Obtaining the Critical Screening Constants of Two-electron Yukawa Atom via a Combination of Variational Method and Algorithmic Solving of Schrodinger Equation

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One- and two-electron Yukawa atom are of considerable interest because they mimic screened atoms. This finds a direct application in the study of terrestrial and astrophysical plasma. At a sufficient screening, the atom ceases to be bound. In a previous work, Hylerras algorithm is used to estimate the two electrons critical screening which is a very tedious method. In this work, we try to compare the fidelity of these results by employing the variational method using various wavefunctions.

Introduction

Here we consider the One- and two- electron Yukawa atom (non-relativistic) which essentially is the Coulomb potential factored with an exponentially decaying term. This term further confines the potential spatially and in comparison with the Coulomb potential.

$$\mathcal{H}_{1e} = -1/2\ \nabla^2 - Z\ exp(-\lambda r)/\ r,$$

$$\mathcal{H}_{2e} = -1/2\ \nabla_1{}^2 - 1/2\ \nabla_2{}^2 - Z\ exp(-\lambda r_1)/\ r_1 - Z\ exp(-\lambda r_2)/\ r_2 + exp(-\lambda r_{12})/\ r_{12}$$

As λ is increased in a two-electron system the ground state energy slowly changes and at a certain critical screening (λ_2) one of the two electrons becomes unbound. From this point on the system is simply a one-electron system until another critical screening is reached for the one-electron atom (λ_1) where the one-electron ground state becomes unbound. In their paper K.D. Sen, H. E. Montgomery and Jacob Katriel [1] show that using the Hylleras algorithm one could obtain the two-electron critical screening (λ_2). In this project, we employ the Variational Method to try and obtain λ_2 and attempt to determine a good wavefunction used to variationally obtain the ground state energy of the two-electron Yukawa atom.

One-electron Yukawa Atom

The one-electron Yukawa atom ground state can be obtained by directly solving the Schrodinger equation for the same. We employed the Numerovs algorithm to solve the Radial equation (1) [2].

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V(r)-E)R(r) = l(l+1)R(r).$$

Eq(1): Radial Equation

In the above equation substitution $\chi = r\mathbf{R}(r)$ to get it in a suitable form. Since we cannot solve the differential equation over zero to infinity we set an r_{max} which, we assume, is large enough to be considered as infinity. The two boundary conditions that are imposed are that χ is zero at r=0 and $r=r_{max}$. We solve the radial equation from either side and then we match at an intermediate point which we choose as the classical turning point for the particular energy. Since the wave function should be continuous and differentiable, at the intermediate point, we check if the slope fo the two solutions are matching. Continuity is not a concern since the solutions can be rescaled to be made continuous at the intermediate point.

We obtain the ground state energy for various values of the screening constants until the ground state energy becomes smaller than 10^{-10} Hartree. The screening at which the ground state energy becomes so small is taken as the critical screening constant. The critical screening constants obtained for various Z (Atomic number) values are shown in Table (1).

Two-electron Yukawa Atom

The critical screening constants for two-electron Yukawa atom are obtained by observing E_1-E_2 (Where E_1 is the ground state energy for the one-electron Yukawa atom and E_2 is the ground state energy for two-electron Yukawa atom for the same value of the screening constant λ). As the screening constant approaches to critical screening constant this value (E_1-E_2) approaches zero. Henceforth the problem essentially becomes a one-electron Yukawa atom and the critical screening constant can be obtained as was shown in the previous section.

Table(1):

		ψ_{Zeff}	ψ_{CS}	$\psi_{hyllera}$
Z	λ_1	λ_2	λ_2	λ_2
1	1.1867	Not Bound	0.5947	1.125
2	2.3665	1.4238	1.7369	2.30
3	3.5556	2.4265	2.7507	3.48
4	4.732	3.3922	3.7541	NA

The two-electron ground state energy is variationally obtained using two different wave functions. Screened wavefunction and Chandrashekhar wavefunction are given below:

$$\psi_{Zeff}=C_n e^{-Zeff(r1+r2)}$$

$$\psi_{CS}=C_n\{exp(-[Z_1r_1+Z_2r_2])+exp(-[Z_2r_1+Z_1r_2])\}$$

The critical screening constants for the two wave functions and of the Hylleras algorithm from Sen et. al. have been shown in Table(1) for comparison.

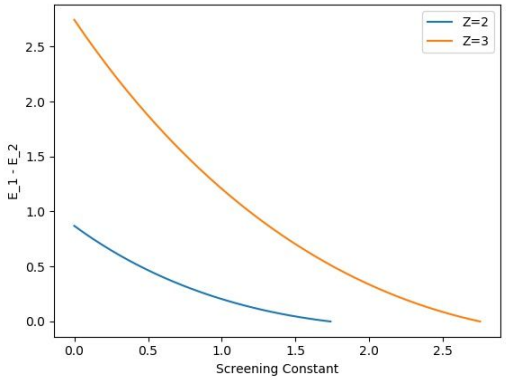

Fig: E_1-E_2 vs λ for Chandrashekhar Wavefunction

Conclusion

It is very clear that the two variational wavefunctions used are not very useful in estimating the two-electron ground state energy. These pattern in the critical screening constants can be explained by the boundedness of the three wave functions which goes as follows:

$$\psi_{Zeff} < \psi_{CS} < \psi_{hyllera}$$

And this loosely bound wavefunction becomes unbound at a screening constant smaller than that of Hyllera's. In fact, in the case of ψ_{Zeff} and Z=1 is not bound for any non-zero screening constants. That is a better candidate for a variational wave function would be the Le Sech wave function. The reason for its candidature is that it provides a much accurate estimation of the Helium atom when compared to Chandrashekhar wave function.

Reference

[1] Critical screening in the one- and two-electron Yukawa atoms PHYSICAL REVIEW A 97, 022503 (2018) K. D. Sen et. al.

[2] "A method of extrapolation of perturbations", Monthly Notices of the Royal Astronomical Society, 84: 592–601, Bibcode:1924MNRAS..84..592N, doi:10.1093/mnras/84.8.592