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Research Article

SERIES SOLUTION OF A CENTRAL POTENTIAL PROBLEM WITH THREE-TERM RECURSION RELATION

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ABSTRACT
The series solution of the radial part of the Schrödinger equation for simultaneous coulomb and harmonic potential involves three-term recursion relation and is thus difficult to solve for bound states. We have suggested a simple method to solve for low lying states. Finite polynomial solutions exist only if the coulomb and oscillator potentials are nontrivially related.

***Key Words*:** *Three-term Recursion Relation, Central Potential, Series Solution*

INTRODUCTION

In the quantum mechanics text books (Schiff, 1968; Bransden and Joachain, 2000; Zettili, 2009; and Griffiths, 2006), the radial part of the Schrödinger equation for a central potential problem is solved by Frobenius' method where in general the two-term recursion relation relates one coefficient of the series to another one. Normally one needs to truncate the series to a finite polynomial to have normalizable bound state wavefunctions. We also get the energy eigenvalues from the condition of the series truncation. But we find very rare comments about the recursion relation involving more than two coefficients as they are difficult to solve. In a popular quantum mechanics book, in the context of hydrogen atom problem, the three-term recursion relation has been commented as "enormously more difficult to work with" compared to a two-term recursion relation (Griffiths (2006)). We can avoid the three-term recursion relation in hydrogen atom by choosing the functional form of the radial wavefunction from its behavior at small and large r. Here we discuss one such interesting example where we cannot avoid a three-term recursion relation. Consider the Schrödinger equation in three dimensions when both coulomb and harmonic oscillator potentials are present together, i.e., the potential is given by

$$V(r) = -\alpha \frac{1}{r} + \frac{1}{2} m\omega^2 r^2 \tag{1}$$

(Where $\alpha = e^2 / (4\pi\grave{o}_0)$ for hydrogen atom problem).The series solution of the radial part for this potential involves a three-term recursion relation. For the bound state solution the series needs to be truncated to a polynomial. The main difficulty of this problem is that the analytic solution for any arbitrary energy level in general form is very difficult to obtain. In Foldy and Stansfield (1987), a similar type of problem was addressed with anisotropic harmonic oscillator with frequency ratio of the oscillators in different directions chosen in such a way that separation of variables in the parabolic co-ordinates works. If one takes isotropic oscillator, then it is not possible to make the separation of variables for all three parabolic coordinates. The authors of that paper tried a series solution which again resulted in the three-term recursion relation which cannot be solved analytically and they solved numerically in two dimensions for a special case when the coulomb term is zero. Hall *et al.*, (2011) solved the isotropic case in d-dimensions with more rigorous mathematical approach. They showed that to have polynomial solutions, the parameters in the potential need to satisfy specific conditions depending on the order of the polynomial.

In this paper, we have suggested a very simplistic method to obtain the low lying energy eigenvalues without much mathematical complications. Converting the recursion relations involving three coefficients

to relations involving only two, we can find out the conditions for the series to be terminated to give normalizable bound state wavefunctions and the energy eigenvalues.

The Radial Equation

We write the Schrödinger equation in spherical polar coordinates. After the separation of variables, the angular part of the Schrödinger equation can very easily be solved and can be found in any standard quantum mechanics book, the solution is given by the spherical harmonics $Y_{lm}(\theta,\phi)$. The radial equation is given by,

$$-\frac{\hbar^2}{2m}\frac{d^2u(r)}{dr^2}+[-\frac{\alpha}{r}+\frac{1}{2}m\omega^2r^2+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}]u(r)=Eu(r) \tag{2}$$

Where l is the azimuthally quantum number. The effective potential

$$V_{eff}=-\frac{\alpha}{r}+\frac{1}{2}m\omega^2r^2+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \tag{3}$$

Let us define

$$k=\frac{\sqrt{2mE}}{\hbar},\ \rho=kr,\ \rho_0=\frac{2m\alpha}{\hbar^2k},\ \text{and}\ \rho_1=\frac{m\omega}{\hbar k^2} \tag{4}$$

Then the radial equation (Equation 2) can be written as

$$\frac{d^2u}{d\rho^2}=[\rho_1^2\rho^2+\frac{l(l+1)}{\rho^2}-\frac{\rho_0}{\rho}-1]u \tag{5}$$

The asymptotic behavior is determined by

$$\frac{d^2u}{d\rho^2}=\rho_1^2\rho^2u \tag{6}$$

The general solution of this equation is given by the parabolic cylinder functions (Abramowitz and Stegun (1972)) $C_1D_{-1/2}(\sqrt{2\rho_1}\,\rho)+C_2D_{-1/2}(i\sqrt{2\rho_1}\,\rho)$ (where C_1 and C_2 are constants). With the condition that the wavefunction vanishes at infinity, the solution for $\rho\to\infty$ goes as

$$u\sim e^{-\rho_1\rho^2/2} \tag{7}$$

Whereas the behavior at small distances ($\rho\to 0$) is given by

$$u\sim\rho^{l+1} \tag{8}$$

So, we assume that the general form of radial wavefunction is given by

$$u(\rho)=\rho^{l+1}e^{-\rho_1\rho^2/2}v(\rho) \tag{9}$$

With this substitution, Equation (5) becomes

$$\rho\frac{d^2v}{d\rho^2}+2(l+1-\rho_1\rho^2)\frac{dv}{d\rho}+[\rho_0-\rho\{-1+(2l+3)\rho_1\}]v=0 \tag{10}$$

Series Solution

Substituting,

$$v(\rho) = \sum_{i=0}^{\infty} c_i \rho^i \tag{11}$$

In Equation (10) we get

$$\sum_{i=0}^{\infty} i(i+1)c_{i+1}\rho^i + 2(l+1)\sum_{i=0}^{\infty}(i+1)c_{i+1}\rho^i - 2\rho_1\sum_{i=0}^{\infty} i c_i \rho^{i+1} + \rho_0\sum_{i=0}^{\infty} c_i\rho^i - [(2l+3)\rho_1 - 1]\sum_{i=0}^{\infty} c_i \rho^{i+1} = 0 \tag{12}$$

The coefficients c_i satisfies the recursion relation

$$c_{i+1} = \frac{[a + 2\rho_1(i-1)]c_{i-1} - \rho_0 c_i}{(i+1)(2l+2+i)} \tag{13}$$

Where $a = -1 + (2l+3)\rho_1$ and

$$c_1 = -\frac{\rho_0}{2(l+1)} c_0 \tag{14}$$

Looking at the solution for very large i, the approximate behavior of the series solution is given by

$$v(\rho) \sim c_o \sum_{i=1,3,5\ldots}^{\infty} \frac{\sqrt{2\rho_1}}{(i+1)!!}(\sqrt{2\rho_1}\rho)^i + c_1 \sum_{i=2,4\ldots}^{\infty} \frac{1}{(i+1)!!}(\sqrt{2\rho_1}\rho)^i \tag{15}$$

Each of the terms in the above expression goes as $e^{\rho_1\rho^2}$ and thus spoils the asymptotic behavior of the radial wavefunction $u(r)$. So, we need to truncate the series. Note that here the recursion relation Equation (13) involves three coefficients c_{i+1}, c_i, c_{i-1} and the truncation is very tricky. If we want to truncate the series in the conventional way that is if we set the coefficient $c_{n+1} = 0$, it does not guarantee the termination of the series. On top of that, if we set $c_{n+1} = 0$, then it implies from Equation (13) that

$$\frac{c_n}{c_{n-1}} = \frac{a + 2\rho_1(n-1)}{\rho_0} \tag{16}$$

increases as n increases i.e., the series does not converge which contradicts the original recursion relation! In its present form, we cannot set Equation (13) to be zero.

To truncate the series we need the recursion relation with only two coefficients. For this purpose we rewrite the first few coefficients in term of the lowest coefficient c_0:

$$c_1 = -\frac{\rho_0}{2(l+1)}c_0$$
$$c_2 = \frac{ac_0 - \rho_0 c_1}{2(2l+3)} = \frac{(2l+2)a + \rho_0^2}{2(2l+2)(2l+3)}c_0$$
$$c_3 = \frac{(a+2\rho_1)c_1 - \rho_0 c_2}{3(2l+4)} = -\frac{\rho_0[2(2l+3)(a+2\rho_1) + (2(l+1)a + \rho_0^2)]}{6(2l+2)(2l+3)(2l+4)}c_0 \quad (17)$$

etc. Alternatively, one can write down the coefficient c_n in terms of c_{n-1} as,

$$c_1 = -\frac{\rho_0}{2(l+1)}c_0$$
$$c_2 = \frac{ac_0 - \rho_0 c_1}{2(2l+3)} = -\frac{2(l+1)a + \rho_0^2}{2(2l+3)\rho_0}c_1$$
$$c_3 = \frac{(a+2\rho_1)c_1 - \rho_0 c_2}{3(2l+4)} = -\frac{\rho_0[2(2l+3)(a+2\rho_1) + (2(l+1)a + \rho_0^2)]}{(2(l+1)a + \rho_0^2)3(2l+4)}c_2 \quad (18)$$

and so on. It is not possible to write down the recursion relation for a general term c_n in these forms, but we can write down as many terms as we wish. So, in place of a general solution let us look at the low lying solutions. The lowest possible term that can be set to zero is c_2 (this corresponds to $i=1$ in Eq.(13)). If $c_2 = 0$ then $c_3 = 0$ only if the coefficient of c_1 in the recursion relation for c_3 i.e., $(a+2\rho_1) = 0$ which puts an additional constraint on the energy eigenvalues. The conditions that $c_2 = 0$ is given by

$$2(l+1)a + \rho_0^2 = 0. \quad (19)$$

Since $\rho_1 = \frac{\hbar\omega}{2E}$ and $\rho_0^2 = \frac{2m\alpha^2}{\hbar^2 E}$, Equation (19) gives the energy eigenvalues

$$E_{1l} = (2l+3)\frac{1}{2}\hbar\omega + \frac{m\alpha^2}{(l+1)\hbar^2} \quad (20)$$

The condition that c_3 also be zero is given by

$$a + 2\rho_1 = 0 \quad (21)$$

which gives another expression for energy eigenvalue

$$E_{1l} = \frac{1}{2}(2l+5)\hbar\omega \quad (22)$$

Equation (22) together with Equation (20) gives the condition

$$\beta = \frac{m\alpha^2}{\hbar^2} / (\hbar\omega) = l + 1 = \text{integer} \tag{23}$$

Thus, the infinite series can be terminated into a finite polynomial only if the parameters in the effective potential satisfy a nontrivial condition! The above results exactly agree with the results in Hall, Saad, and Sen (2011). The minimum value of the ratio β is one thus this method is not applicable with $\alpha = 0$. With this condition the energy eigenvalue Equation (20) becomes

$$E_{1l} = (l + \frac{5}{2})\hbar\omega = \frac{3}{2}\hbar\omega + \frac{m\alpha^2}{\hbar^2} \tag{24}$$

It is interesting to note that though we have never assumed any particular value for l, the final expression for the energy (Eq. (24)) corresponds to $l = 0$ in Equation (20).

Now, let us set $c_3 = 0$ (i.e., $i = 2$ in Equation (13)) with the condition that $a + 4\rho_1 = 0$ so that c_4 also becomes zero and the series terminates to a second order polynomial. Then from Equation (17) we get

$$2(a + 2\rho_1)(2l + 3) + [2(l + 1)a + \rho_0^2] = 0 \tag{25}$$

which gives

$$E_{2l} = \frac{3(2l + 3)(l + 2)}{2(3l + 4)}\hbar\omega + \frac{m\alpha^2}{(3l + 4)\hbar^2} \tag{26}$$

and the condition on the oscillator frequency and the strength of the coulomb potential is given by the dimensionless ratio

$$\beta = 4l + 5 \tag{27}$$

in agreement with Hall, Saad, and Sen (2011). With this condition the energy eigenvalue reduces to

$$E_{2l} = (l + \frac{7}{2})\hbar\omega = \frac{9}{4}\hbar\omega + \frac{m\alpha^2}{4\hbar^2} \tag{28}$$

which again corresponds to $l = 0$ in Equation (26). If we set the coefficient $c_n = 0$ then the series terminates if the pre-factor of c_{n-1} in the recursion relation for c_{n+1} is zero i.e., $[a + 2\rho_1(n - 1)] = 0$. This gives the energy eigenvalue

$$E_{nl} = (n + l + \frac{3}{2})\hbar\omega,\ n = 1, 2, 3\cdots \tag{29}$$

This condition ensures that the ratio c_n / c_{n-1} in Equation (16) is zero and the divergence of the series does not arise. As the general condition for $c_n = 0$ cannot be written down, we cannot determine the condition amongst ω, α and l for arbitrary n.

CONCLUSION

We have proposed a very simplistic method to extract the low lying eigenvalues by truncating a series involving three-term recursion relation. We have considered the quantum mechanical problem with both harmonic oscillator and coulomb potentials. The series solution of the radial equation results in a recursion relation involving three coefficients and is difficult to truncate the series into a polynomial. We

have shown that the low lying eigenvalues and eigenfunctions can be obtained by a very simple method by writing the coefficient c_n in terms of the lowest order coefficient c_0 or the preceding coefficient c_{n-1}. The series truncation needs an extra condition on the harmonic oscillator frequency and the coulomb strength. Depending on the order of the polynomial, the relation between ω and α comes out to be different, but the dimensionless ratio β always takes only integer values. The energy eigenvalues can be written as purely harmonic oscillator or hydrogenic energy levels. And the eigenvalues then depends on angular momentum l, on the other hand the energies can also be written in combination of both harmonic oscillator and hydrogen atom energies by completely eliminating l which is exactly same as the eigenvalue for $l = 0$ without the additional constraint between α and ω. Using our method we can obtain a general expression for the energy eigenvalue for terminating the series at any arbitrary n-th order polynomial, but we cannot evaluate the relation between α and ω in the general form. Thus this method provides a very simple way to extract the low lying eigenvalues when the recursion relation involves more than two coefficients.

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