

## Logarithmic perturbation expansions for an inverse square weak perturbing potential

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### Abstract

We have computed ground and first excited state energies of an electron for a hydrogen atom under an inverse square weak perturbing potential (repulsive) using Rayleigh-Schrodinger (RS) perturbation and Logarithmic perturbation (LP) methods. The energy values obtained from LP and RS methods are tabulated for different perturbation parameters. They are found to be quite close, thus verifying the credibility of the LP method.

### 1. Introduction

Our objective in quantum mechanics is to solve Schrodinger equation for different systems. In theory we assume that in a hydrogen atom the only potential is the Coulomb potential but in reality it is not so. Many other factors come into play such as other potentials which act as perturbations. These kinds of phenomena bring about changes in the energy spectra of the hydrogen atom. So what we need are suitable methods to solve the perturbed potential problems. The most popular and widely used method is the Rayleigh-Schrodinger (RS) which is mostly included in all texts and courses of quantum mechanics. In RS method, calculation of energy correction to first order is easy but for higher orders summation over all possible eigen states is involved which we cant always explicitly perform. It is inherently an approximate method. So we look for other methods which give us maximum output with limited input. Here we

focus our attention to the Logarithmic perturbation (LP) method. In the LP method we transform the unperturbed wave function into  $S(x) = \ln\psi(x)$  and then expand it in the coupling constant. So, only the information about  $\psi(x)$  is sufficient to carry out this method while other intermediate eigen states are not necessary. But this method has shortcomings of its own due to the presence of nodes in wave functions while calculating the corrections of higher excited states. But methods of avoiding these difficulties can be coped up with by the suggestions made in several papers [1], [2] and [3]. It is also seen that with trigonometric wave functions LP method becomes rather troublesome shown by Ndefru and Duwa [4]. Several perturbation problems have been solved by this LP method as by Dobrovolska et al in [5] and [6]. But the problem that we have taken up here proves to be a very good and innovative application of the LP method. We describe the LP method following Imbo and Sukhatme 1984 [7], Cooper et al 2000 [8].

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Time independent Schrodinger equation is

$$-\frac{\hbar^2 d^2 \psi}{2m dx^2} + [V_0(x) + g(V_1(x))]\psi(x) = E\psi(x) \quad (1)$$

where  $V_0(x)$  = unperturbed potential,  $V_1(x)$  is the perturbation with coupling constant  $g$ . After replacing  $\psi(x) = e^{S(x)}$  we get

$$-\frac{\hbar}{2m} [S''(x) + S'(x)^2] + V_0(x) + gV_1(x) - E = 0 \quad (2)$$

which is Riccati's equation.

Now we write  $E$  and  $S'(x)$  as follows:

$$E_i = E_i^{(0)} + gE_i^{(1)} + g^2 E_i^{(2)} + \dots$$

(for the  $i$ -th state and the superscripts denote the orders of corrections) and

$$S'(x) = C_0(x) + gC_1(x) + g^2 C_2(x) + \dots$$

Substituting these in (2) and equating like powers of  $g$ :

$$C'_0(x) + C_0^2(x) = \frac{2m}{\hbar^2} [V_0(x) - E_i^{(0)}] \quad (3)$$

$$C'_1(x) + 2C_0(x)C_1(x) = \frac{2m}{\hbar^2} [V_1(x) - E_i^{(1)}] \quad (4)$$

In general:  $C'_n(x) + 2C_0(x)C_n(x) =$

$$-\frac{2m}{\hbar^2} E_i^{(n)} - \sum_{s=1}^{n-1} C_s(x)C_{n-s}(x); \quad n = 2, 3, 4, \dots \quad (5)$$

Equation (3) is just the unperturbed problem, so we need not solve it. To integrate equation (4) we use  $|\psi(x)|^2$  as the integrating factor where  $\psi(x)$  is the unperturbed ground state normalized wave function so that equation (4) becomes

$$\begin{aligned} C'_1(x)|\psi(x)|^2 + 2C_0(x)C_1(x)|\psi(x)|^2 \\ = \frac{2m}{\hbar^2} [V_1(x) - E_i^{(1)}]|\psi(x)|^2 \end{aligned}$$

which may be written as

$$\frac{d}{dx} [C_1(x)|\psi(x)|^2] = \frac{2m}{\hbar} [V_1(x) - E_i^{(1)}]|\psi(x)|^2$$

The purpose of this is to make the left hand side of equation (4) a derivative so that it can be integrated by inspection. In the just above equation if we put  $\psi(x) = e^{S(x)}$  and  $S'(x) = C_0(x)$  as  $g = 0$  for the unperturbed case, we can reproduce equation (4). Thus the just above equation and equation (4) are equivalent if we consider  $\psi(x)$  to be the unperturbed ground state normalized wave function.

$\psi(x)$  tends to 0 when  $x$  tends to  $-\infty$ . So

$$C_1(x)|\psi(x)|^2 = \frac{2m}{\hbar^2} \int_{-\infty}^x [V_1(x) - E_i^{(1)}]|\psi(x)|^2 dx$$

Again as  $x$  tends to  $\infty$  left hand side of the above equation becomes zero. So

$$E_i^{(1)} = \int_{-\infty}^{\infty} [V_1(x)|\psi(x)|^2] dx \quad (6)$$

Similarly we can find  $E_i^{(2)}$  as

$$E_i^{(2)} = -\frac{\hbar}{2m} \int_{-\infty}^{\infty} [C_1^2(x)|\psi(x)|^2] dx \quad (7)$$

Again

$$C_2(x)|\psi(x)|^2 = -\int_{-\infty}^x \left[ \frac{2m}{\hbar^2} E_i^{(2)} + C_1^2(x) \right] |\psi(x)|^2 dx \quad (8)$$

$$E_i^{(3)} = -\frac{\hbar}{2m} \int_{-\infty}^{\infty} 2C_1(x)C_2(x)|\psi(x)|^2 dx \quad (9)$$

and so on. In the following sections we have made corrections in  $E$  upto second order for the ground state,  $2s$  and  $2p$  states and compared those with  $E$  obtained from RS method.

## 2. Calculations for the Energies by Logarithmic Perturbation Method

An atomic nucleus of charge  $Ze$  and an electron of charge  $-e$  interacts through Coulomb potential

$$V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}$$

where  $r$  = distance between two particles.

In atomic scale the nucleus is a point particle. So if we separate out the centre of mass motion then the Schrodinger equation becomes a one particle motion. So we work with the reduced mass which is

$$m = \frac{m_e M_n}{m_e + M_n}$$

where  $m_e$  is the mass of electron and  $M_n$  is the mass of the nucleus. Here we consider hydrogen atom as the system to verify the credibility of the LP method. The radial Schrodinger equation in spherical polar co-ordinates for the perturbed hydrogen atom reads as follows:

$$-\frac{\hbar^2}{2m} \frac{d^2 u(r)}{dr^2} + \left[ -\frac{Ze^2}{4\pi\epsilon_0 r} + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right] u(r) + g \frac{\hbar^2}{2mr^2} u(r) - Eu(r) = 0 \quad (10)$$

$$\therefore -\frac{\hbar^2}{2m} \frac{d^2 u(r)}{dr^2} + V_0(r)u(r) + gV_1(r)u(r) - Eu(r) = 0 \quad (11)$$

where  $u(r) = rR(r)$ ,  $-\frac{Ze^2}{4\pi\epsilon_0 r} + \frac{\hbar^2}{2mr^2}l(l+1) = V_0(r)$ ,  $V_1(r) = \frac{\hbar^2}{2mr^2}$  and here 'm' is taken to be the reduced mass. It is true that the change appears in the Hamiltonian only due to  $\frac{g\hbar^2}{2mr^2}$ . Our intention is to expand the energy as:

$$E_i = E_i^{(0)} + gE_i^{(1)} + g^2E_i^{(2)} + \dots \quad (i = 1, 2, 3, \dots)$$

where subscript is for states while superscript denotes order of corrections of  $E$ .  $E_i^{(0)}$  is the energy only due to the effective potential that is  $-\frac{Ze^2}{4\pi\epsilon_0 r} + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}$  of the unperturbed problem.

If we mix the centrifugal part of the potential to the perturbed potential and write  $\frac{\hbar^2}{2mr^2}[l(l+1) + g]$  as  $\frac{\hbar^2}{2m} \frac{k(k+1)}{r^2}$ , then we fail to expand  $E_i$  and  $S'(x)$  in powers of  $g$ . As the expansion of  $E_i$  and  $S'(x)$  in powers of  $g$  is central to the LP method we cannot use the form  $\frac{\hbar^2}{2mr^2}k(k+1)$ .

First order correction for ground state energy can be expressed as

$$E_{1s}^{(1)} = \int_0^1 V_1(r)|u(r)|^2 dr \quad (12)$$

$$\text{Here } u_{1s}(r) = \left( \frac{4Z^3}{a^3} \right)^{\frac{1}{2}} r e^{-\frac{Zr}{a}}$$

where 'a' is the Bohr radius and  $Z = 1$ . Therefore

$$E_{1s}^{(1)} = \frac{\hbar^2}{2m} \int_0^\infty \frac{1}{r^2} \left( \frac{4}{a^3} \right) r^2 e^{-\frac{2r}{a}} dr = \frac{\hbar^2}{ma^2} \quad (13)$$

Now,

$$\begin{aligned} C_1(R)|u_{1s}(R)|^2 &= \frac{2m}{\hbar^2} \int_0^R [V_1(r) - E_{1s}^{(1)}]|u_{1s}(r)|^2 dr \\ &= \frac{2m}{\hbar^2} \int_0^R \left[ \frac{\hbar^2}{2mr^2} - \frac{\hbar^2}{ma^2} \right] \left( \frac{4}{a^2} \right) r^2 e^{-\frac{2r}{a}} dr \\ &= \frac{4}{a^3} \int_0^R e^{-\frac{2r}{a}} dr - \frac{8}{a^5} \int_0^R r^2 e^{-\frac{2r}{a}} dr \\ &= \frac{4}{a^2} \frac{R}{a} e^{-\frac{2R}{a}} \left( 1 + \frac{R}{a} \right) \end{aligned} \quad (14)$$

$$\begin{aligned} E_{1s}^{(2)} &= -\frac{\hbar}{2m} \int_0^\infty |u_{1s}(R)|^{-2} [C_1(R)|u_{1s}(R)|^2]^2 dR \\ &= -\frac{5}{2} \frac{\hbar^2}{ma^2} \end{aligned} \quad (15)$$

Equation (13) and (15) represent the 1st and 2nd order energy corrections to the 1s state of the perturbed system.

The unperturbed wave function for the 2s state is

$$u_{2s}(r) = \frac{rZ^{\frac{3}{2}}}{\sqrt{2}} a^{-\frac{3}{2}} \left( 1 - \frac{Zr}{2a} \right) e^{-\frac{Zr}{2a}} \quad (\text{here } Z = 1).$$

Similarly first order correction for 2s is

$$\begin{aligned} E_{2s}^{(1)} &= \int_0^\infty V_1(r)|u_{2s}(r)|^2 dr \\ &= -\frac{\hbar}{2m} \int_0^\infty \frac{1}{r^2} \frac{r^2}{2a^3} \left( 1 - \frac{r}{2a} \right)^2 e^{-\frac{r}{a}} dr \\ &= \frac{\hbar^2}{8ma^2} \end{aligned} \quad (16)$$

$$\begin{aligned}
 C_1(R)|u_{2s}(R)|^2 &= \frac{2m}{\hbar^2} \int_0^R [V_1(r) - E_{2s}^{(1)}]|u_{2s}(r)|^2 dr \\
 &= \frac{2m}{\hbar^2} \int_0^R \left[ \frac{\hbar^2}{2mr^2} - \frac{\hbar^2}{8ma^2} \right] \frac{r^2}{2a^3} \left(1 - \frac{r}{2a}\right)^2 e^{-\frac{r}{a}} dr \\
 &= \frac{R^2}{32a^6} e^{-\frac{R}{a}} \tag{17}
 \end{aligned}$$

Now,

$$\begin{aligned}
 E_{2s}^{(2)} &= -\frac{\hbar}{2m} \int_0^\infty |u_{2s}(R)|^{-2} [C_1(R)|u_{2s}(R)|^2]^2 dR \\
 &= -\frac{3}{16} \frac{\hbar^2}{ma^2}
 \end{aligned}$$

which is the second order energy correction for first excited state (2s).

Unperturbed wave function for 2p state is

$$u_{2p}(r) = \frac{r^2 Z^{\frac{5}{2}}}{a\sqrt{24}} a^{-\frac{3}{2}} e^{-\frac{Zr}{2a}} \quad (\text{here } Z = 1).$$

Therefore the first order correction for 2p is

$$\begin{aligned}
 E_{2p}^{(1)} &= \int_0^\infty V_1(r)|u_{2p}(r)|^2 dr \\
 &= \frac{\hbar}{2m} \int_0^\infty \frac{1}{24r^2 a^5} r^4 e^{-\frac{r}{a}} dr = \frac{1}{24} \frac{\hbar}{ma^2}
 \end{aligned}$$

So,

$$\begin{aligned}
 C_1(R)|u_{2p}(R)|^2 &= \frac{2m}{\hbar^2} \int_0^R [V_1(r) - E_{2p}^{(1)}]|u_{2p}(r)|^2 dr \\
 &= \frac{2m}{\hbar^2} \int_0^R \left[ \frac{\hbar^2}{2mr^2} - \frac{\hbar^2}{24ma^2} \right] \frac{r^2}{24a^5} e^{-\frac{r}{a}} dr \\
 &= \frac{R^3}{72a^5} e^{-\frac{R}{a}} \left(1 + \frac{R}{4a}\right) \tag{18}
 \end{aligned}$$

Therefore second order energy correction for 2p is

$$\begin{aligned}
 E_{2p}^{(2)} &= -\frac{\hbar}{2m} \int_0^\infty |u_{2p}(R)|^{-2} [C_1(R)|u_{2p}(R)|^2]^2 dR \\
 &= -\frac{13}{432} \left( \frac{\hbar^2}{2ma^2} \right)
 \end{aligned}$$

To evaluate all these integrals of equations (14), (17) and (18) we used Gradshteyn and Ryzhik [9].

### 3. Energy Values as Given by The Rayleigh-Schrodinger Method

In this method [10] we can write the corrected energy up to second order as

$$E_i = E_i^{(0)} + H'_{ii} + g^2 \sum_{k \neq i} \frac{|H'_{ki}|^2}{E_i^{(0)} - E_k^{(0)}}$$

where  $H'_{ii}$  is the expectation value of the perturbing potential with respect to the unperturbed wave-function corresponding to  $i$ -th state,  $g$  is the coupling constant,  $E_i^{(0)}$  is the zeroth order energy of the  $i$ -th state and  $E_k^{(0)}$  is the zeroth order energy values for the states other than  $i$ -th state. In our calculation  $k(\neq i)$  is only for 1s, 2s and 2p. Here  $H'_{ii}$  is equal to that of first order corrected energy as found from the LP method.

Now we obtain that;

$$\begin{aligned}
 E_{1s} &= -13.59833551 + \frac{g\hbar^2}{ma^2} \\
 &\quad + g^2 \left[ \frac{\left(\frac{4\sqrt{2}\hbar^2}{18ma^2}\right)^2}{-10.2} + \frac{\left(\frac{7\hbar^2}{24\sqrt{3}ma^2}\right)^2}{-12.08888889} \right]
 \end{aligned}$$

$$\begin{aligned}
 E_{2s} &= -3.399583878 + \frac{g\hbar^2}{8ma^2} \\
 &\quad + g^2 \left[ \frac{\left(\frac{4\sqrt{2}\hbar^2}{18ma^2}\right)^2}{10.2} + \frac{\left(\frac{296\hbar^2}{1875\sqrt{6}ma^2}\right)^2}{-1.888888889} \right]
 \end{aligned}$$

$$\begin{aligned}
 E_{2p} &= -3.399583878 + \frac{g}{24} \left( \frac{\hbar^2}{ma^2} \right) \\
 &\quad + g^2 \left[ \frac{\left(\frac{2\hbar^2}{9\sqrt{6}ma^2}\right)^2}{10.2} + \frac{\left(\frac{31\sqrt{2}\hbar^2}{625ma^2}\right)^2}{-1.888888889} \right]
 \end{aligned}$$

(Here the units of  $E_{1s}$ ,  $E_{2s}$  and  $E_{2p}$  are in electron volts.)

So now we are in a position to make tables for comparing the energy values obtained from both the LP and RS methods for different values of coupling constant  $g$ .

**Table for Energy Values Obtained from LP and RS Method for Different Values of Coupling Constant**

Coupling Constant	State	Energy by RS Method (eV)	Energy by LP Method (eV)
$g = 0.1$	$1s$	-10.96143851	-11.55360911
	$2s$	-3.003170433	-3.063911924
	$2p$	-3.299351765	-3.290090043
$g = 0.01$	$1s$	-13.32659937	-13.33252108
	$2s$	-3.364948848	-3.366016287
	$2p$	-3.388357925	-3.388265308
$g = 0.001$	$1s$	-13.57108143	-13.57114065
	$2s$	-3.396170438	-3.396181113
	$2p$	-3.398449255	-3.398448329

#### 4. Conclusion

The above table shows that for  $g \sim 10^{-3}$ ; energy values for different states using RS and LP method matches very well; both results converge up to 3 decimal place for  $1s$  but for  $2s$  and  $2p$  states it is up to 4 and 5 decimal places respectively. But as we go on increasing the perturbation strength  $g$ ; it is seen that deviation increases between the two results but they are more or less in good agreement. These two methods work very well only for weak perturbations. Among these two methods, LP is easier to work with to evaluate the energy values.

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