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## DETERMINATION OF THE ENERGY SPECTRA OF YUKAWA POTENTIAL VIA VARIATIONAL AND PERTURBATION FORMULATIONS

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### ABSTRACT

In this paper, we obtained the energy spectra of Yukawa potential using the variational and perturbation formulations. The variation of energy  $E$  (eV) with variational parameter  $\alpha$  and perturbation parameter  $a_0$  are also reported. From the variational technique, the value of variational parameter ( $\alpha$ ) which minimizes the energy is  $5.25 \times 10^{11} \text{m}$  which is approximately Bohr's radius  $a_0$  with the corresponding energy  $E(\alpha) = -13.53 \text{eV}$ . This value is close to the ground state energy of hydrogen atom (H-atom) of  $-13.6 \text{eV}$ . From the perturbation formulation, numerical value for the energy  $E(\alpha)$  is  $-17.24 \text{eV}$  which deviates more from the ground state energy of hydrogen atom. Under appropriate choice of parameter, Yukawa potential reduces to a well known Coulomb potential and its corresponding energy calculated analytically. The results of this work indicates that variational technique under appropriate choice of trial wave function gives a better approximate value for the energy eigenvalue of a system than perturbation formation.

### INTRODUCTION

One of the important tasks of quantum mechanics is to find exact solution of the wave equations (non-relativistic and relativistic) for certain potentials of physical interest since they contain all the necessary information regarding the quantum system under consideration (Dong *et al.*, 2007). However, most problems in physics cannot be solved exactly, hence the need to be dealt with approximately (Antia *et al.*, 2015).

There are different approximation methods commonly used in quantum mechanics among them are perturbation theory (Soliveroz, 1981), variational method (Friedberg *et al.*, 2001 and Ikot *et al.*, 2009), Wentzel-Kramers-Brillouin method (WKB) (Saxena, 2007) and others. The increasing interest of finding the energy spectra of Yukawa potential under non-relativistic treatment is due to the fact that the potential is one of the exponential potentials in physical sciences whose applications goes beyond doubt. The Yukawa potential is a screened coulomb potential which is widely used in physics being a good approximation to short-range interactions between charged particles in various area of physics (Yukawa, 1935).

In plasma physics, the Yukawa potential is known as the Debye Huckel potential which describes the shielding effect of ions embedded in plasma (Kar and Ho, 2007). It has also been used to play a fundamental role in (dusty/complex) plasma and colloidal suspensions (Antia, 2013). In solid state, atomic and nuclear physics, it is called Thomas-Fermi or screened coulomb potential due to the cloud of electronic charges around the molecules. In high energy physics the potential is used to model the interaction of hadrons in short range gauge theories where coupling is mediated by the exchange of massive scalar meson (Roy and Nigam, 1967).

The aim of this research was to determine the energy spectra of Yukawa potential using two approximation methods; the variational method and perturbation theory.

The Yukawa potential in this paper is defined as  $V(r) = \frac{V_0 e^{-\mu r}}{r}$ , 1

where  $\mu$  is the screening parameter,  $V_0$  is the potential depth and is given as  $V_0 = -\frac{e^2}{4\pi\epsilon_0}$ .

### VARIATIONAL METHOD

The variational method is one of the approximation methods used in solving problems in quantum mechanics. This method involves choosing a “trial wave function” depending on one or more parameters, and finding the values of these parameters for which the expectation value of the energy is the lowest possible (Griffiths, 1995). The wave function obtained by fixing the parameters to such values is then an approximation to the ground state wave function, and the expectation value of the energy in that state is an upper bound to the ground state energy.

Consider a system described by the Hamiltonian  $H$ , which possesses a complete set of eigen functions  $U_1, U_2, U_3, \dots, U_n$  and corresponding eigenvalues  $E_1, E_2, E_3, \dots, E_n$  such that

$$E_1 \leq E_2 \leq E_3 \leq \dots \leq E_n. \tag{2}$$

Any state of the system can be expanded in terms of the eigen states  $U$  as

$$\Psi = \sum_{n=1}^{\infty} C_n U_n, \tag{3}$$

where  $C_n$  is the expansion coefficient. The expectation value of the energy in the state is then

$$\text{given by } \langle H \rangle = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\sum_{n=1}^{\infty} |C_n|^2 E_n}{\sum_{n=1}^{\infty} |C_n|^2} \tag{4}$$

$$\text{Since } E_n \geq E_1 \text{ for all } n, \text{ it follows that } \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_1. \tag{5}$$

Equation (5) is the basis for approximation of the ground state energy and it means that the expectation value of the Hamiltonian  $H$  for every normalized state is an upper bound to the ground state energy  $E_1$  (Drake and Zong-Chao, 1994). The equality applies only if  $\Psi$  is an eigen function of  $H$  with eigenvalue  $E_1$ .

The trial function  $\Psi_T(\alpha_1, \alpha_2, \alpha_3, \dots, \alpha_s)$  is chosen such that

$$\Psi_T = \Psi_T(\alpha_1, \alpha_2, \alpha_3, \dots, \alpha_s) \tag{6}$$

and the ground state energy is calculated, thus

$$E(\alpha_1, \alpha_2, \dots, \alpha_s) = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \tag{7}$$

Then by minimizing Eq. (7) with respect to the variational parameters  $\alpha_1, \alpha_2, \alpha_3, \dots, \alpha_s$  and

$$\text{solving the equation } \frac{\partial E}{\partial \alpha_i}(\alpha_1, \alpha_2, \dots, \alpha_s) = 0, \tag{7b}$$

for  $i = 1, 2, 3, \dots, s$ , we obtain the variational parameter. The resulting minimum value of  $E$  represents the best estimate of the ground state energy for the trial function of Eq. (6)

### PERTURBATION METHOD

In quantum mechanics, perturbation theory is a set of approximation schemes directly related to mathematical perturbation for describing a complicated quantum system in terms of a simpler one. The idea of perturbation theory is to start with a simple system for which a mathematical solution is known and add an additional “perturbing” Hamiltonian representing a weak disturbance to the system.

$$\text{The Hamiltonian is modified as } H = H^0 + H^1, \tag{8}$$

where  $H^1$  is a small perturbation to the Hamiltonian (Frasca, 2007).

Expanding the total wave function up to first order contributions as

$$\Psi_n = \Psi_n^0 + \Psi_n' \tag{9}$$

Using Schrödinger equation  $H\Psi_n = E_n \Psi_n$  10

with  $E_n = E_n^0 + E_n'$  11

substituting Eq. (8), (9) and (11) into Eq. (10) and simplifying we have:

$$H' \Psi_n^0 + H^0 \Psi_n' = E_n' \Psi_n^0 + E_n^0 \Psi_n' \tag{12}$$

In order to solve Eq. (12) for  $\Psi_n'$  and  $E_n'$ , we multiply the left hand side of Eq. (12) by  $\Psi_n^{0*}$  and integrate to obtain

$$E_n' = \int d\tau \Psi_n^{0*} H' \Psi_n^0 \tag{13}$$

The energy correction becomes  $E_n = E_n^0 + E_n'$  14

For the wave function  $\Psi_n$ , we write as

$$\Psi_n = \Psi_n^0 + \sum_{j \neq n} a_{nj} \Psi_j^0 \tag{15}$$

Multiplying Eq. (15) by  $\Psi_k^{0*}$  and integrating, we get

$$a_{nk} (E_k^0 - E_n^0) = E_n' \int d\tau \Psi_k^{0*} \Psi_n^0 - \int d\tau \Psi_k^{0*} H' \Psi_n^0 \tag{16}$$

Now, we consider two cases,  $k = n$  and  $k \neq n$ ,

For  $k = n$ ;  $E_n = \int d\tau \Psi_n^{0*} H' \Psi_n^0$  17

For  $k \neq n \rightarrow a_{nk} = \frac{\int d\tau \Psi_k^{0*} H' \Psi_n^0}{E_n^0 - E_k^0} = \frac{H'_{kn}}{E_n^0 - E_k^0}$  18

Thus, the first order correction to the wave function is given as:

$$\Psi_n = \Psi_n^0 + \sum_{j \neq n} \left( \frac{\int d\tau \Psi_j^{0*} H' \Psi_n^0}{E_n^0 - E_j^0} \right) \Psi_j^0 \tag{19}$$

where  $d\tau = r^2 dr \sin \theta d\theta d\phi$ .

### ENERGY SPECTRA OF YUKAWA POTENTIAL VIA VARIATIONAL METHOD

The trial wave function for the Yukawa potential of Eq. (1) is given as

$$\Psi_T = A e^{-\frac{r}{\alpha}}, \tag{20}$$

where  $\alpha$  is the variational parameter and  $A$  is the normalization constant.

Normalizing the trial function, we get  $A = \left( \frac{1}{\pi \alpha^3} \right)^{\frac{1}{2}}$  21

Substituting Eq. (21) with Eq. (20), we obtained the normalization wave function as

$$\Psi_T = \left( \frac{1}{\pi \alpha^3} \right)^{\frac{1}{2}} e^{-r/\alpha} \tag{22}$$

The Hamiltonian of the system is obtained as

$$H = -\frac{\hbar^2 \nabla^2}{2m} + \frac{V_0 e^{-ur}}{r}, \tag{23}$$

where the first term on the right hand side of Eq. (23) is the kinetic energy and the second term is our Yukawa potential.

Using Eq. (7), the expectation value of the Hamiltonian for a normalized wave function is

$$E = \langle \Psi_T | H | \Psi_T \rangle = \langle \Psi_T | T + V | \Psi_T \rangle \tag{24}$$

Eq. (24) can be written as:

$$E = \langle \Psi_T | T | \Psi_T \rangle + \langle \Psi_T | V | \Psi_T \rangle \quad 25$$

The expectation value of the kinetic energy part of the Hamiltonian is obtained as

$$\langle T \rangle = \left\langle \Psi_T \left| \frac{-\hbar^2}{2m} \nabla^2 \right| \Psi_T \right\rangle$$

Substituting Eq. (22) into Eq. (25) and by simple algebraic, we obtain the expectation value as

$$\langle T \rangle = \frac{\hbar^2}{2m\alpha^2} \quad 26$$

Similarly, the expectation value for the potential energy counterpart is obtained as

$$\langle V \rangle = \langle \Psi_T | V | \Psi_T \rangle = \left\langle \Psi_T \left| \frac{V_0 e^{-2r/\alpha}}{r} \right| \Psi_T \right\rangle \quad 27$$

Using Eq. (22) in Eq. (27), we obtain the expectation value as 28

$$\langle V \rangle = \frac{V_0}{\alpha \left(1 + \frac{\mu\alpha}{2}\right)^2}$$

By Taylor expanding Eq. (28), we now rewrite the expectation value of potential energy for this system as

$$\langle V \rangle = \frac{V_0}{\alpha} \left(1 - \mu\alpha + \frac{3}{4}\mu^2\alpha^2 + \dots\right). \quad 29$$

Combining Eqs. (26) and (29), the expectation value of Hamiltonian ( $H$ ) is written as

$$E = \langle H \rangle = \langle T \rangle + \langle V \rangle = \frac{\hbar^2}{2m\alpha^2} + V_0 \left[ \frac{1 - \mu\alpha + \frac{3}{4}(\mu\alpha)^2 + \dots}{\alpha} \right]. \quad 30$$

Minimizing Eq. (30) using Eq. (7b), we obtain

$$\frac{\partial \langle H \rangle}{\partial \alpha} = \frac{-\hbar^2}{m\alpha^3} - V_0 \left( \frac{1}{\alpha^2} - \frac{3\mu^2}{4} \right) = 0. \quad 31$$

Eq. (31) is a cubic equation, but we only need the variational solution which is the leading order solution. Neglecting the  $\mu^2$  term, yields:

$$\alpha \approx \frac{-\hbar^2}{mV_0} = a_0 \quad 32$$

Now we can write  $\alpha = a_0 + \delta$  an expand for small  $\delta$ . Substituting  $\alpha = a_0 + \delta$  into Eq. (31) and after a simple simplification, we obtain the term  $\delta$  as

$$\delta = \frac{3}{4} a_0^3 \mu^2. \quad 33$$

This implies that  $\alpha = a_0 + \frac{3}{4} a_0^3 \mu^2 = a_0 \left(1 + \frac{3}{4} \mu^2 a_0^2\right)$  34

Substituting Eq.(34) in to Eq. (30) gives the expectation value energy spectra for the Yukawa potential as

$$E = \frac{\hbar^2}{2ma_0^2 \left(1 + \frac{3}{4} \mu^2 a_0^2\right)^2} + \frac{V_0 \left[1 - \mu a_0 \left(1 + \frac{3}{4} \mu^2 a_0^2\right) + \frac{3}{4} \mu^2 a_0^2 \left(1 + \frac{3}{4} \mu^2 a_0^2\right)^2\right]}{a_0 \left(1 + \frac{3}{4} \mu^2 a_0^2\right)} \quad 35$$

If  $a_0\mu \ll 1$ , thus  $a_0^2\mu^2 \rightarrow 0$ , Eq. (35) reduces to  $E = \frac{\hbar^2}{2ma_0^2} + \frac{V_0}{a_0} [1 - \mu a_0]$  36

where  $\frac{\hbar^2}{2ma_0^2} = R_y$  is the ground state energy for hydrogen atom.

### ENERGY SPECTRA OF YUKAWA POTENTIAL UNDER PERTURBATION FORMULATION

In this case our perturbative potential,  $H'$  is the Yukawa potential of Eq. (1) and substituting into Eq. (8), we obtain the Hamiltonian of the system as

$$\hat{H} = H^0 + \frac{V_0 e^{-\mu r}}{r}, \tag{37}$$

where  $H^0$  is the quantum mechanical model of the hydrogen atom given as (Schiff, 1968)

$$\hat{H}^0 = \frac{-\hbar^2 \nabla^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0 r}. \tag{38}$$

The correction  $\Delta E$  is calculated as an infinite series of increasing smaller corrections

$$\Delta E = E^{(1)} + E^{(2)} + E^{(3)} + \dots \tag{39}$$

$E^{(1)}$  is the first order correction energy.

For most cases, the size of the correction decreases drastically with order i.e. the first correction is almost equal to  $\Delta E$ .

The energy correction is the expectation value or average of the perturbation. Thus

$$E^{(1)} = \langle \Psi^0 | H' | \Psi^0 \rangle = \int_{-\infty}^{\infty} \Psi^{(0)*} H' \Psi^{(0)} d\tau \tag{40}$$

For Hydrogen atom (Schiff, 1968)  $\Psi^0 = \left( \frac{1}{\pi a_0^3} \right)^{\frac{1}{2}} e^{-r/a_0}$  41

Substituting Eq. (41) into Eq. (40) and integrating with simple algebraic we obtain

$$E_1^{(1)} = \frac{4V_0}{a_0^3} \left[ \frac{1}{(2/a_0 + \mu)^2} \right] = \frac{4V_0}{a_0(2 + a_0\mu)^2} \tag{42}$$

The second order correction is evaluated using

$$E_s^{(2)} = \sum_{k \neq s} \frac{|\langle U_k | H' | U_s \rangle|^2}{E_s - E_k} \tag{43}$$

$E_s^{(2)} \approx E_1^{(2)}$  is negative since  $E_s - E_k \approx E_1 - E_2$  which is always negative. Using the closure relation and replacing  $E_s - E_k$  by  $E_1 - E_2$ , we write Eq. (43) as

$$-E_1^{(2)} \leq \left( \frac{1}{E_2 - E_1} \right) \sum_{k \neq 1} \langle U_1 | H' | U_k \rangle \langle U_k | H' | U_1 \rangle = \left( \frac{1}{E_2 - E_1} \right) \left( \langle U_{100} | H'^2 | U_{100} \rangle - E_1^{(1)2} \right) \tag{44}$$

But the energy spectra of Hydrogen is given as (Schiff, 1968)

$$E_n = \frac{-ze^2}{2a_0 n^2}, \tag{45}$$

Substituting into Eq. (44) and carrying out all the necessary integration yields

$$E_1^{(2)} = \frac{32V_0^2}{3e^2 a_0 (2 + a_0\mu)^2} \left[ 1 - \frac{4}{(2 + a_0\mu)^2} \right] \tag{46}$$

Using Eqs. (42), (46) and (39) gives the second order correction to the energy for the system as

$$\Delta E = E^{(1)} + E^{(2)} = \frac{4V_0}{a_0(2 + a_0\mu)^2} + \frac{32V_0^2}{3e^2 a_0 (2 + a_0\mu)^2} \left[ 1 - \frac{4}{(2 + a_0\mu)^2} \right] \tag{47}$$

The total energy of the system is defined as  $E = E_{nl} + \Delta E$  48

where  $E_{nl}$  is the unperturbed energy of the Yukawa potential (Hamzavi et al. 2012),

$$E_{nl} = \frac{-\alpha^2 \hbar^2}{2m} \left[ \frac{mV_0 - (n+1)^2 - l(2n+l+2)^2}{(n+l+1)} \right]^2 \quad 49$$

where  $\alpha$  is the fine structure  $= \frac{1}{137.037 m}$  (Hamzavi et al., 2012)

substituting Eqs. (47) and (49) into Eq. (48) we obtained the total energy for this system as

$$E = E_{nl} + \Delta E = -\frac{\alpha^2 \hbar^2}{2m} \left[ \frac{mV_0 - (n+1)^2 - l(2n+l+2)^2}{(n+l+1)} \right]^2 + \frac{4V_0}{a_0(2+a_0\mu)^2} + \frac{32V_0^2}{3e^2 a_0(2+a_0\mu)^2} \left[ 1 - \frac{4}{(2+a_0\mu)^2} \right] \quad 50$$

For  $n = 1, l = 0$ , Eq. (49) becomes  $E_1 = \frac{-\alpha^2 \hbar^2}{8m} \left( \frac{mV_0}{\alpha} - 4 \right)^2 \quad 51$

### DISCUSSION

If we set  $\mu \rightarrow 0$ , the potential in Eq. (1) reduces to Coulomb potential of the form

$$V(r) = \frac{V_0}{r}, \quad 52$$

with the corresponding energy as  $E = \frac{\hbar^2}{2ma_0^2} + \frac{V_0}{a_0} \quad 53$

The energy level  $E(eV)$  of this system for various variational parameter  $\alpha$  with  $h = 6.626 \times 10^{-34} Js, m = 9.11 \times 10^{-34} Kg, V_0 = 0.023 \times 10^{-23}, \epsilon_0 = 8.85 \times 10^{-12} c^2 N^{-1} m^{-2}$  is in Table 1.

Table 1: Energy levels  $E(eV)$  for various variational parameters ( $\alpha$ )

$\alpha \times 10^{-11}$	$E(eV)$
1.00	237.33
2.00	23.44
4.00	- 12.09
6.00	- 13.35
8.00	- 11.99
10.00	- 10.54
12.00	- 9.32

In Fig. 1, the variation of Energy  $E(eV)$  against  $\alpha$  is shown. From the graph the value of  $\alpha$ , which minimizes the energy is about  $5.29 \times 10^{-11}$  which is approximately equal to the Bohr's radius  $a_0$ . The corresponding minimum energy  $E(\alpha)$  for this value of  $\alpha$  is about -13.53eV. This value of energy is close to the ground state energy of hydrogen atom (- 13.6eV) (Griffiths, 1995).

The energy levels for this system is also computed for the perturbation method for various perturbation parameter values of  $a_0$  (Table 2).

Table 2: Energy levels  $E(eV)$  for various  $a_0$

$a_0(m) ( \times 10^{-11})$	$E(eV)$
1.00	- 35.89
2.00	- 24.39
4.00	- 18.64
6.00	- 16.72
8.00	- 15.77

10.00	- 15.19
12.00	- 14.81
50.00	- 13.35

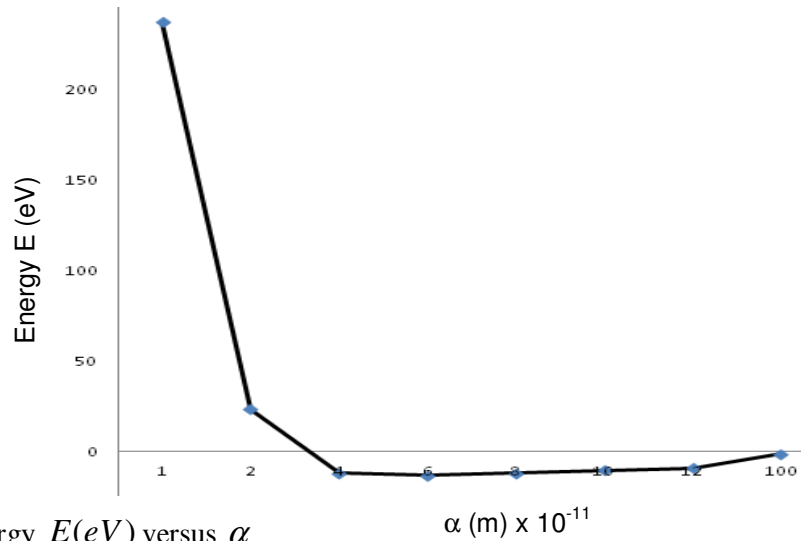


Fig. 1: Energy  $E(eV)$  versus  $\alpha$

The variation of energy against the perturbation parameter  $a_0$  is reported in Fig. 2. In Fig 3, the variation of energy for the two methods (variational and perturbation) against  $\alpha$  is reported.

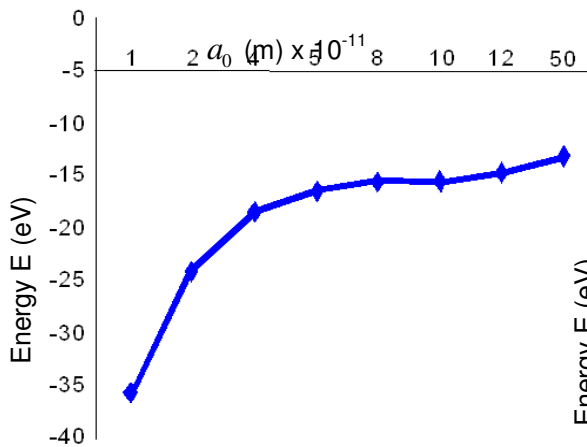


Fig. 2: Energy  $E(eV)$  versus  $a_0$

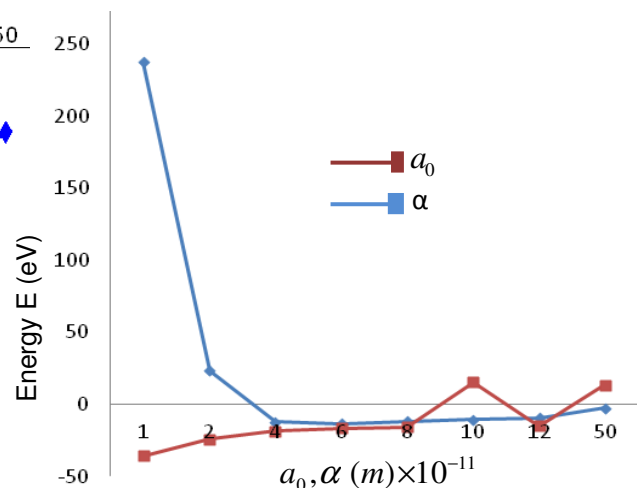


Fig.3: Energy  $E(eV)$  versus  $a_0, \alpha$

### CONCLUSION

In this work, we have used two methods; variational techniques and the perturbation approach to study the energy spectra of Yukawa potential. In the variational technique, the value of  $\alpha$  which minimizes the energy is  $\alpha = 5.29 \times 10^{-11}$  from the graph and this is approximately equal to the Bohr's radius  $a_0$  and the corresponding minimum energy is  $-13.5eV$  which is close to the ground state energy of hydrogen atom ( $-13.6eV$ ). Perturbation formulation gives a result,  $E(a_0) = -17.24eV$ , which deviate more from the ground state energy of  $H$  atom. Thus from the results of our calculations we can conclude that with the appropriate choice of trial wave

function, variational method gives more accurate approximation to the ground state energy of a system than the perturbation formulation.

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