

ANALYTICAL SOLUTIONS OF THE MODIFIED COULOMB POTENTIAL USING THE FACTORIZATION METHOD.

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ABSTRACT

We have solved exactly Schrödinger equation with modified Coulomb Potential under the framework of factorization method. Energy levels and the corresponding wave functions in terms of associated Laguerre function are also obtained. For further guide to interested readers we have computed the energy eigenvalue for some selected elements for various values of n and l .

KEYWORDS

Modified coulomb potential, Schrodinger equation, bound state solution, factorization method.

INTRODUCTION

The exact bound-state solutions of the Schrödinger equation with physically significant potentials play a major role in quantum mechanics. And one of the important tasks in theoretical physics is to obtain exact solution of the Schrödinger equation for special potential. In recent years, exact and approximate solutions of Schrödinger equation with different potentials have attracted much interest [1-12].

The exact solutions of the Schrödinger equation are only possible for some potentials of physical interest [7, 13, 14]. It is well known that these exact solutions of the wave equations are only possible in cases such as harmonic oscillator, pseudoharmonic and Mie-type potentials [5,15]. However, for an arbitrary l –state, many potential of the quantum system could only be solved by approximation method [16, 17].

Different methods have been developed in obtaining the exact or approximate solutions of Schrödinger, Klein-Gordon and Dirac equations for any potential of interest. Among such methods include the shape invariant method [18], supersymmetric quantum mechanics approach (SUSYQM) [19], Nikiforov-Uvarov (NU) [20], asymptotic iteration method (AIM) [21], $\frac{1}{N}$ expansion method [22], factorization method [23] and others [24].

The relativistic Coulomb and oscillator potential problems including their bound-state spectra and wave functions have already been established for a long time [25], and ref. therein and their non-relativistic limits reproduce the usual Schrödinger Coulomb and Schrödinger oscillator solutions respectively. Chen and Dong [26] obtained the exact solution of the Schrödinger equation for the

Coulomb potential plus ring-shaped potential which has possible applications to ring-shaped organic molecules like cyclic polyenes and benzene.

In this paper we consider the modified Coulomb potential defined as

$$V(r) = I - \frac{Ze^2}{r}, \quad 1$$

where I is the threshold potential, Z is the atomic number of the atom, e is the charge of electron. The effective potential $V_{eff}(r)$ of Eq. (1) is given as

$$V_{eff}(r) = I - \frac{Ze^2}{r} + \frac{l(l+1)\hbar^2}{2\mu r^2} \quad 2$$

This potential has great applications in many branches of physics and chemistry such as nuclear, atomic and molecular physics, nuclear chemistry and other related areas. The aim of this paper is to solve the Schrödinger equation under modified Coulomb potential within the framework of factorization method [27].

FACTORIZATION METHOD

In the spherical coordinates, the Schrödinger wave equation is

$$\begin{aligned} & \frac{-\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right] \Psi(r, \theta, \varphi) \\ & + V_{eff}(r) \Psi(r, \theta, \varphi) = E \Psi(r, \theta, \varphi), \end{aligned} \quad 3$$

where $V_{eff}(r)$ in this case is the effective potential of the modified Coulomb potential of Eq. (2). In order to find exact solution of Eq. (3), we give spherical total wave function as

$$\Psi(r, \theta, \varphi) = R(r)\Theta(\theta)\Phi(\varphi) \quad 4$$

Substituting Eq. (4) into Eq. (3) yields the wave equation for the effective potential separated into independent variable as the following equations:

$$\frac{d^2 R(r)}{dr^2} + \frac{2}{r} \frac{dR(r)}{dr} + \frac{2\mu}{\hbar^2} [E - V_{eff}(r)] R(r) = 0, \quad 5$$

$$\frac{d^2 \Theta(\theta)}{d\theta^2} + \cot \frac{d\Theta(\theta)}{d\theta} + \left[\lambda - \frac{m^2}{\sin^2 \theta} \right] \Theta(\theta) = 0, \quad 6$$

$$\frac{d^2 \Phi(\varphi)}{d\varphi^2} + m^2 \Phi(\varphi) = 0, \quad 7$$

where $\lambda = l(l+1)$ and m^2 are separation constants. Equation (6) and (7) are spherical harmonic $Y_{lm}(\theta, \varphi) = \Theta(\theta)\Phi(\varphi)$ whose solution is well known [28]. Therefore, our interest is on Eq. (5).

THE SOLUTIONS OF THE RADIAL PART OF THE SCHRÖDINGER WITH MODIFIED COULOMB POTENTIAL

Substituting Eq. (2) into Eq. (5), we can rewrite the radial part of the Schrödinger equation with the effective potential as

$$\frac{d^2 R(r)}{dr^2} + \frac{2}{r} \frac{dR(r)}{dr} + \frac{2\mu}{\hbar^2} \left[E - I + \frac{Ze^2}{r} - \frac{\lambda \hbar^2}{\mu r^2} \right] R(r) = 0 \quad 8$$

By a change of variable of the form

$$\rho = \alpha r, \quad 9$$

Eq. (8) is written as

$$\rho R''(\rho) + 2R'(\rho) + \left[\frac{2\mu}{\hbar^2 \alpha^2} (E - I) \rho + \frac{2\mu Ze^2}{\hbar^2 \alpha} - \frac{\lambda}{\rho} \right] R(\rho) = 0 \quad 10$$

Writing ansatz for the function in eq. (10) as

$$R(\rho) = U(\rho) L_{n,m}^{(\alpha,\beta)}(\rho), \quad 11$$

and substituting Eq. (11) into Eq. (10), and after a little algebraic, we get

$$\rho L''(\rho) + \left(\frac{2\rho U'(\rho)}{U(\rho)} + 2 \right) L'(\rho) + \left(\frac{\rho U''(\rho)}{U(\rho)} + \frac{2U'(\rho)}{U(\rho)} + \frac{2\mu}{\hbar^2 \alpha^2} (E - I) \rho + \frac{2\mu Ze^2}{\hbar^2 \alpha} - \frac{\lambda}{\rho} \right) L(\rho) = 0. \quad 12$$

To obtain the wave function $U(\rho)$ we compare Eq. (12) with the following associated Laquerre

deferential equation [27] and ref there in.

$$\rho L_{n,m}^{(\alpha,\beta)''}(\rho) + (1 + \alpha - \beta\rho) L_{n,m}^{(\alpha,\beta)'}(\rho) + \left[\left(n - \frac{m}{2} \right) \beta - \frac{m}{2} \left(\alpha + \frac{m}{2} \right) \frac{1}{\rho} \right] L_{n,m}^{(\alpha,\beta)}(\rho) = 0; \quad 13$$

So we obtain the $U(\rho)$ as

$$U(\rho) = e^{-\frac{\beta\rho}{2}} \rho^{\frac{(\alpha-1)}{2}} \quad 14$$

Substituting Eq. (14) into Eq. (11) yields the wave function for this system as

$$R(\rho) = e^{-\frac{\beta\rho}{2}} \rho^{\frac{(\alpha-1)}{2}} L_{n,m}^{(\alpha,\beta)}(\rho) \quad 15$$

where $L_{n,m}^{(\alpha,\beta)}(\rho)$ is the associated Laquerre polynomial.

Here, we note that the solution of associated Laquerre in the Rodriques representation are:

$$L_{n,m}^{(\alpha,\beta)}(x) = \frac{A_{n,m}(\alpha, \beta)}{(\rho)^{\alpha + \frac{m}{2}} e^{-\beta\alpha\rho}} \left(\frac{d}{dx} \right)^{n-m} \left(\rho^{n+\alpha} e^{-\beta\alpha\rho} \right), \quad 16$$

where $A_{n,m}(\alpha, \beta)$ is the normalization constants which is also obtained as

$$A_{n,m}(\alpha, \beta) = (-1)^m \sqrt{\frac{\beta^{\alpha+m+1}}{\Gamma(n-m+1)\Gamma(n+\alpha+1)}} \quad 17$$

To obtain the energy eigenvalue we substitute Eq. (14) into Eq. (12) and carry out the required derivative to have:

$$\rho L''(\rho) + (1 + \alpha - \beta\rho)L'(\rho) + \left[\left(\frac{\beta^2}{4} + \frac{2\mu}{\hbar^2 \alpha^2} (E - I) \right) \rho - \frac{(\alpha + 1)}{2} \beta + \frac{2\mu Z e^2}{\hbar^2 \alpha} + \left(\frac{1}{4} (\alpha - 1)(\alpha - 3) + (\alpha - 1) - \lambda \right) \frac{1}{\rho} \right] L(\rho) = 0$$

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Comparing Eq. (18) with Eq. (13), we have

$$\beta = \frac{4\mu Z e^2}{\hbar^2 \alpha (2n - m + \alpha + 1)}, \tag{19}$$

$$m = -\alpha \pm \sqrt{4\lambda + 1}, \text{ where } \lambda = l(l + 1), \tag{20}$$

$$E = I - \frac{16\mu Z^2 e^4}{8\hbar^2 (2n - m + \alpha + 2)^2} \tag{21}$$

Where α, β, m are polynomial parameters. α and β are the arbitrary numbers, n is the quantum number and m is the magnetic quantum number.

Equation (21) is the energy eigenvalue of the modified coulomb potential. Using the magnetic quantum number m the energy eigenvalue of Eq. (21) becomes

$$E = I - \frac{16\mu Z^2 e^4}{8\hbar^2 (2n + 2\alpha + 1 - \sqrt{4\lambda + 1})^2} \tag{22}$$

But for ordinary Laquerre polynomial, $\alpha = 0$ thus Eq. (22) becomes

$$E_{n,l} = I - \frac{16\mu Z^2 e^4}{8\hbar^2 (2n + 1 - \sqrt{4l(l + 1) + 1})^2} \tag{23}$$

If $I = 0$ and we set $\mu \rightarrow \frac{\mu}{4}$ for $l = 0$, Eq. (23) reduces to the Coulomb energy of the form

$$E_n^C = -\frac{\mu Z^2 e^4}{8\hbar^2 n^2}. \tag{24}$$

The energy states eigenvalue of Eq. (24) for the five(5) selected elements Hydrogen (H), Lithium (Li), Sodium (Na), Potassium (K) and Copper (Cu) have been calculated. The threshold potential $I(eV)$ of these elements is presented in Table 1. The numerical behaviours of the energy of the selected elements with various values of n and l for $\mu = \hbar = 1$ and $e = 1.6 \times 10^{-19} C$ are presented in Tables 2 – 6. From the computed results it can be observed that the degeneracies exist as expected in tables 2 – 6.

Table 1: Threshold potential I for some selected elements

Element	$I(eV)$
Hydrogen H	13.6
Lithium Li	5.39
Sodium Na	5.14
Potassium K	4.74
Copper Cu	7.73

Table 2: Energy eigenvalue for Hydrogen, H

n	Energy eigenvalue $E_{n,l}(eV) \times 10^{-8}$		
	$l = 0$	$l = 1$	$l = 2$
1	-231.1	-102.5	-57.8
2	-102.5	-57.8	-37.0
3	-57.8	-37.0	-25.7
4	-37.0	-25.7	-18.9
5	-25.7	-18.9	-14.4

Table 3: Energy eigenvalue for Lithium, Li

n	Energy eigenvalue $E_{n,l}(eV) \times 10^{-8}$		
	$l = 0$	$l = 1$	$l = 2$
1	-6238.5	-2772.7	-1559.6
2	-2772.7	-1559.6	-998.2
3	-1559.6	-998.2	-693.2
4	-998.2	-693.2	-509.3
5	-693.2	-509.3	-389.9

Table 4: Energy eigenvalue for Sodium (Na)

n	Energy eigenvalue $E_{n,l}(eV) \times 10^{10}$		
	$l = 0$	$l = 1$	$l = 2$
1	-3075.3	-1366.8	-768.8
2	-1366.8	-768.8	-492.1
3	-768.8	-492.1	-341.7
4	-492.1	-341.7	-251.0
5	-341.7	-251.0	-192.2

Table 5: Energy eigenvalue for Potassium (K)

n	Energy eigenvalue $E_{n,l}(eV) \times 10^{-11}$		
	$l = 0$	$l = 1$	$l = 2$
1	-1584.8	-704.4	-396.2
2	-704.4	-396.2	-253.6
3	-396.2	-253.6	-176.1
4	-253.6	-176.1	-129.4
5	-176.1	-129.4	-99.1

Table 6: Energy eigenvalue for Copper (Cu)

n	Energy eigenvalue $E_{n,l}(eV) \times 10^{-11}$		
	$l = 0$	$l = 1$	$l = 2$
1	-5633.6	-2503.8	-1408.4
2	-2503.8	-1408.4	-901.4
3	-1408.4	-901.4	-626.0
4	-901.4	-626.0	-459.9
5	-626.0	-459.9	-352.1

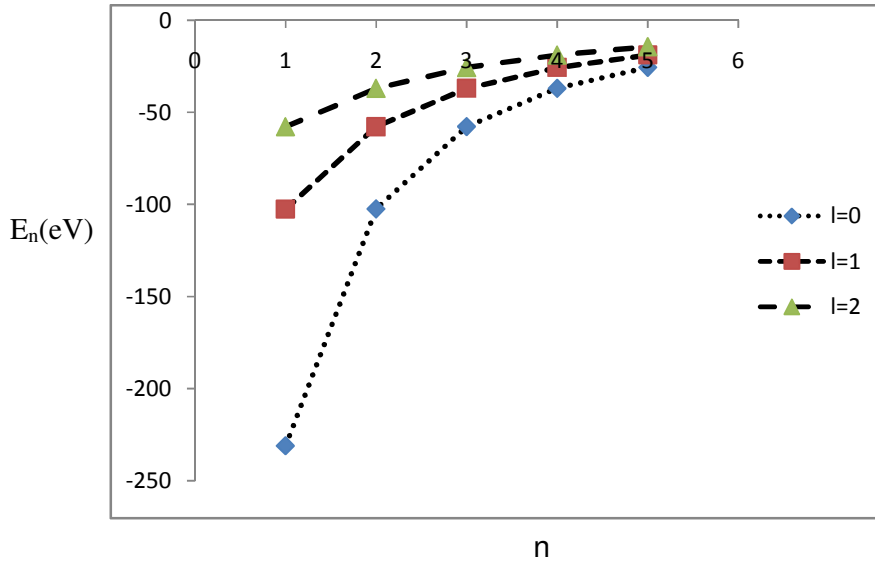


Fig. 1: Energy E_n (eV) versus n for Hydrogen (H)

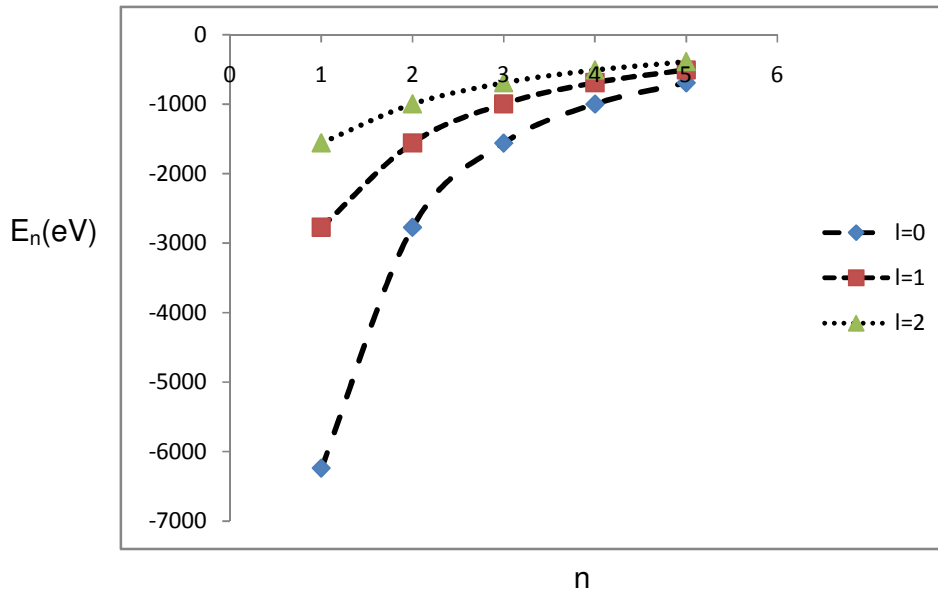


Fig. 2: Energy E_n (eV) versus n for Lithium (Li)

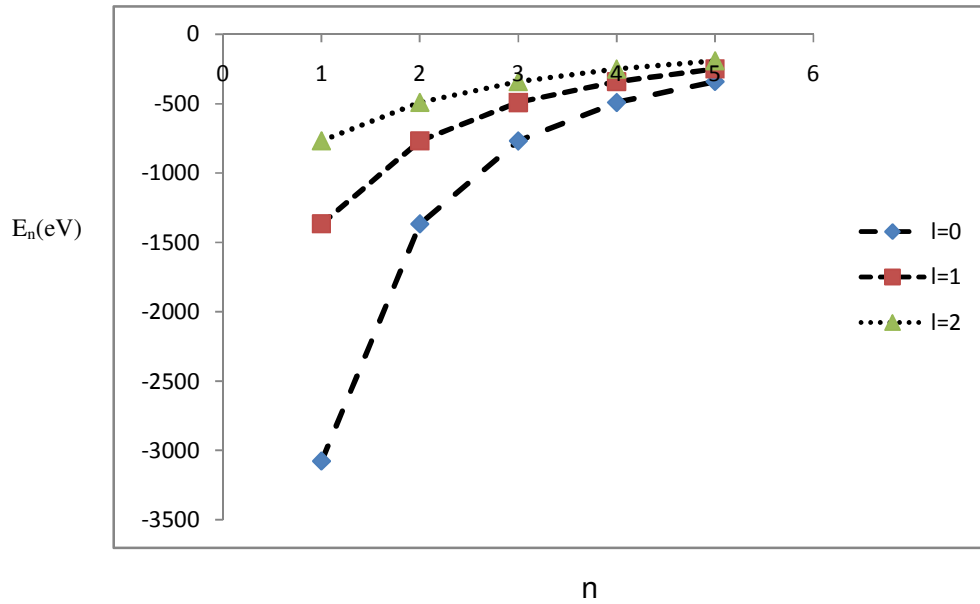


Fig. 3: Energy E_n (eV) versus n for Sodium (Na)

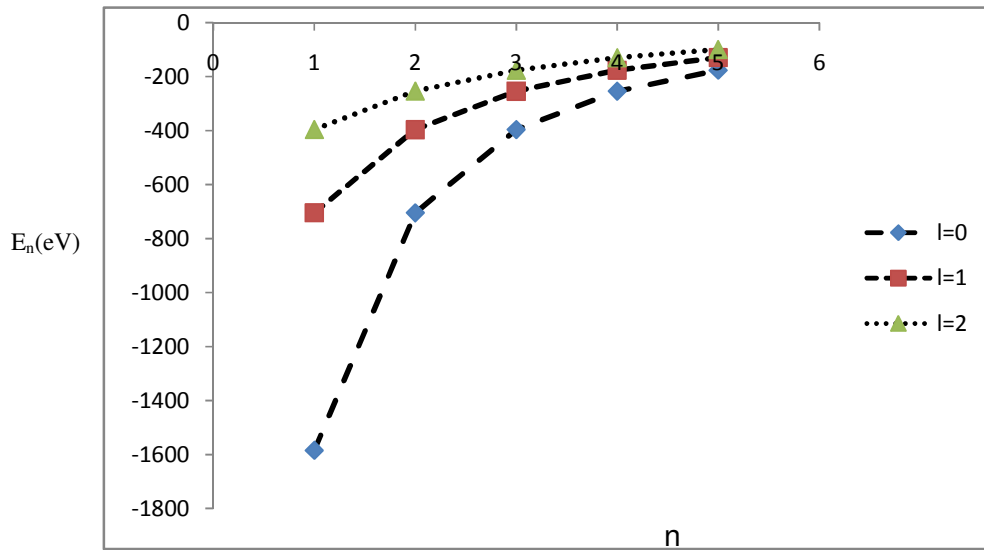


Fig. 4: Energy E_n (eV) versus n for Potassium (K)

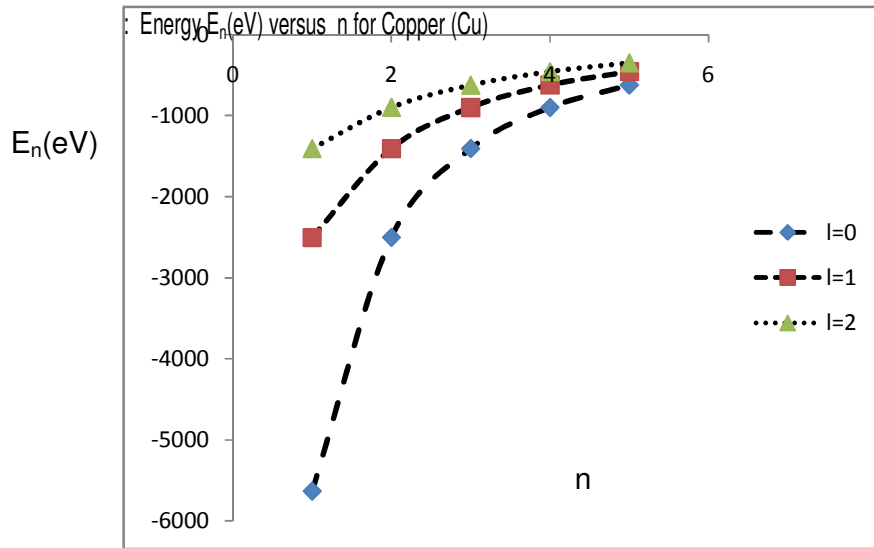


Fig 5: Energy E_n (eV) versus n for Copper (Cu)

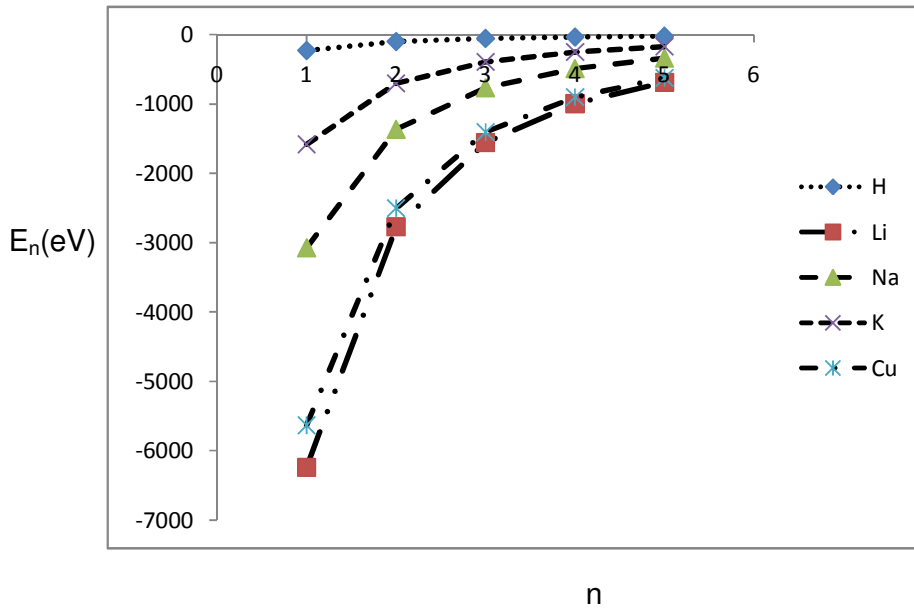


Fig. 6: Energy E_n (eV) comparison for selected elements for $l=0$

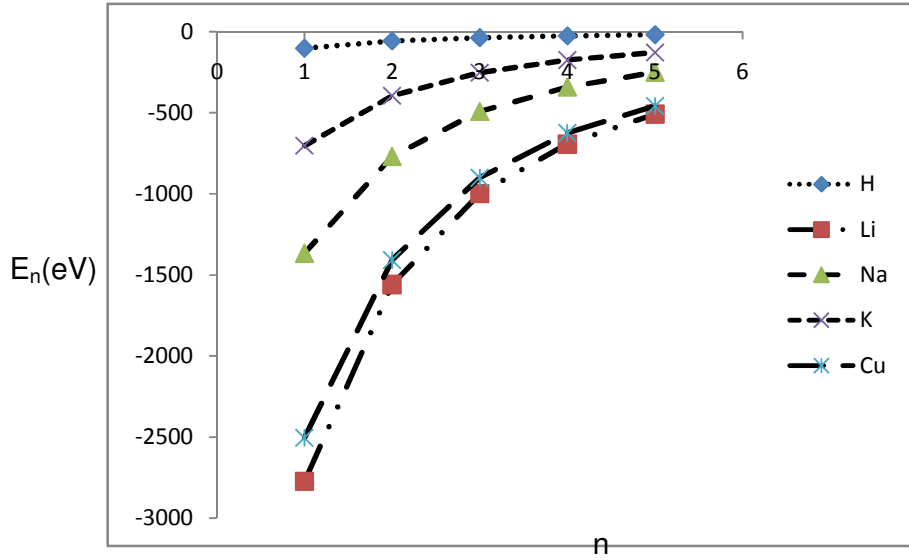


Fig. 7: Energy E_n (eV) comparison for selected elements for $l=1$

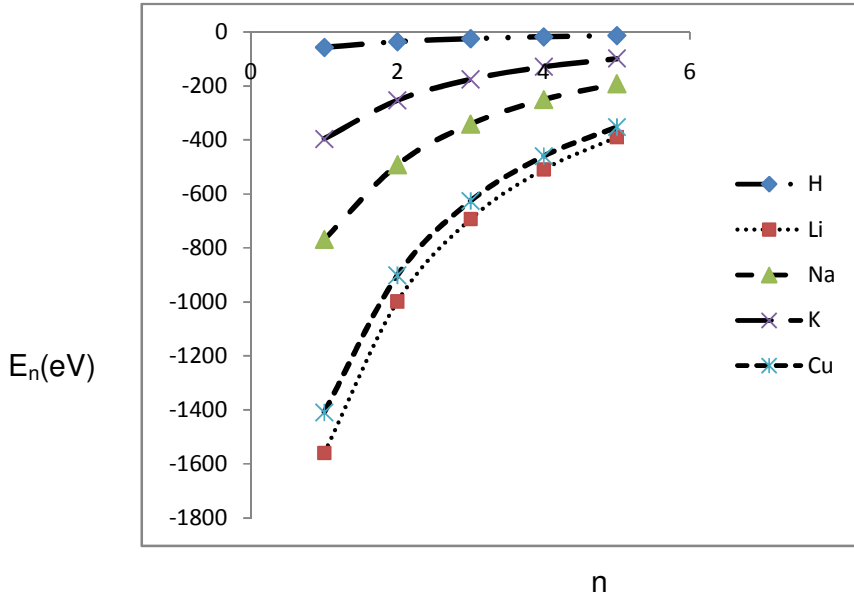


Fig. 8: Energy E_n (eV) comparison for selected elements for $l=2$

CONCLUSION

In this paper, we have obtained the exact solutions of the Schrödinger equation for modified Coulomb potential using the factorization method. The energy eigenvalue and the wave function expressed in terms of associated Laguerre function are obtained. Numerical data for the energy spectrum are discussed for some selected elements like H, Li, Na, K and Cu indicating usefulness for other physical systems.

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