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Eigenvalues Obtained by Perturbation and Exact Methods for Short and Long Range Potentials II

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ABSTRACT. Three Potentials, one long range, Kratzer and two short range, Hulthén and Pöschl-Teller, were used to investigate the range of validity of the perturbation method developed by Müller-Kiresten.

Eigenvalues obtained exactly for these potentials are compared with those obtained by perturbation methods. These results are discussed in the conclusion.

1. Introduction

In a previous paper (refered to as I) (Abdulmomen *et al.* 1983) we investigated the validity of the perturbation method developed over the years by Müller and Schilcher (1968) and (1970), to calculate eigenvalues and eigenfunctions for variety of potentials. The three potentials we had already investigated, the Yukawa, the Gauss and the exponential had their wide applications in atomic, molecular, nuclear and particle physics. Our previous investigation had shown (Table 6 of I) that for the case of the exactly solvable potential (the exponential) the eigenvalues obtained by perturbation method are quite different from those eigenvalues obtained from exact calculations.

To clarify this and other points and to extend the investigation to a wide range of potentials, we have chosen three more exactly solvable potentials with wide physical and intrinsic interests. These potentials are: the Kratzer, eq. (2), the modified Pöschl-Teller, eq. (3) and the Hulthén, eq. (4). These potentials when

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put in the radial Schrodinger equation give exact S-wave eigenfuntions and eigenvalues. We note that the Kratzer potential is a long range and has a singularity like the centrifugal term (r^{-2}), at the origin. The Hulthén Potential has a singularity like the Coulomb term (r^{-1}) while the Pöschl-Teller is regular at the origin. The latter potential has wide applications in the physics of many body problems, where it represents a mean field of the interaction with a $\delta-$function two body force (Calogero 1975). Furthermore, the Pöschl-Teller potential represents the non-relativistic limit of the sine– Gordon equation (Zamolodchikov and Zamolodchikov 1979). The Schrodinger equation with these three potentials are discussed by Flügge (1974).

The bound and scattering states of the Pöschl-Teller potential can also be shown to be connected with unitary representation of some group (Alhassid *et al.* 1983). We give the general perturbation calculational method for the eigenvalues for these potentials in section 2. Section 3 contains the exact solutions for the Schrodinger equation with these potentials along with expressions for their eigenvalues. In section 4 we discuss our results.

2. Energy Eignevalues by Assymptotic Expansion

We start with the radial Schrodinger equation:

$$\frac{d^2\psi(r)}{dr^2} + \frac{2\mu}{\hbar^2}(E - \frac{\hbar^2\ell\,(\ell+1)}{r^2} - V(r))\,\psi(r) = 0 \tag{1}$$

(We set $\hbar = c = 2\mu = 1$) with the potentials

$$V(r) = -g^2\,(\frac{a}{r} - \frac{1}{2}\frac{a^2}{r^2}) \tag{2}$$

$$V(r) = -g^2\,\frac{\lambda\,(\lambda-1)}{\cosh^2 gr} \tag{3}$$

and

$$V(r) = -g^2\,\frac{e^{-r/a}}{1-e^{-r/a}} \tag{4}$$

We expand the potentials in power of the coupling constants g to obtain the sets of energy eigenvalues for each potential. We first obtain eigenvalues for eq. (1) with the expanded potentials. To do this we set:

$$\alpha = 2\mu E/\hbar^2, \quad \gamma = \ell(\ell+1) \equiv L^2 - \frac{1}{4} \tag{5}$$

and $r = e^Z$, while $\psi = e^{Z/2}\rho$

Equation (1) then assumes the form

$$\frac{d^2\rho}{dz^2} + (\alpha \cdot e^{2z} - L^2 - V(z)\, e^{2z})\, \rho(z) = 0 \tag{6}$$

or

$$\frac{d^2\rho}{dz^2} + [- L^2 + v(z)]\, \rho(z) = 0 \tag{7}$$

where $v(z) = e^{2z} (\alpha - V(z))$ (8)

The eigenvalue equation then reads:

$$\frac{1}{\hbar^2} \left(- L^2 - v(z_0) \right) = \frac{1}{2}\, q \tag{9}$$

where $q = 2n + 1, \qquad n = 0, 1, 2, ---$

The value of $z = z_0$ is the position of the minimum of $V(z)$,

$$v' \ (z_0) = 0$$

and $h = [+ 2v''(z_0)]^{1/4}$ (10)

These are the main steps to obtain the energy eigenvalues for a large class of regular potentials.

The perturbative solutions for eq. (1), with the expansions obtained for eqs. (2) – (4) (s–wave only), are briefly given here.

We start by letting

$$V(r) = v(r) + v(r_0) \tag{11}$$

where $v(r_0)$ is the value of the potential at $r = r_0$

The expansion of $V(r)$ is

$$v(r) = v(r_0) + \sum_{i=2}^{\infty} \frac{(r-r_0)^i}{i\,!}\, v^{(i)}\, (r_0) \tag{12}$$

We set $h = + [2v''(r_0)]^{1/4}$ (13)

and $\omega = h\, (r-r_0)$ (14)

to have

$$\frac{d^2\rho(\omega)}{d^2\omega} + (\frac{E_n - v(r_0)}{h^2} - \frac{\omega^2}{4})\, \rho(\omega) = \sum_{i=3}^{\infty} \frac{v^{(i)}\,(r_0)\,\omega^2}{2v^{(2)}\,(r_0) i\,!\, h^{i-2}}\, \rho\,(\omega) \tag{15}$$

For large enough value of h(in the R.H.S. of eq. (15), we can determine the energy eigenvalues,

$$(E_n - v(r_0)) \simeq \tfrac{1}{2}\, q\, h^2 \tag{16}$$

$$(q = 2n+1, \quad n = 0,1,2, \text{----})$$

The Kratzer Potential (eq. (2))

We use eq.(16) to obtain

$$\left.\begin{aligned} &\frac{2\mu}{\hbar^2}\, E = \alpha = v(r_0) + \tfrac{1}{2}\, q\, h^2 \\ &q = 1,\ 3,\ 5,\ \text{-------} \\ &\text{where } v(r_0) = -\frac{\delta}{2},\ h^2 = \sqrt{2\delta} \end{aligned}\right\} \tag{17}$$

$$\text{and} \qquad \delta = (\frac{2\mu}{\hbar^2})q$$

We take a = 1 and consider large enough values for δ such that $h >> 1$.

We also note that for the cases of

$$\left.\begin{aligned} &v = 0\,, \quad q = 1 \\ \text{and} \\ &v = 1\,, \quad q = 3 \end{aligned}\right\} \tag{18}$$

we have different eigenvalues.

The Pöschl - Teller Potential (eq. (3))

Again eq.(16) provides an expression for the eigenvalues for this potential, or

$$\frac{2\mu}{\hbar^2 q^2} E = \lambda(\lambda-1) + q\sqrt{\lambda(\lambda+1)}$$
$$= v(r_0) + \tfrac{1}{2} q h^2 \tag{19}$$

Here again values for λ must be chosen such that $h >> 1$.

The Hulthén Potential (eq.(4))

For this potential eq. (16) gives an expression for the eigenvalues as follows:

$$E_q = \frac{\delta}{2} + [\frac{3\beta}{2}\{\frac{3}{2}q + \sqrt{f(q) + \frac{\delta}{\beta^{1/3}}\ g(q)}\}]^{2/3} \tag{20}$$

where $\beta = \delta/12$ and $f(q)$ and $g(q)$ are polynomials, calculated according to the procedures given by Müller (1968). We again note that the values of h and δ are given such that for $\delta << 1$, $h >> 1$.

Both $f(q)$ and $g(q)$ are calculated by perturbation method (Table 1). It is important to indicate that this perturbative spectrum (eq. (20)), results from a approximation of the Hulthén potential by the expansion.

$$V(r) \simeq g\,(-\frac{1}{r} + \frac{1}{2} - \frac{r}{12} + \text{----}) \tag{21}$$

This perturbative eigenvalues spectrum obtained for eq.(4) should also be compared with those obtained for the first order approximation potential, *i.e.,*

$$V(r) \simeq -g/r$$
$$\text{where} \quad \frac{2\mu E}{\hbar^2} = -\frac{\delta^2}{4n^2} \tag{22}$$

is the eigenvalue spectrum. This is clearly the spectrum for the Coulomb potential.

3. Energy Eigenvalues From Exact Solution of Eq.(1)

In this section we give the exact spectrum of the energy eigenvalues for the three chosen potentials (eq.(2)−(4)). We start with:

The Kratzer Potential eq.(2)

With this potential, the Schrodinger eq.(1) can be solved exactly. The explicit solution for eq.(1) is:

$$\psi(r) = C_0\, e^{-Br}{}_1F_1\left(\lambda - \frac{\gamma^2}{\beta}, 2\lambda ; 2\beta r\right) \tag{23}$$

Here C_0. is a normalization constant

$$\beta^2 = -a^2E, \text{ and } \gamma^2 = \frac{2\mu}{\hbar^2}\, g\, \frac{a^2}{2} = \frac{\delta a^2}{2}$$

For $\ell = 0$, eq.(23) yields the eigenvalues

$$\frac{2\mu E}{\hbar^2} = -\frac{1}{a^2}\, \frac{\gamma^4}{(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \gamma^2})^2} \tag{24}$$

The Pöschl-Teller Potential (eq.(3))

Here again the exact solution for eq.(1) with this potential is:

$$\psi(r) = \cosh \alpha r\, {}_2F_1 (a, b, \tfrac{1}{2}, -\sinh^2 \alpha r) \tag{25}$$

Only even eigenvalues are present for this solution.

The odd eigenvalues are obtained from:

$$\psi(r) = \cosh \alpha r \sinh \alpha r\, {}_2F_1 (a + \tfrac{1}{2}, b + \tfrac{1}{2}\tfrac{3}{2}; -\sinh^2 \alpha r) \tag{26}$$

Here

$$a = \tfrac{1}{2}(\lambda + ik/\alpha)$$

and

$$b = \tfrac{1}{2}(\lambda - ik/\alpha) \tag{27}$$

the general expression for the eigenvalue spectrum is:

$$\frac{2\mu E}{\hbar^2 \alpha^2} = -\chi (\lambda - 1 - n)^2$$

where

$$\chi = \begin{cases} \lambda - 1 - 2 \\ \lambda - 2 - 2 \end{cases} \tag{28}$$

and $n \leq \lambda - 1$, $\quad n = 0, 1, 2,$ ----

The Hulthén Potential (eq. (4))

The Schrodinger eq.(1), for this potential, has the eigensolution

$$\psi(r)=C_0 e^{\alpha r}(1-e^{-r})\,{}_2F_1(2\alpha+1+n,\quad 1-n, 2\alpha+1, e^{-r}) \tag{29}$$

C_0 is the normalization constant,

$$\begin{aligned} &\alpha - \gamma = n, \qquad n = 1,2,\text{----} \\ &\gamma = \sqrt{\alpha^2+\beta^2}, \quad \beta^2 > n^2, \ \beta^2 = \frac{2\mu g}{\hbar^2}\, a^2 > 0 \\ &\alpha^2 = -\frac{2\mu E}{\hbar^2}\, a^2 > 0 \end{aligned} \tag{30}$$

The energy eigenvalues are:

$$E_n = -g\left(\frac{\beta^2 - n^2}{2n\beta}\right)^2 \tag{31}$$

Finally we compare,

(i) Eigenvalues obtained from eq. (17) and eq. (24) (Table 2)
(ii) Eigenvalues obtained from eq.(19) and eq.(28) (Table 3) and
(iii) Eigenvalues obtained from eq.(22) and eq.(31) (Table 4)

Table 1. Values of the functions f(q) and g(q); eq.(20)

q	f(q)	g(q)
1	0.78441	− 2.44575
3	1.29595	− 3.39112
5	2.29508	− 3.42526
7	3.79006	− 5.40592

Table 2. Eigenvalues computed by exact solution eq. (24) and perturbative method eq.(17) for $\ell = 0$. (For Kratzer Potential).

δ	$E_{per.}$	$E_{ext.}$	$\frac{(E_{ext.} - E_{per})}{E_{ext.}} \times 100$
300	− 137.752 (q = 1) − 113.257 (q = 3)	− 138.242 (v = 0) − 118.876 (v = 1)	0.35 (q = 1, v = 0) 4.70 (q = 3, v = 1)
350	− 116.771 (q = 1) − 135.314 (q = 3)	− 162.262 (v = 0) − 140.989 (v = 1)	0.30 (q = 1, v = 0) 4.00 (q = 3, v = 1)
400	− 185.858 (q = 1) − 157.574 (q = 3)	− 186.349 (v = 0) − 163.297 (v = 1)	0.26 (q = 1, v = 0) 3.50 (q = 3, v = 1)
450	− 210.000 (q = 1) − 180.000 (q = 3)	− 210.492 (v = 0) − 185.763 (v = 1)	0.23 (q = 1, v = 0) 3.10 (q = 3, v = 1)

Table 3. Eigenvalues computed by exact solution eq. (28) and perturbative method eq.(19) for $\ell = 0$. (For the Pöschl-Teller Potential).

λ	$E_{ext.}$	$E_{per.}$	$\frac{(E_{ext.} - E_{per})}{E_{ext.}} \times 100$
25.1	− 616.311 (n = 10, odd State)	− 580.315	6.0
26.2	− 645.248 (n = 11, even State)	− 634.545	1.7
40.2	−1438.208 (n = 18, odd State)	−1536.143	6.8
50.3	−2282.577 (n = 23, even State)	−2429.992	6.5

Table 4. Eigenvalues computed by exact solution eq.(31) and perturbative method eq.(22) (For the Hulthén Potential).

δ	β	E_{coul}	$E_{ext.}$ (q=1)	$E_{per.}$ (n=1)	$\frac{(E_{ext.} - E_{per})}{E_{ext.}} \times 100$
0.05	0.00417	0.0256	0.07254	0.11280	55.5
0.04	0.00333	0.0204	0.11520	0.06442	44.2
0.02	0.00167	0.0101	0.12000	0.04030	33.6
0.01	0.00083	0.0500	0.12250	0.02477	79.8

4. Conclusions

In this investigation we used one long range, the Kratzer potential and two short range, the modified Pöschi-Teller and the Hulthén potentials to extend the range of validity of the perturbation method of Müller-Kiresten. We found that the degree of singularities at the origin which is like r^{-2} (eq. (2)) does not invalidate the expansion for the perturbation solution. All our calculations were done for the case of s-wave where we can work with exact solutions for the three cases.

We may summarize our findings as follows:

i) Table (2) shows that eigenvalues obtained from exact solution for the case of Kratzer potential are within 0.35% of the eigenvalues obtained perturbatively for this potential. We should choose our values for the quantities q ad v to be q = 1 and ad v = 0 respectively to obtain very good agreement. However for q = 3 and v = 1, the agreement is marginal.

ii) For the Pöschl-Teller potential, the agreement is good to within 5%.

iii) There is a marked difference in eigenvalues obtained by perturbation method and the exact values in case of the Hulthén potential they are off by 50%. The reason may very well lie in the fact that the expansion was possible in the region of r = 0, which renders the Hulthén potential to be a two-terms potential, linear plus coulomb potentials, so the perturbation method does not lend itself very easily for this type of potential *i.e. further expansion may be needed.*

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القيم الذاتية لدوال الجهد القصير والطويلة المدى المحسوبة بطريقة نظرية الاضطرابات وطريقة الحلول الكاملة(٢)

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تم استخدام ثلاثة جهود، إحدهما طويل المدى (كراتزر) وإثنان قصيرا المدى (هليثن وبوشل - تيلر) وذلك لدراسة مدى انطباق طريقة الاضطراب التي طورت من قبل مولر - كرستين.

وإن القيم الذاتية التي تم حسابها تماماً لهذه الجهود قد قورنت مع القيم الذاتية التي تم الحصول عليها بواسطة طرق الاضطراب. وقد تمت مناقشة هذه النتائج في فقرة الاستنتاج في نهاية البحث.

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