Modeling a helium atom from a collision of an electron with an ionized helium atom

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Abstract. A method which is based on quantum scattering theory and, particularly, on the Jost functions, is presented for solving the bound states problem of helium atom. Within this approach, the energies of bound states of helium atom were obtained as the sum of energies of a hydrogen atom and the energies that one electron needs to bind to an ionized helium atom in a collision process. We calculated the ground state energy and the energies of the first excited states of helium atom, and obtained remarkable results. This method could then be used as basis to study atoms with more electrons.

1. Introduction

The eigenvalues equation of helium atom in general does not have an analytic solution; for that reason, the scientists have developed certain methods of approximation in order to solve this equation and to try to understand this atom. The first theoretical studies on the helium atom took place in 1929 by Hylleraas\cite{1} who used variational methods. The authors in\cite{2} used the perturbations method up to first order to calculate the ground state energy of helium atom and they reported an error of the 5.3\% with respect to the experimental value of -79.01 eV\cite{2}. Until now, it has not been possible to calculate the correction of second order using only the perturbation method, but using a combination of the variational method and the perturbation method with functions of proof with 100 terms. Scherr and Knight calculated up to the thirteenth order energy corrections\cite{3} and found an energy of -2.90372433(e^2/a_0) (with e^2/a_0=27.208 eV). Corrections up to the twenty-first order were obtained in\cite{4}. On the other hand, the authors in\cite{2} found an energy of -77.48 eV using only the variational method, taking as function of proof the hydrogenoid functions and taking as variational parameter the Z atomic number; if we compare this value with the experimental value (-79.01 eV) we found an error of 1.9\% that is less than what was obtained using the perturbation method with the first order energy correction. Using complicated functions of proof with six terms, Hylleraas found an energy value that is only 0.01 eV higher than the experimental value of the ground state\cite{1}. Hylleraas’s work has been expanded by other authors. Pekeris found an energy value of -2.9037244375(e^2/a_0) using a variational function with 1078 terms\cite{5}. Frankowski and Pekeris obtained better values than those obtained by Pekeris -2.9037437703(e^2/a_0) with an error of 10^{-11}(e^2/a_0) with respect to the correct non-relativistic energy\cite{6}. An accuracy of 10^{-14} was obtained by Drake and Zong-Chao using linear variational functions\cite{7}. Although the methods mentioned above produce excellent results\cite{1,3–7}, they are very difficult to apply. In this way,
the main objective of this paper is to developed a method to solve the bound states problem of helium atom that is easy to understand, easy to apply and that produces excellent result. Therefore, the scattering theory was used in this paper in order to model the helium atom from a collision of an electron with an ionized helium atom.

2. Theory

In scattering theory, the Jost function is the theoretical concept that permits to study bound states, virtual states, resonance states and scattering states [8, 9], but the majority of research works which utilize this function are those that deal with scattering and resonance [10–14]; Furthermore, in the literature, there are few methods which allow to calculate it [15,16]; in this paper, we used the method proposed in [17] in order to find this function, i.e, the Equation (1) was solved.

\[
F''_L(k, r) - \left( \frac{U'(r)}{U(r)} + 2 \frac{h^+_L(kr)}{h^+_L(kr)} \right) F'_L(k, r) - U(r)F_L(k, r) = 0, \tag{1}
\]

where \( U(r) \) is a spherical potential of interaction between an incident particle and a target; \( h^+_L(kr) \) are the Hankel functions which depend on the angular momentum \( L \), the wave number \( k \) and the distance \( r \) between the particles; and \( F_L(k, r) \) are known as the Jost solutions. In each case, the prime index means to derive with respect to \( r \). After that the Equation (1) is solved we can find the Jost functions \( f_L(k) \) through Equation (2).

\[
f_L(k) = \lim_{r \to \infty} F_L(k, r) \tag{2}
\]

In addition, the energies of bound states are calculated through \( E = k^2 \hbar^2 / 2m \), where \( m \) is the reduced mass of the system and the values of \( k \) satisfy \( \text{Im}(k) > 0 \) and \( \text{Re}(k) = 0 \) and for which \( f_L(k) = 0 \).

3. Method

The electronic Hamiltonian in atomic units for a helium atom is given in Equation (3).

\[
\hat{H} = -\frac{1}{2} \nabla^2 r_1 - \frac{1}{2} \nabla^2 r_2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{|r_2 - r_1|} \tag{3}
\]

where the first and second term correspond to the kinetic energies of two electrons, the third and fourth term are the electron-nucleus interactions, and the last one is the electron-electron interaction. The Hamiltonian in Equation (3) can be written as \( \hat{H} = \hat{H}^0 + \hat{H}^1 \) with the Equation (4) and Equation (5).

\[
\hat{H}^0 = -\frac{1}{2} \nabla^2 r_1 - \frac{2}{r_1} \tag{4}
\]

\[
\hat{H}^1 = -\frac{1}{2} \nabla^2 r_2 - \frac{2}{r_2} + \frac{1}{|r_2 - r_1|} \tag{5}
\]

In Equation (4), \( \hat{H}^0 \) represents the Hamiltonian of a hydrogenoid atom (of atomic number \( Z = 2 \)) with energies of bound states given by \( E^0 = -\frac{1}{2} \frac{Z^2}{n^2} \) (in atomic units). While from Equation (5), \( \hat{H}^1 \) can be interpreted as the collision of one electron with a nucleus (of \( Z = 2 \)) and other electron; thus, the effective potential that the electron experiments due to the interactions with the nucleus and with the charge distribution originated by the other electron is given by Equation (6) and Equation (7) [2].
\[ V(r) = -\frac{Z_1}{r} + \int \frac{\Phi(r', Z_2)^2}{|r-r'|} dr' \]  \hfill (6)

\[ V(r) = \frac{1}{r} - \frac{Z_1}{r} + \frac{1}{r}[(1 + Z_2 r)e^{-2Z_2 r}], \]  \hfill (7)

where \( \Phi(r, Z_2) = \sqrt{\frac{2Z_3}{\pi}} e^{-Z_2 r} \) and \( Z_i \) is the effective charge that each electron experiments. In Equation (6) and Equation (7) when \( Z_1 = Z_2 = 2 \), it is known as non screened-potential and the Equation (7) takes the form shown in Equation (8).

\[ V(r) = -\frac{1}{r} - \frac{1}{r}[(1 + 2r)e^{-4r}] \]  \hfill (8)

while if \( Z_1 = 2 \) and \( Z_2 = 2 - 5/16 \) [2], now it is named screened-potential and the Equation (7) can be written in the form presented in Equation (9).

\[ V(r) = -\frac{1}{r} - \frac{1}{r}[(1 + \frac{27}{16}r)e^{-2(\frac{27}{16}r)}] \]  \hfill (9)

Also, the relationship between the reduced potential \( U \) in Equation (1) and the effective potential \( V \) given in Equation (8) and Equation (9) is given by \( U(r) = 2mV(r)/\hbar^2 \). Now we may use Equation (1) and Equation (2) in order to calculate the bound states energies \( E_1 \) that correspond to \( \hat{H}^1 \) by means of \( E_1 = k^2/2 \). Finally the total electronic energies are found with \( E = E^0 + E_1 = -\frac{1}{2} \frac{Z^2}{n^2} + \frac{k^2}{2} \). Where \( n \) is the main quantum number.

4. Results and discussion
In general terms, the solutions of Equation (1) are complex functions due the fact that Hankel functions are complex functions too. Figure 1 shows an arbitrary solution of Equation (1), where we used the potential given by Equation (8) and the arbitrary values \( k = 1 \) and \( L = 0 \). It is observed that when the \( r \) distance tends to infinity, the \( F(k = 1, r) \) function tends to be constant, which it is the behavior predicted by the Equation (2), and in this way we have calculated the Jost function \( f_{L=0}(k = 1) \). We repeat this process, using both potentials shown in Equation (8) and in Equation (9), in order to find the \( k \) values that satisfy both relations \( Im(k) > 0 \) and \( Re(k) = 0 \) and for which \( f_{L,k} = 0 \).

![Figure 1](image_url)  \hfill (a)

**Figure 1.** Solution of Equation (1) for the non screened-potential and for \( k = 1 \) and \( L = 0 \), (a) real part and (b) imaginary part.
In Table 4, the bound state energies calculated for the ground state and the first three excited states of helium atom are shown. Comparing the energies obtained with the screened-potential with the experimental values, we found errors of 0.039%, -0.541%, -0.077% and 0.713%, respectively. It can be observed that the error obtained in this work for the ground state energy is lower than the errors calculated with the perturbation method (with first order energy correction) and the variational method (with hydrogenoid function as function of proof), 5.3% and 1.9% respectively. This demonstrates that the method proposed in this paper produces excellent results.

Table 1. Bound state energies of helium atom calculated with a non screened-potential and with screened-potential.

| States        | Non screened-potential | Screened-potential | Experimental values |
|---------------|------------------------|--------------------|---------------------|
|               | $k$ $E$                | $k$ $E$            | $E_{exp}$           |
| Ground state  | 1.28036$i$ -2.81967    | 1.34358$i$ -2.90260| -2.90372            |
| First excited state | 0.55312$i$ -2.15297    | 0.56142$i$ -2.15759| -2.14597            |
| Second excited state | 0.26783$i$ -1.96413    | 0.35453$i$ -2.06285| -2.06127            |
| Third excited state | 0.19442$i$ -1.98110    | 0.19546$i$ -2.01910| -2.03359            |

5. Conclusions
In this theoretical work we have modeled the helium atom from a collision of one electron with a hydrogenoid atom (of $Z = 2$). It was possible because we considered the Hamiltonian of helium atom as the joint of two Hamiltonian, i.e, $\hat{H} = \hat{H}^0 + \hat{H}^1$, where $\hat{H}^0$ represents a hydrogen atom and $\hat{H}^1$ was interpreted as a collision of one electron with a hydrogenoid atom (of $Z = 2$); therefore, the scattering theory was used to calculate the bound state energies of $\hat{H}^1$. Finally, we found the electronic energies as the sum of energies that correspond to $\hat{H}^0$ and $\hat{H}^1$. The results that have been found to match those of the experimental values.

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