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IONIZATION ENERGY OF SCREENED HELIUM BY VARIATIONAL QUANTUM MONTE CARLO METHOD

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ABSTRACT
Variational quantum Monte Carlo method was used to determine the ground state energies of the screened Helium atom and its ion under the context of Born-Oppenheimer approximation. The ground state energies at different values of screening parameters were presented for both screened Helium atom and its ion and were further used to obtain the ionization energy of Helium. The most probable wavefunctions were used to calculate the ground state energies, this facilitates in obtaining the idealized value of the ionization energy. The screening parameter in the Helium was found to be inversely proportional to the ionization energy and directly proportional to the ground state energy of both the Helium atom and ion.

KEYWORDS;- Ionization energy and Screening parameter *etc.*

INTRODUCTION

Many body columbic particle problems are persistently challenging issues in the field of theoretical condensed matter physics. The drawbacks of the theory in its inability to describe precisely, the system stimulated many mathematicians and physicist to devote themselves in using various methods to obtain the energies and other expectation values. Few-electron systems like helium are typical models.There are two electrons out of the nucleus of helium atom; and each of them has three freedoms (without considering its spin) so the system can be described by a 6-D Schrödinger equation taking in to consideration the Born-Oppenheimer approximation. The mean field theory has been usual approach in quantum mechanics where each electron is considered independently to be in the central electric field formed by the nucleus and other electrons. The original problem is transferred into a system of nonlinear partial differential equations of low-dimension then solves it iteratively. The other usual method named variational method (Bueckert, H. Rothstein,S. M. and Vrbik, J. (1992)) searches the status function to find the minimum energy value, which has been proved to be close to the precise value. The variational method has been applied to the helium atom at different settings, Theodorakis *et al* considered optimization method to find the approximate solutions of field equations, Lobanova *et al* and Biaye *et al* used variational method in calculating energies of excited states of helium to illustrate the importance of electron correlation effects, Komasa and Bychelwski considered correlated Gaussian functions in variational calculations to estimate the ground state energy of helium dimmer, Banerjoe and Flores-Riveros *et al* studied energy spectrum of spherically confined helium atom. The helium atom is a three particle problem; two electrons which will be labeled 1 and 2, orbit around the nucleus, which consist of two protons with a charge *e* each and two neutral neutrons. Each electron is attracted to the nucleus and the two electrons repel each other as in fig 1. It is assumed that there are no other forces other than electromagnetic ones which are necessary to describe the dynamics of the helium atom with the help of quantum mechanics (Born-Oppenheimer approximation). In this work the Columbic electrostatic interaction between any two charges is replaced by screened Coulomb potential.

The Helium Atom

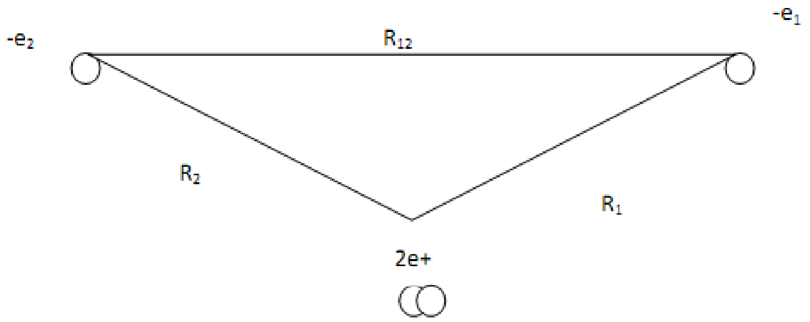


FIGURE 1 coordinates used in describing the helium atom

THEORETICAL BACKGROUND

The effect of electron screening of the nuclear charge is considered, therefore each electron represents a collection of negative charges which partially spans the nucleus, so that the second electron observes an effective nuclear charge, hence the Hamiltonian of the system is given by

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{Z}{r_1} + \frac{Z}{r_2}\right) + \frac{e^2}{4\pi\varepsilon_0}\left(\frac{Z-2}{r_1} + \frac{Z-2}{r_2}\right) + \frac{1}{|r_1 - r_2|} \quad 2.1$$

The trial wavefunctions in the variational method used for the helium atom and its ion are $\psi = e^{\alpha(r_1+r_2)}e^{\beta r_{12}}$ and $\psi = e^{-\propto r}$, respectively. The factor r_{12} in the wavefunction for the atom is the correlation factor which is the effect of the interelectronic interaction to the energy values.

The expectation value of the Hamiltonian in (2.1.1) is given by

$$\langle H\rangle = 2Z^2E_N^0 + 2(Z-2)\left(\frac{e^2}{4\pi\varepsilon_0}\right)\langle\frac{1}{r}\rangle + \langle V_{ee}\rangle \quad 2.2$$

Where V_{ee} represents the electron-electron interaction which is given by

$$V_{ee} = \frac{e^2}{4\pi\varepsilon_0 r_{12}} \quad 2.3$$

The Hamiltonian in the screened Helium atom can be represented as

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2e^{-\sigma r_1}}{r_1} - \frac{2e^{-\sigma r_1}}{r_2} + \frac{e^{-\sigma r_{12}}}{r_{12}} \quad 2.4$$

Where σ is considered as the screening parameter.

The Hamiltonian in the screened Helium ion and due to the choice of the wavefunction can be represented as

$$H = -\frac{1}{2}\nabla^2 - \frac{2e^{-\sigma r}}{r} \quad 2.5$$

COMPUTATIONAL PROCEDURES

The Variational quantum Monte Carlo technique is being developed to calculate the lowest available energies of the Helium atom and the ion systems. The values of the energies obtained are used to determine the ionization energy of the screened Helium.

The Variational quantum Monte Carlo (VQMC) is a scheme for the study of properties of many-body systems at low temperatures. This method relies on the availability of an appropriate trial wavefunction that is reasonably good approximation of the true ground state wavefunction and is a combination of the famous variational principles and the Monte Carlo procedures for the evaluation of the integrals.

The VQMC methodology after the determination of the trial wavefunction that gives the most accurate ground state energy, it also involves the utilization of Metropolis algorithm which can be as follows

a) Start the walker at random position **R.**

b) Make a trial move to a new position R' chosen from some probability density function $T(R' \leftarrow R)$ after the trial move the probability that the walker initially at **R** is now in the volume element dR' is dR' X $T(R' \leftarrow R)$

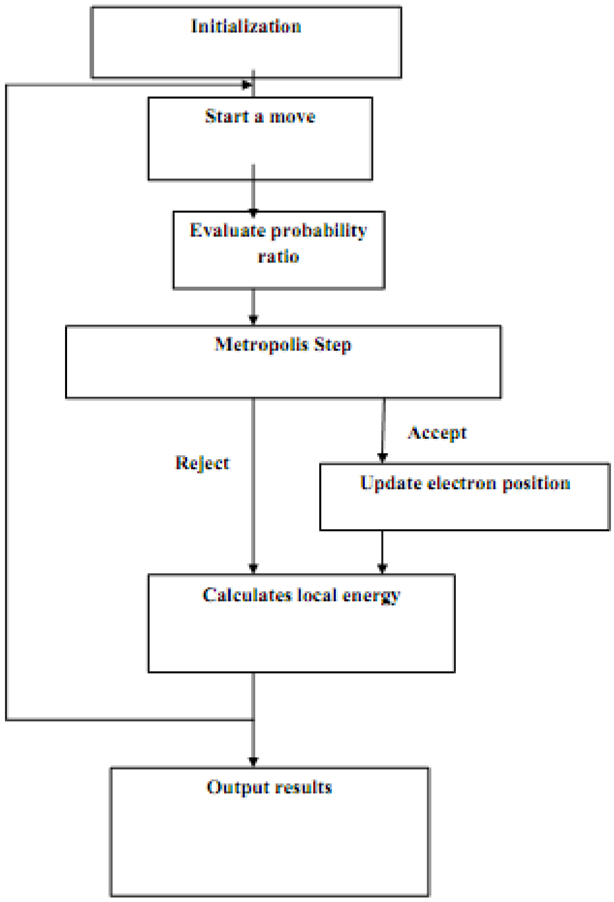
c) Accept the trial move to R' with probability

$$A\ (R' \leftarrow R) = Min\left(1\frac{T(R \leftarrow R')\rho(R')}{T(R' \leftarrow R)\rho(R)}\right).$$

If the trial move is accepted the point R' becomes the next point on the walk; if the trial move is rejected, the point R becomes the next point on the walk. If $\rho(R)$ is high, most trial moves away from **R** will be rejected and the point **R** may occur many times in the set of points making up the random walks.

d) Return to step b and repeat.

The flow chart of the VQMC code can be illustrated as in overleaf,



The value of the screening parameter is varied at some stable intervals and corresponding ionization energy is calculated.

RESULTS AND DISCUSSION

An appropriate wavefunction was used to determine the ground state energies for both the Helium atom and its ion. The interelectronic repulsion factor contributes a lot in lowering the energy levels; therefore the variational parameters were used throughout the computational procedures to calculate the corresponding ground state energy for different values of screening parameters at stable intervals. The corresponding ionization energies were obtained by making appropriate relations between the Helium atomic ground state energy and the ground state energy of the helium ion. The values of GSE in Helium atom and its ion with their corresponding ionization energies at different values of screening parameters were presented in the overleaf table.

The graphic representations of the results are shown below

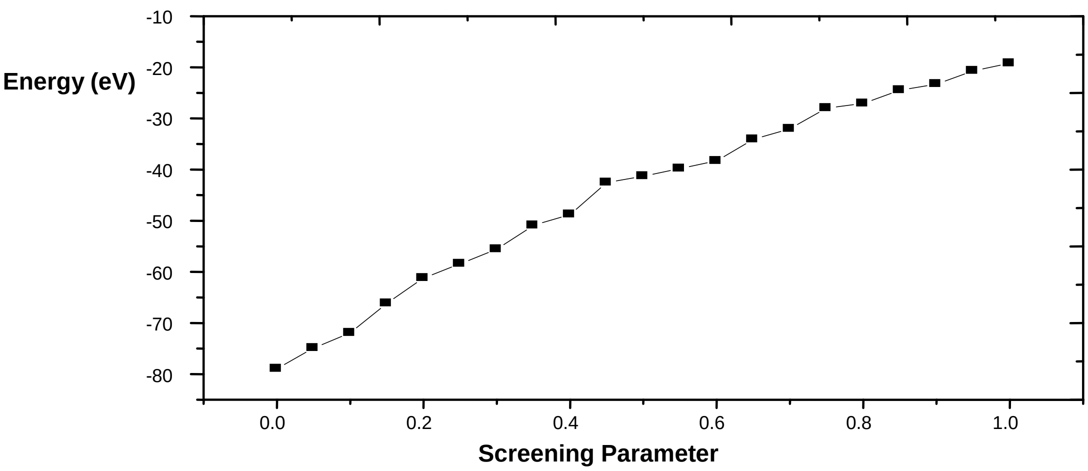


Figure 1 Graph of GSE of Helium atom Vs The Screening Parameter

TABLES: 1 Helium atom and its ion with their corresponding ionization energies at different values

Screening parameter(σ)	GSE (Screened He atom) eV	GSE (Screened He ion) eV	Ionization energy (eV)
0	-78.94256	-54.59494	24.34762
0.05	-74.89792	-52.088	22.80992
0.1	-71.92496	-49.88752	22.03744
0.15	-66.14496	-46.68336	19.4616
0.2	-61.20272	-44.5536	16.64912
0.25	-58.43376	-41.87736	16.5564
0.3	-55.57232	-40.67512	14.8972
0.35	-50.93472	-36.76352	14.1712
0.4	-48.77504	-35.36272	13.41232
0.45	-42.55984	-30.464	12.09584
0.5	-41.28688	-29.7311	11.55578
0.55	-39.79904	-29.43856	10.36048
0.6	-38.2894	-28.76588	9.52352
0.65	-34.1088	-26.61248	7.49632
0.7	-32.0008	-25.81008	6.19072
0.75	-27.98064	-22.35296	5.62768
0.8	-27.05856	-21.59136	5.4672
0.85	-24.48816	-19.32016	5.1680
0.9	-23.28592	-18.16848	5.11744
0.95	-20.67472	-16.43968	4.23504
1.0	-19.2032	-15.2025	4.0007

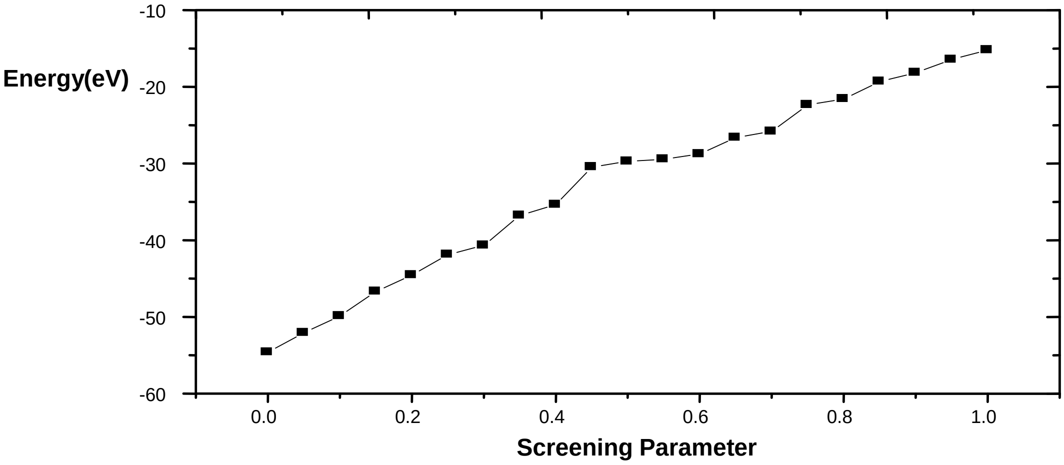


Figure 2 Graph of GSE of Helium Ion Vs The Screening parameter

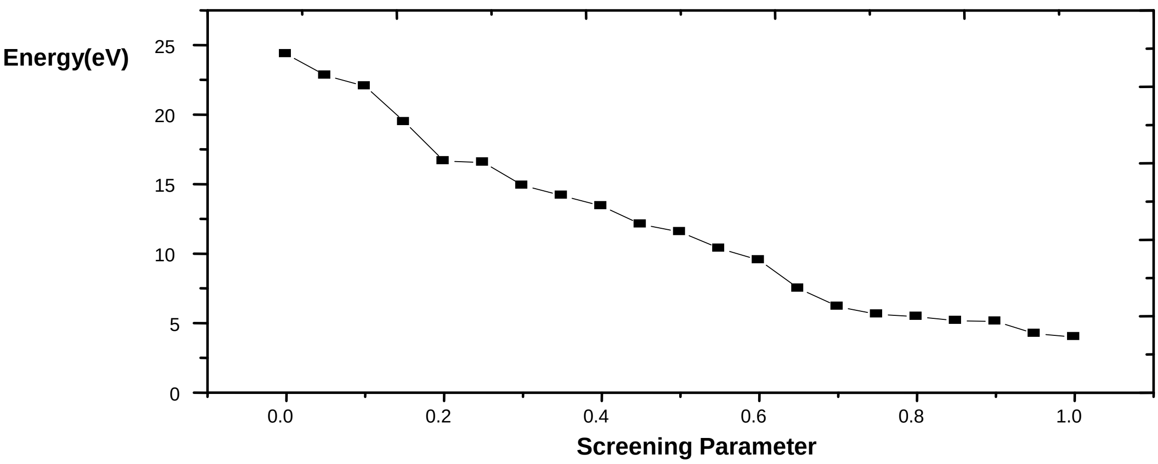


Figure 3 Graph of Ionization Energy Vs Screening Parameter for Helium

DISCUSSION

The results indicated that the ground state energies of both helium atom and its ion are directly proportional to the screening parameter by employing the class of wavefunctions used in this report, while the ionization energy was found to be inversely proportional to the screening parameter. This is represented graphically in Figs 1, 2, and 3 respectively, this method of calculations reveals that the ionization energy of helium atom is in consistent with the experimental value of 24.5eV(Kinoshita, T 1957) which indicates an accuracy of about 99.4%.

CONCLUSION

The nonrelativistic ground state energy levels of screened helium atom and its ion were calculated using the variational quantum Monte Carlo method under the context of Born-Oppenheimer approximation. An appropriate wave function was chosen to satisfy the electron-electron cusp condition. The ionization energies of helium at each point of the screening parameter were determined by making the proper mathematical relationship between the ground state energies of the helium atom and its ion.

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