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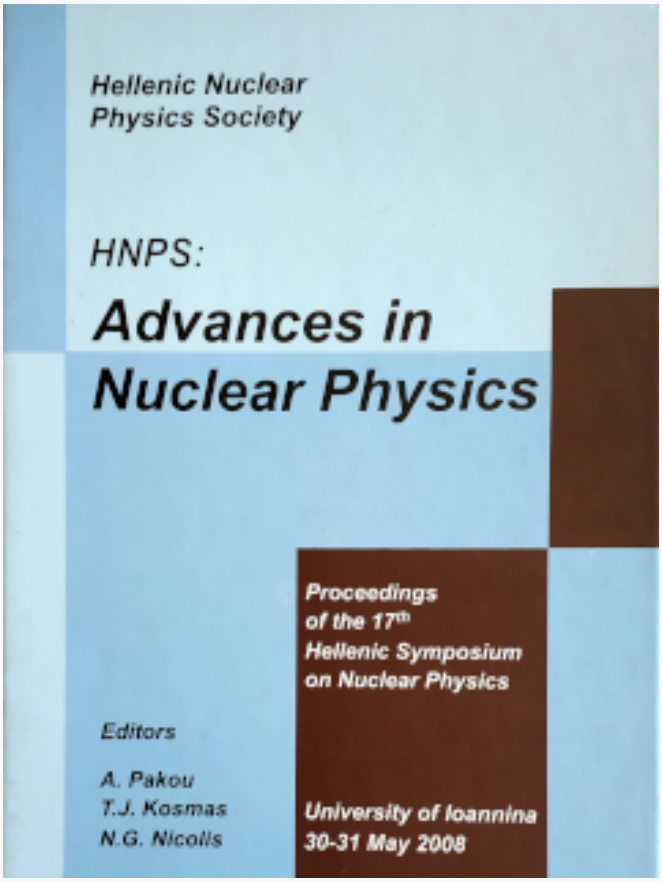

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A RENORMALIZED HVT APPROACH

FOR A CLASS OF CENTRAL POTENTIAL WELLS

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Abstract

An investigation is carried out to consider a renormalized HVT approach in the context of s- power series expansions for the energy eigenvalues of a particle moving non- relativistically in a central potential well belonging to the class $V(r)=-D\,f(r/R),\ D>0$ where f is an appropriate even function of $x=r/R$ and the dimensionless quantity $s=\left(\hbar^2/2\mu D R^2\right)^{1/2}$ is assumed to be sufficiently small. Previously, the more general class of central potentials of even power series in r is considered and the renormalized recurrence relations from which the expansions of the energy eigenvalues follow, are derived. The s- power series of the renormalized expansion are then given for the initial class of potentials up to third order in s (included) for each energy-level $E_{n\ell}$. It is shown that the renormalization parameter K enters the coefficients of the renormalized expansion through the state- dependent quantity $a_{n\ell}\,\chi^{1/2}=a_{n\ell}\left(1+K/\left(\left(-d_1\,D\right)/R^2\right)\right)^{1/2}, a_{n\ell}=\left(2n+\ell+3/2\right)$. The question of determining χ is discussed. Our first numerical results are also given and the utility of potentials of the class considered (to which belong the well- known Gaussian and reduced Poschl- Teller potentials) in the study of single–particle states of a Λ in hypernuclei is pointed out.

1 Introduction

The Quantum – Mechanical Hypervirial Theorem (HVT) approach has been since its introduction [1] a very useful technique in various branches of Physics and Chemistry [2,3], where Quantum Mechanics has been the basic theoretical tool. Its use in approximation methods is worth- mentioning. We note in particular its use in treating the motion of a particle in a given potential model. This method avoids the use of wave functions, thus resulting to considerable simplifications, when for example there is a small parameter involved in the problem in question.

It was realized, however, when expansions were obtained on the basis of the HVT technique, usually for the energy eigenvalues, that a suitable modification of the expansion may offer advantages and might be advisable to be pursuit. We mention in particular, in this direction, the use of reformulated expansions, the so-called "renormalized HVT " expansions (see references [4,5,6]).

The object of this contribution to the symposium is to report our first results concerning a renormalized expansion for the energy eigenvalues for a fairly wide class of potential wells. For potentials of that class, consideration of the standard HVT technique led to the so called s-power series expansions, an appropriate truncation of which can lead to simple approximate analytic expressions, easy to be used in practice, if we relax the need in obtaining highly accurate numerical results for which, however, more complicated numerical methods exist. The same is the scope of the present investigation. We may recall in connection to this matter that there are physical problems for which high accuracy is not needed since the experimental values are known with rather large errors.

In the following section 2, the more general class of the even power- series central potentials is considered and the recurrence relations are given from which the recurrence relations for the class of potentials more often used in practice follows. In section 3, the renormalized expansion for the energy eigenvalues $E_{n\ell}$ is given for the latter potentials and in the final section our first numerical results are displayed.

2 The renormalized recurrence relations for the class of even power series central potentials.

Let us consider first the more general class of the even power series central potentials, that is:

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

In this potential we introduce a renormalization parameter K by adding and subtracting the same harmonic oscillator potential $K r^2$, in a way analogous to that of ref [4] for the perturbed one- dimensional oscillator. Thus, potential (1) takes the form

$$V^R(r) = \left(-D + V_0^R \, r^2\right) + \left[\left(\sum_{k=1}^{\infty} V_k^R \, \lambda^k \, r^{2k+2} \right) - K r^2 \right] \tag{2}$$

where: $V_0^R = V_0 + K$, $V_k^R = V_k$ for $k = 1, 2, 3, \ldots$

The corresponding radial Schrödinger equation may be written in this case as follows, in analogy with the usual HVT:

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2} + \sum_{k=0}^{\infty} V_k^R \, \lambda^k \, r^{2k+2} - K r^2 \right] u_{n\ell}^R(r) = E'^R_{n\ell} \, u_{n\ell}^R(r) \tag{3}$$

where

$$E'^R_{n\ell} = E^R_{n\ell} + D \tag{4}$$

that is $E'^R_{n\ell}$ are the shifted energy eigenvalues .

In the case of the potential wells of next section, while $E'^{R}_{n\ell}$ are positive, $E^{R}_{n\ell}$ are measured from the bottom of the well $-D$.

The corresponding unperturbed Schrödinger eigenvalue problem which provides us with the zeroth–order energy eigenvalues $E'^{R(0)}_{n\ell}$ and the zeroth- order energy eigenfunctions $u^{R(0)}_{n\ell}(r)$ is obviously the following:

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}+V_0^R\, r^2 \right] u^{R(0)}_{n\ell}(r)= E'^{R(0)}_{n\ell}\, u^{R(0)}_{n\ell}(r) \tag{5}$$

Writing the following expansions for the energy eigenvalues $E'^{R}_{n\ell}$ and for the moments $\left\langle r^N \right\rangle^R_{n\ell}$

$$E'^{R}_{n\ell}=\sum_{k=0}^{\infty} E^{R(k)}\lambda^k \tag{6}$$

$$\left\langle r^N \right\rangle^R_{n\ell}=\sum_{p=0}^{\infty} C_N^{R(p)}\lambda^p \tag{7}$$

and using also the Hellmann-Feynmann theorem we end up, after a rather lengthy algebra with the following recurrence relations on the basis of which we can obtain the quantities of interest:

$$(N+2)V_0\, C^{R(k)}_{N+2}=\frac{\hbar^2}{2\mu}N\left[\frac{(N+1)(N-1)}{4}-\ell(\ell+1)\right]C^{R(k)}_{N-2}+(N+1)E^{R(0)}C^{R(k)}_{N}+$$

$$+\sum_{q=1}^{k}\left\{(N+1)E^{R(q)}C^{R(k-q)}_{N}-(N+q+2)V_q C^{R(k-q)}_{N+2q+2}\right\}$$

where:

$$C_0^{R(k)}=\delta_{k0} \text{ and } E^{R(q)}=\frac{1}{q}\sum_{m=1}^{q} m\, V_m C^{R(q-m)}_{2m+2}\ ,\ \begin{cases} k=0,1,2,3,... \\ q=1,2,3,... \\ m=1,2,3,... \end{cases}$$

3 The renormalized s-power series expansion of $E_{n\ell}$ for the class of potential wells considered

We use now the results of the previous section for a particle of mass μ moving non-relativistically in a central potential well belonging to the class of potentials of the following form:

$$V(r) = -D\, f(r/R) \tag{8}$$

where $D > 0$ is the potential depth, $R > 0$ its "radius" and f $(f(0) = 1)$ the potential form- factor which determines its shape and is assumed to be an appropriate analytic function of even powers of $x = r/R$ with $-d^2 f / dx^2 \big|_{x=0} > 0$, that is they behave like an harmonic oscillator near the origin. Typical examples are the (reduced) Poeschl-Teller and the Gaussian potentials:

$$V(r) = -D \cosh^{-2}(r/R) \text{ and } V(r) = -D\, e^{-(r/R)^2} \tag{9}$$

In the case of potentials of class (8) after a lengthy algebra on the basis of expansions (6) and (7) and the recurrence relations at the end of the previous section, the expansion of the renormalized energy eigenvalue $E_{n\ell}$ can be obtained in terms of the (small) dimensionless parameter s:

$$s = \left(\hbar^2 / 2\mu D R^2\right)^{1/2} \tag{10}$$

so that we can write with a reasonable approximation:

$$\frac{E^R_{n\ell}}{D} = e^{R(0)}_{n\ell} + e^{R(1)}_{n\ell}\, s + e^{R(2)}_{n\ell}\, s^2 + e^{R(3)}_{n\ell}\, s^3 + O\left(s^4\right) \tag{11}$$

where

$$e^{R(0)}_{n\ell} = -1 \tag{12}$$

$$e^{R(1)}_{n\ell} = 2\,(-d_1)^{1/2}\, a_{n\ell}\, \chi^{1/2} \tag{13}$$

$$e^{R(2)}_{n\ell} = -\frac{d_2}{8|d_1|}\left[3 - 4\ell(\ell+1) + 12\, a^2_{n\ell}\, \chi\right] \tag{14}$$

$$e^{R(3)}_{n\ell} = \frac{a_{n\ell}\, \chi^{1/2}}{8|d_1|^{5/2}}\left\{\left(20 d_1 d_3 - 17 d_2^2\right) a^2_{n\ell}\, \chi + \left(25 d_1 d_3 - \frac{67}{4} d_2^2\right) - 3\ell(\ell+1)\left(4 d_1 d_3 - 3 d_2^2\right)\right\} \tag{15}$$

and $a_{n\ell} = (2n + \ell + 3/2)$. The renormalization parameter χ is related to the Killingbeck renormalization parameter K with the relation:

$$\chi = 1 + \frac{K}{\left(\dfrac{-d_1 D}{R^2}\right)}$$

and it is seen that this parameter enters formula (11) only in combination with the state - dependent number $a_{n\ell}$.
Finally, the numbers d_k are related to the derivatives of f and are defined as follows:

$$d_k = \frac{1}{(2k)!}\frac{d^{2k}}{dx^{2k}} f(x)\Big|_{x=0} \quad , k = 0,1,2,3...$$

It is seen that when $K = 0$ that is when $\chi = 1$, formula (11) becomes identical to the one in the HVT case [7,8,9]. Thus, depending on the value of χ formula (11) incorporates both the HVT and the RHVT results.

4 Preliminary numerical results.

In this final section we give some preliminary numerical results. We choose the (reduced) Poeschl-Teller potential which has certain additional analytic advantages and we give the energy eigenvalues E_{00}^{R}/D for certain small values of the dimensionless parameter s, namely for $s = 0.02, 0.04, 0.06, 0.08$ and 0.1. Obviously, the estimated eigenvalues depend on the assumed value of the renormalization parameter. It seems in this respect that the so called ''plateaux criterion'' of ref. [4,5], although it is desirable to be used, does not appear to be suitable in our case in which only a few terms of the expansion are taken into account, in view of the scope of our investigation, as mentioned in the introduction.
Thus, one has to try other possibilities. For purposes of a rather rough estimate we could choose the unperturbed (zeroth- order) potential to be an harmonic oscillator which passes through $r = 0$ and through $r = R$ $(\chi = 1)$. In this case the parameter χ is given by $\chi = 1 - f_{PT}(1) = 1 - 1/\cosh^2(1) = 0.580026$. A somehow more improved value is expected to be obtained if integral expressions are used in the spirit of reference [10]. If the above value of χ is used the values of table 1 are obtained which, however, are less satisfactory than the HVT $(\chi = 1)$ results (table 2), if they are compared with the exact analytic results.
In an effort of another attempt of determining χ (and therefore of the theoretical determination of the eigenvalue E_{00}) which in fact can be related to a problem of physical interest, namely to the ground state energies of a $\Lambda-$ particle in hypernuclei, we considered a number of them and we took χ, along D and r_0 (in the rigid core model expression $R = r_0 A_C^{1/3}$) as fitting parameters, using as far as possible, recent experimental results (see ref. [11,12] and refs therein) for the Λ binding energies. The best fit values found were $D = 40.00\ MeV$, $r_0 = 0.8802\ fm$ and $\chi = 0.92078$. The corresponding eigenvalues E_{00}^{R}/D for certain values of s (though very small) are displayed in table 3. If only the first two terms of the expansion are taken into account, the best fit values become $D = 35.19\ MeV$, $r_0 = 1.198\ fm$ and $\chi = 0.760$. The fit is fairly satisfactory , but it is considerably better when the best fit values are $D = 39.95\ MeV$, $r_0 = 0.9205\ fm$ and χ is determined on the basis of an HVT

expression $\chi=\left(1-\frac{5}{6}s+\frac{1}{8}s^2\right)^2$.The problem of determining χ is still (August 2008) under further investigation.

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Table 1 $(\chi=0.580026)$

s	$e_{00}^{R(0)}$	$e_{00}^{R(1)}s$	$e_{00}^{R(2)}s^2$	$e_{00}^{R(3)}s^3$	E_{00}^R/D
0.02	-1.000000	0.045696	-0.000622	0.000002	-0.954924
0.04	-1.000000	0.091391	-0.002488	0.000018	-0.911078
0.06	-1.000000	0.137087	-0.005598	0.000062	-0.868449
0.08	-1.000000	0.182783	-0.009952	0.000146	-0.827023
0.10	-1.000000	0.228478	-0.015550	0.000286	-0.786786

Table 2 $(\chi=1)$

s	$e_{00}^{R(0)}$	$e_{00}^{R(1)}s$	$e_{00}^{R(2)}s^2$	$e_{00}^{R(3)}s^3$	E_{00}^R/D
0.02	-1.000000	0.060000	-0.001000	0.000003	-0.940997
0.04	-1.000000	0.120000	-0.004000	0.000024	-0.883976
0.06	-1.000000	0.180000	-0.009000	0.000081	-0.828919
0.08	-1.000000	0.240000	-0.016000	0.000192	-0.775508
0.10	-1.000000	0.300000	-0.025000	0.000375	-0.724625

Table 3 $(\chi=0.92078)$

s	$e_{00}^{R(0)}$	$e_{00}^{R(1)}s$	$e_{00}^{R(2)}s^2$	$e_{00}^{R(3)}s^3$	E_{00}^R/D
0.02	-1.000000	0.057575	-0.000929	0.000003	-0.943351
0.04	-1.000000	0.115150	-0.003715	0.000023	-0.888542
0.06	-1.000000	0.172725	-0.008358	0.000078	-0.835556
0.08	-1.000000	0.230300	-0.014860	0.000184	-0.784375
0.10	-1.000000	0.287875	-0.023218	0.000360	-0.734983

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