form :

$$V(r) = -V_0 f(\frac{r}{R}) \qquad 0 \leq r < \infty \tag{1}$$

where $V_0 > 0$, $R > 0$.

The class of potentials we are interested in, is further specified by assuming that f is an even analytic function of $x = \frac{r}{R}$, with $\frac{d^2 f}{dx^2} |_{x=0} < 0$. Thus, such potentials behave like an harmonic oscillator potential near the origin.

It will be also assumed in this note that the function f tends to zero at large r.

Typical examples of that oscillator-like class of potentials is the Gaussian and the Poeschl-Teller-type potential $V(r) = -V_0 \cosh^{-2}\left(\frac{r}{R}\right)$. Another example is the potential of the form:

$$V(r) = -\frac{V_0}{1 + e^{\left(\frac{r}{R}\right)^2}} \tag{2}$$

There has been shown [7] that the application of the Hypervirial Theorems technique enables one to study the class of potentials (1) in quite a general way and obtain approximate expressions not only for the energy eigenvalues but also for other quantities of physical interest, such as the expectation values of the kinetic and the potential energy operators of a particle moving non-relativistically in such a potential and of the mean-square radius of its orbit in a given energy eigenstate. In the present study use is made of those results by considering , in the interest of simplicity, the ground-state of a particle ,of mass μ , moving in a potential of the above mentioned class.

In an effort to obtain an approximate ground-state eigenfunction for a potential belonging to the class specified at the beginning, using the above mentioned approximate expressions for E_{nl} and $< r^2 >_{nl}$(with $n = 0$ and $l = 0$),we proceed as follows:

We break up the desired eigenfunction into two parts :

$$u_{00}(r) = \begin{cases} u_{in}(r) & 0 < r < R_0 \\ u_{ex}(r) & R_0 < r < \infty \end{cases} \tag{3}$$

As long as R_0 is sufficiently large, the "external" wave function $u_{ex}(r)$ is:

$$u_{ex}(r) = Ce^{-kr} \tag{4}$$

where

$$k = \sqrt{\frac{2\mu}{\hbar^2}|E_{00}|} \tag{5}$$

On the other hand, the solution in the internal region, $u_{in}(r)$, can be approximated by the ground- state eigenfunction of an appropriately specified harmonic oscillator (HO):

$$u_{in}(r) = Nre^{-\frac{r^2}{2b^2}} \tag{6}$$

A plausible requirement, for the determination of the H.O. parameter b, is that the mean square radius (m.s.r) of the H.O. ground state orbit equals the corresponding one obtained through the HVT scheme:

$$< r^2 >_{00}^{HO} = < r^2 >_{00} \tag{7}$$

where the expectation values are calculated with respect to the ground state harmonic oscillator wave function and that of the given potential, respectively. Note that $< r^2 >_{00}$ (as well as E_{00}) is known approximately in terms of the potential parameters, through the formulae mentioned above.Therefore, the parameter b of the H.O. potential follows immediately from Eq(7):

$$b = \sqrt{\frac{2}{3} < r^2 >_{00}} \tag{8}$$

The radius R_0 can be determined by the continuity condition of the wave function and its derivative:

$$u_{in}(R_0) = u_{ex}(R_0) \tag{9}$$

$$\left(\frac{du_{in}(r)}{dr}\right)_{R_0} = \left(\frac{du_{ex}(r)}{dr}\right)_{R_0} \tag{10}$$

These conditions yield the following equations:

$$NR_0 e^{-\frac{R_0^2}{2b^2}} = Ce^{-kR_0} \tag{11}$$

$$\left(1 - \frac{R_0^2}{b^2}\right) Ne^{-\frac{R_0^2}{2b^2}} = -Cke^{-kR_0} \tag{12}$$

By solving the above equations with respect to R_0 one obtains:

$$R_0 = \frac{1}{2}kb^2 \left[1 + \sqrt{1 + 4(kb)^{-2}}\right] \tag{13}$$

Since k and b are given in terms of the potential parameters, so is R_0.

Having determined R_0, $u_{ex}(r)$ follows readily, as from Eq(11) we have:

$$C = NR_0 e^{-\frac{R_0^2}{2b^2}} e^{kR_0} \tag{14}$$

Therefore:

$$u_{ex}(r) = NR_0 e^{-\frac{R_0^2}{2b^2}} e^{-k(r-R_0)} \tag{15}$$

Considering the unit-step function : $\theta(t) = \begin{cases} 0 & t \leq 0 \\ 1 & 0 < t \end{cases}$ the eigenfunction $u_{00}(r)$ can be written as :

$$u_{00}(r) = \widetilde{N}_{00} \left\{ [1 - \theta(r - R_0)] re^{-\frac{r^2}{2b^2}} + \theta(r - R_0) R_0 e^{-\frac{R_0^2}{2b^2}} e^{-k(r-R_0)} \right\} \tag{16}$$

$0 \leq r < \infty$

The constant $\widetilde{N_{00}}$ will be determined through the normalization condition:

$$\int_0^{\infty} u_{00}^2(r)\, dr = 1 \tag{17}$$

After some algebra one obtains:

$$\widetilde{N_{00}} = \left\{ \frac{\pi^{\frac{1}{2}} b^3}{4} - \frac{b^3}{2} \Gamma\left(\frac{3}{2}, \frac{R_0^2}{b^2}\right) + \frac{R_0^2}{2k} e^{-\frac{R_0^2}{b^2}} \right\}^{-\frac{1}{2}} \tag{18}$$

where use has been made of the incomplete Gamma function $\Gamma(q, x)$ (See e.g. ref [9]).

Owing to the fact that R_0 is, in many cases, sufficiently large, Eq(18) can be further simplified so that :

$$\widetilde{N_{00}} = 2b^{-\frac{3}{2}} \left\{ \pi^{\frac{1}{2}} - 2\frac{R_0}{b} e^{-\frac{R_0^2}{b^2}} \left[1 + \frac{1}{2}\left(\frac{b}{R_0}\right)^2 - R_0 \left(kb^2\right)^{-1} \right] \right\}^{-\frac{1}{2}} \tag{19}$$

In order to test the accuracy of the ground state wave function, which can be obtained in the described approximate way, we consider the Gaussian potential

$$V(r) = -V_0 e^{-\frac{r^2}{R^2}} \tag{20}$$

To be more specific and close to a problem of physical interest we considered such a potential as a first approximation to the self-consistent Λ-nucleus potential-as in certain other studies [10, 11]. Then the potenial radius R may be expressed in terms of the mass number of the core nucleus A_c (using the rigid-core model [12]) by means of the relation

$$R = r_0 A_c^{\frac{1}{3}} \tag{21}$$

where r_0 is a parameter which may be expressed in terms of the potential depth V_0 and the volume integral of the spin-averaged $\Lambda-$nucleon potential: $\left|\overline{V}_{\Lambda N}\right|$.

The existing two potential parameters, namely the potential depth V_0 and the radius parameter r_0 have been determined by least-squares fitting some known experimental values of the Λ-particle binding energy in hypernuclei and are the following [11]: $V_0 = 34,16 MeV$ $\quad r_0 = 1,199 fm$

Visualization of the results can be achieved by plotting the eigenfunctions obtained through the present method against those obtained by numerical integration One can easily observe that the heavier the hypernuclei the better the coincidence of the plots which validates the proposed approach for the analytic determination of the wave function, especially for heavy hypernuclei. This is clear from fig.1 and fig.2 in which the ground-state wave functions correspond to $A_c = 20$ and $A_c = 40$.

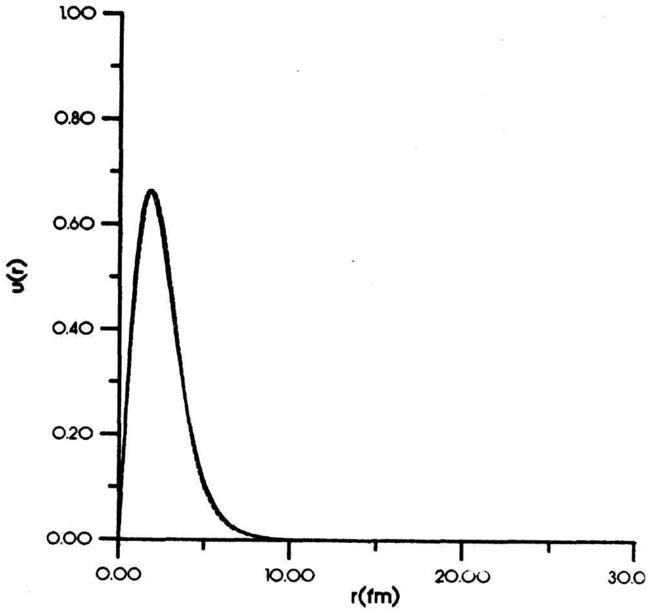

Fig.1 Plot of the analytic eigenfunction u_{00} (broken line) for $A_c = 20$ against the corresponding u_{num} (solid line) obtained through numerical integration of the Schroedinger equation

We further note that a measure of the quality of the achieved approximation is the value of the integral:

$$I_{00} = \int_0^\infty |u_{num}(r) - u_{00}(r)|^2 \, dr \tag{22}$$

where $u_{num}(r)$ is the corresponding normalized eigenfunction obtained through numerically integrating the Schroedinger equation .For various hypernuclei one obtains:

A_c	I_{00}
20	0,025
40	0,005
80	0,004

where Ac is the mass number of the core nucleus of the hypernucleus.

It is seen that the value of I_{00} decreases considerably with A_c so that the heavier the nuclei the better the approximation.

In conclusion, the present approach appears to provide a quite simple and efficient way of obtaining approximate analytic ground state wavefunctions for quite a wide class of potentials of physical interest, by using the results of the Hypervirial Theorems technique.

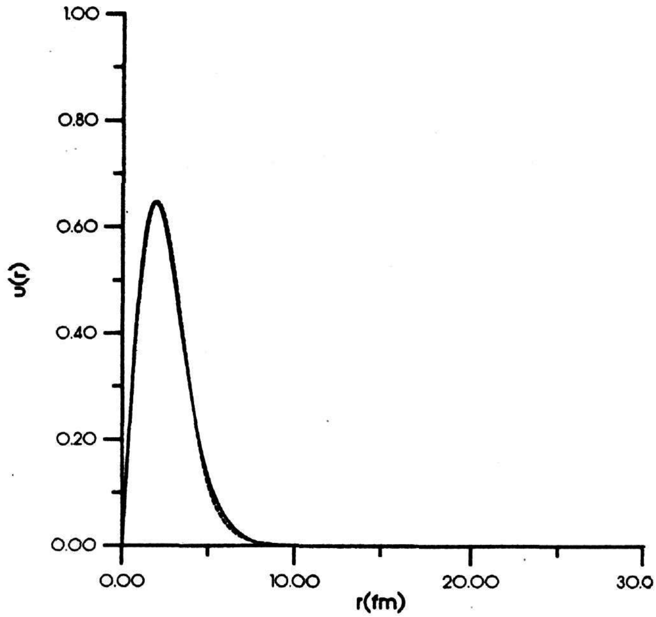

Fig.2 Plot of the analytic eigenfunction u_{00} (broken line) for $A_c = 40$ against the corresponding u_{num} (solid line) obtained through numerical integration of the Schroedinger equation

References

[1] J.O. Hirschfelder, J.Chem.Phys.33, (1960)1462

[2] (a) G.Marc and W.G. McMilllan, Adv.Chem.Phys.58, (1985)209; (b) F.M. Fernandez and E.A. Castro, Hypervirial Theorems, Lecture notes in Chemistry, Vol.43 (Springer-Verlag) (1987);(c) S.M. McRae and E.R. Vrscay, J.Math.Phys.33,(1992)3004

[3] R.J. Swenson and S.H. Danforth, J.Chem.Phys.57, (1972) 1734

[4] (a) J. Killingbeck, Phys.Lett.65A, (1978)87; (b) J. Killingbeck, J.Phys.A 18, (1985)L1925; (c) J. Killingbeck, J.Phys.A 18, (1985)245

[5] (a) C.S. Lai, J.Phys.A16, (1983)L181; b) C.S. Lai, Phys.Rev.A23, (1981)455; c) C.S. Lai,Phys.Rev.A 26, (1982)2245

[6] (a) M.R.M Witwit, J.Phys.A 24, (1991)5291; (b) M.R.M Witwit, J.Phys.A 24, (1991)4535; (c) M.R.M Witwit, J.Phys.A 24, (1991)3053

[7] T.E. Liolios and M.E. Grypeos "Advances in Nuclear Physics" (Proceedings of the 5th Hellenic Symposium of Nuclear Physics, Patras, Greece. p.104, ed.by C.Syros and C.Ronchi, European Commission (EUR 16302 EN) (1995)

[8] (a) H.Hellmann, Einfuhrung in die Quantenchemie (Deuticke, Vienna, 1937); (b) R.P.Feynman,Phys.Rev.56,(1939)340

[9] G.Arfken ,Mathematical methods for physicists, p471 (Academic Press) 1970

[10] R.Dalitz and B.Downs, Phys.Rev.111, (1958)967; b) R.Dalitz "Nuclear interactions of hyperons", Oxford University Press, London , (1965)

[11] G.A.Lalazissis, Phys. Rev. C 49, (1994)1412, and private communication

[12] A.Gal, "Advances in Nuclear Physiscs", (Plenum Press, New York-London), (1975)