Non-relativistic energy states of embedded Hydrogen-like Atomic Systems in Plasma medium

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Part01:

Introduction

Obtaining precise solutions for the energy levels and wavefunctions of the Schrödinger equation across a range of quantum systems with different potentials is a major challenge in quantum mechanics. Among these significant potentials are the screened Coulomb potentials $[1]$, which are used to describe confined systems in various environments. Due to the unavailability of exact solutions for these potentials, several numerical $[2, 3]$ and analytical methods $[4, 5]$ have been employed. This work aims to apply a novel theoretical method to derive accurate solutions for the Schrödinger equation with screened Coulomb potentials, which are especially important in plasma physics and particle physics.

The objective of our study

We study the effect of plasma screening on the non-relativistic dynamics of an atomic system represented by a hydrogen-like atom by screened Coulomb potentials in spherical coordinate space. By using suitable approximations , the energy spectrum and its corresponding wave functions are determined with high accuracy using the conventional precise method, considering only two studied cases$(n = 0)$,$(n = 1)$ of our atomic system. Our numerical values are consistent with previous studies. Additionally, at the end of this presentation, we provide graphs of the energy spectrum for different Debye lengths, which show the effect of the plasma medium on the embedded atom.

What are the screened Coulomb potentials?

SCP represent a simple case of the more generalized exponential screened Coulomb potentials (**MGESC**) [6]. These are short-range potentials that effectively describe interactions in many-body environments and are also known as Yukawa and Debye potentials[7 – 8]. They are widely used to describe quantum systems, including hadron interactions in gauge theory[9 – 10], impurity-electron interactions in semiconductors[11 – 12], quantum dots, and the effects of charged particles in plasma.This is the focus of our analysis, given by the equation:

$$V(r) = -\frac{Ze^2}{r}e^{-kr} \tag{1}$$

Where Z is the atomic number, $e^2 = \frac{q^2}{4\pi\varepsilon_0}$ is the coloumb constant and $k = \frac{1}{\lambda}$ corresponding to the screening parameter.

part02:Theoratical method

A detailed reexamination of the Schrödinger equation for certain central potentials:

In spherical symmetry , the radial Schrödinger equation in a central potential is write as :

$$\frac{-\hbar^2}{2\mu}U''_{n,l}(r)+\left(\frac{\hbar^2}{2\mu r^2}l(l+1)+V(r)\right)U_{n,l}(r)=E_{n,l}U_{n,l}(r) \tag{2}$$

Where $U_{n,l}(r)$ is the radial part of the wave function represented in the spherical coordinates (r,θ,φ) in the form:$\psi(r,\theta,\varphi)=\frac{U_{n,l}(r)}{r}Y_l^m(\theta,\varphi)$,$Y_l^m(\theta,\varphi)$ are the spherical harmonics. It is know that the central potential of a free hydrogen -like atoms is given by:

$$V(r)=\frac{-Ze^2}{r} \tag{3}$$

Where Z is the atomic number, $e^2=\frac{q^2}{43c03b5_0}$is the coloumb constant After substituting the potential Eq (3) in the Eq (2) and propose another function of the form :

$$U_{n,l}(r)=r^{l+1}e^{-\lambda r}f_{n,l}(r) \tag{4}$$

With $\lambda=\sqrt{\frac{-2Z\mu E_{n,l}}{\hbar^2}}$ So this function enables us to obtain :

$$f''_{n,l}(r) + 2\left(\frac{l+1}{r} - \lambda\right) f'_{n,l}(r) + 2\left(\frac{-\lambda(l+1)}{r} + \frac{Z\mu e^2}{\hbar^2 r^2}\right) f_{n,l}(r) = 0 \quad (6)$$

The solution to the last equation(5) is an integer powerseries as:$f_{n,l}(r) = \sum_{k=0}^{\infty} C_k r^k$ In the end , the solution obtained for the energy levels and corresponding the wave functions of free hydrogen atom are given by the followig expressions:

$$E_n = \frac{-\mu Z^2 e^4}{2\hbar^2 n^2} \quad (7)$$

And

$$\psi(r,\theta,\varphi) = C_0 \left(\frac{Z}{a_0 n} r\right)^l e^{\left(\frac{-Z}{a_0 n} r\right)} \; {}_1F_1\left(-n+l+1; 2+2l; \frac{2Z}{a_0 n} r\right) Y_l^m(\theta,\varphi) \quad (8)$$

Where $n = (N + l + 1)$ is the principal quantum number ,l is the orbital quantum number and a_0 is boher raduis.

Confined Hydrogen-like atoms:

The radial Schrödinger equation for the confinement potential Eq(1) can be written as:

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}-\frac{Ze^2}{r}e^{-kr}\right)U_{n,l}\left(r\right)=E_{n,l}U_{n,l}\left(r\right) \tag{9}$$

By Taylor's series expansion up to order three in order to make the form of killingbeck potential:

$$-\frac{Ze^2}{r}e^{-kr}=-\frac{a}{r}+br+cr^2+d$$

Where introduce the screening strength parameters:

$$a=Ze^2, b=-\frac{1}{2}\frac{\left(Ze^2\right)}{\lambda^2}, c=\frac{1}{6}\frac{\left(Ze^2\right)}{\lambda^3} \text{ and } d=\frac{Ze^2}{\lambda} \tag{10}$$

After taking the expansion forms of the confining potential,rewrite thenon-relativistic stationary radial Schrodinger equation in the form:

$$\left(\frac{d^2}{dr^2}+C_0+C_1r+C_2r^2+\frac{C_3}{r}+\frac{C_4}{r^2}\right)U_{n,l}(r)=0 \tag{11}$$

With $C_0 = \frac{2\mu\left(E_{n,l} - \frac{Ze^2}{\lambda}\right)}{\hbar^2}, C_1 = \frac{\mu}{\hbar^2}\frac{\left(Ze^2\right)}{\lambda^2}, C_2 = -\frac{\mu}{3\hbar^2}\frac{\left(Ze^2\right)}{\lambda^3}, C_3 = \frac{2\mu\left(Ze^2\right)}{\hbar^2}$ and $C_4 = -l\left(l+1\right)$After considering the solution $U_{n,l}(r) = r^{\alpha}e^{-\left(\beta r+\gamma r^2\right)}g_{n,l}(r)$ and let us use a new transformation $\rho = \sqrt[4]{-C_2}r$ can be obtain the canonical form of BHE:

$$\begin{aligned}\rho\frac{d^2}{d\rho^2} + \left(1+\alpha\text{`} - \beta\text{`}\rho - 2\rho^2\right)\frac{d}{d\rho} + \left(\left(\gamma\text{`} - \alpha\text{`} - 2\right)\rho\right. \\ \left. -\frac{1}{2}\left(\delta\text{`} + \beta\text{`}\left(1+\alpha\text{`}\right)\right)\right)g_{n,l}(\rho) = 0\end{aligned} \tag{12}$$

Subsequently,by introducing the following arbitrary parameters: $\alpha\text{`} = 2l+1$; $\beta\text{`} = \frac{-C_1}{\sqrt{-C_2}}\left(-C_2\right)^{\frac{-1}{4}}$; $\gamma\text{`} = \frac{1}{\sqrt{-C_2}}\left(C_0 + \frac{C_1^2}{4(-C_2)}\right)$and $\delta\text{`} = \frac{-2C_3}{\sqrt[4]{-C_2}}$ In this way the heun's wave function is given by the regular solution:

$$g_{n,l}\left(\rho\right) = H_b\left(\alpha\text{`}, \beta\text{`}, \gamma\text{`}, \delta\text{`}, \rho\right) = \sum_{n\geq 0} a_n \frac{\Gamma\left(1+\alpha\text{`}\right)}{\Gamma\left(1+\alpha\text{`}+n\right)}\frac{\rho^n}{n!} \tag{13}$$

After remplacing the Eq (12) into Eq (11) ,we take a polynomial of degreen n break with two condition if and only:

$$\gamma` - \alpha` - 2 = 2n, n = 0, 1, 2, 3, ... \quad (14)$$

and

$$a_1 = \frac{1}{2}\left(\delta` + \beta`\left(1 + \alpha`\right)\right) = 0 \quad (15)$$

From$(n = 0)$
We obtain

$$E_{0,l} = \sqrt{\frac{\hbar^2 \left(Ze^2\right)}{3\mu\lambda^3}}\left(l + \frac{3}{2}\right) - \frac{\mu\left(Ze^2\right)^2}{2\hbar^2\left(l+1\right)^2} + \frac{\left(Ze^2\right)}{\lambda} \quad (16)$$

With considering the radial wave function:

$$R_{0,l}(r) = A_{0,l} r^l e^{-\left(\left(\frac{-\left(\frac{\mu}{\hbar^2}\frac{\left(Ze^2\right)}{\lambda^2}\right)}{2\sqrt{\frac{\mu}{3\hbar^2}\frac{\left(Ze^2\right)}{\lambda^3}}}\right) r + \left(\frac{1}{2}\sqrt{\frac{\mu}{3\hbar^2}\frac{\left(Ze^2\right)}{\lambda^3}}\right) r^2\right)(a_0)} \quad (17)$$

Where $a_0 = 1$ and $A_{0,l}$ is normalized constant.

And from$(n=1)$

$$E_{1,l} = \sqrt{\frac{\hbar^2\left(Ze^2\right)}{3\mu\lambda^3}}\left(l+\frac{5}{2}-\frac{1}{2\left(l+2\right)}\right)-\frac{\mu\left(Ze^2\right)^2}{2\hbar^2\left(l+1\right)^2}\left(1-\frac{2\left(2l+3\right)}{4\left(l+2\right)^2}\left(1+\sqrt{1+16\left(l+1\right)^2\left(l+2\right)\left(\frac{\hbar}{\sqrt{2\mu}}\right)^3\frac{\sqrt{\frac{1}{6}\frac{\left(Ze^2\right)}{\lambda^3}}}{\left(Ze^2\right)^2}}\right)\right)+\frac{\left(Ze^2\right)}{\lambda} \quad (18)$$

With:

$$R_{1,l}\left(r\right) = A_{1,l}r^l e^{-\left(\left(\frac{-\left(\frac{\mu}{\hbar^2}\frac{\left(Ze^2\right)}{\lambda^2}\right)}{2\sqrt{\frac{\mu}{3\hbar^2}\frac{\left(Ze^2\right)}{\lambda^3}}}\right)r+\left(\frac{1}{2}\sqrt{\frac{\mu}{3\hbar^2}\frac{\left(Ze^2\right)}{\lambda^3}}\right)r^2\right)}\frac{\Gamma\left(2l+2\right)}{\Gamma\left(2l+3\right)}\left(a_0+a_1\left(\sqrt[4]{-C_2}r\right)\right) \quad (19)$$

Where $A_{1,l}$ is normalized constant

The result and discussion:

From the results presented in tables 1 and 2 , it can be observed that the obtained self -energy for $(1s, 2p, 3d, 2s, 3p$ and $4d)$ levels, for various Debye length values in atomic units, are in good agreement with those found using the finite differences approach method in reference $[13]$,as well as with those obtained using the one-dimensional difference method in reference $[14]$ and this only for large Debye lengths .However, discrpancies and lack of agreement are evident for smaller Debye lengths.

Table1:Compared of $1s, 2p$ and $3d$ energy eigenvalues in our studied with results of $[13]$ and$[14]$ for variations (λ_D) values in Atomic units.

	E_{1s}			E_{2p}		
λ	Our results	[13]	$-E$[14]	Our results	[13]	$-E$[14]
200	-0.494694	-0.49999	0.495	-0.119489	-0.12499	0.12005
100	-0.489134	-0.49008	0.49005	-0.113557	-0.11525	0.11525
50	-0.477551	-0.48030	0.4803	-0.100918	-0.11525	0.10595
20	-0.440318	-0.45182	0.4518	-0.058863	-0.08074	0.08075
10	-0.372614	-0.40706	0.40705	0.020644	-0.04653	0.046535

Table2:Compared of $2s, 3p$ and $4d$ energy eigenvalues in our studied with results of $[14]$for variations (λ_D) values in Atomic units.

	E_{2s}		E_{3p}		E_{4d}	
λ	Our results	$-E$[14]	Our results	$-E$[14]	Our results	$-E$[14]
200	-0.119388	0.12005	-0.049706	0.1072	-0.025180	0.26505
100	-0.113268	0.1153	-0.043153	0.09240	-0.018229	0.22225
50	-0.100105	0.10615	-0.028777	0.07570	-0.0027522	0.1494
20	-0.055696	0.08175	0.020978	0.03712	0.051719	0.0158
10	0.029306	...	0.118143	0.00318	0.159625	...

The graphic curve1 and 2 represents the change in the energy spectrum of the hydrogen atom inside the plasma as a function of the Debye lengths. We notice that the curves shift by a very small distance and do not start from zero. We also notice that at small distances separating the electron of the hydrogen atom and the plasma, the energy of diffusion decreases. The hydrogen atom creates coulombic repulsive forces , and they are short-term forces to When we reach a certain distance between the ions,$(\lambda) = (\lambda_c)$, which is called the critical point, where the resultant energy is equal to zero, that is, the potential energy is equal to the kinetic energy, and as the wavelength increases, the energy suddenly turns into a negative amount.

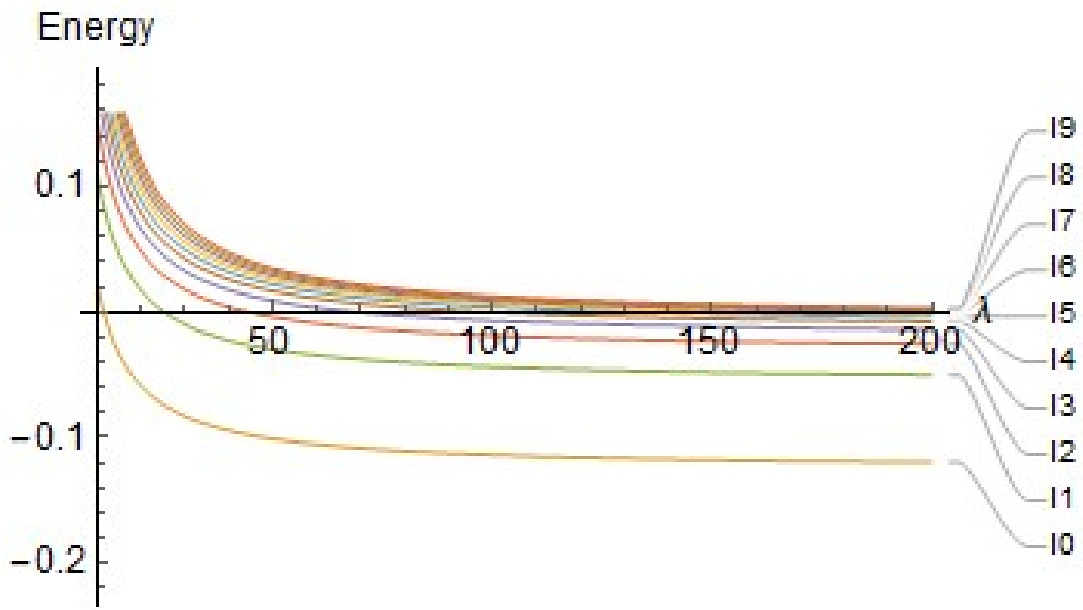

Figure: The variation of the energy levels characterized by different screening parameters (λ) with respect the orbital quantum number(l) in the case $(n = 0)$.

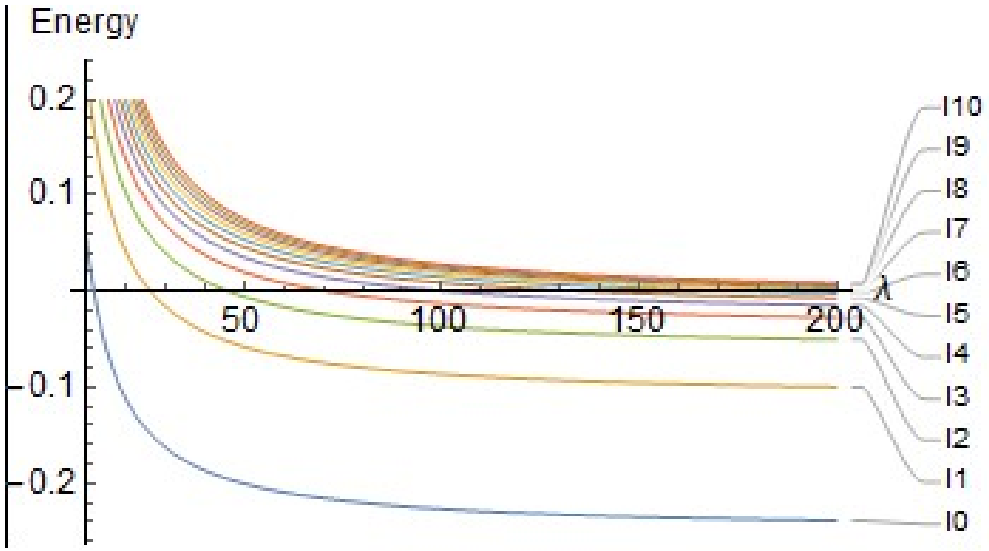

Figure: The variation of the energy levels characterized by different screening parameters (λ) with respect the orbital quantum number(l) in the case $(n = 1)$.

Conclusion:

The main motivation for these studies and theoretical research is a number of calculations that have been carried out on each of the weak atomic systems. And the strong effects of confinement resulting from the environment by mastering existing models using numerical and analytical methods.

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Thank you!