Ionization energy of the helium atom in a plasma

C. S. Lam and Y. P. Varshni
Department of Physics, University of Ottawa, Ottawa K1N 6N5, Canada
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The ground-state energy of the helium atom in a plasma is calculated by the variational method with the static screened Coulomb potential as the interparticle potential. This is used to calculate the ionization energy of the helium atom as a function of the screening parameter. The critical value of the screening parameter at which the ionization energy becomes zero is also estimated.

I. INTRODUCTION

At least for classical charged particles, the effect of the plasma sea on localized two-particle interactions is to replace the Coulomb potential by an effective screened potential.[1] This effective screened Coulomb potential is known in plasma physics as the Debye-Hückel potential and for the attractive case it is given by

$$V(r) = -e^2 e^{-\alpha r}/r \; , \tag{1}$$

where α is a screening parameter. The bound-state energies of an electron in the screened field of a proton have been calculated by a number of authors with a variety of techniques.[2–11] The number of H-atom bound states in such a case is found to be finite and the energy eigenvalues are a function of the density and temperature. The magnitude of the ionization energy decreases as the screening increases.

However, except for a calculation due to Rogers,[12] the problem of plasma screening of two-electron atoms appears to have received very little attention. In the present paper we consider the case of the helium atom in a plasma. We first calculate the energy of the helium atom, with the use of the variational method, when the interaction between the constituent particles is given by the potential (1). We next calculate the ionization energy of the helium atom as a function of the screening parameter. We also estimate the critical value of the screening parameter at which the ionization energy becomes zero. Sometimes, for clarity, a helium atom in which the Coulomb potential is replaced by Eq. (1), shall be referred to as a "screened" helium atom. These calculations are relevant for investigating the behavior and properties of helium atoms in laboratory and astrophysical plasmas.

We shall use atomic units, where the unit of length is $a_0 = \hbar^2/me^2$ and the unit of energy is equal to $-me^4/\hbar^2$. Also $\delta = \alpha a_0$, a dimensionless screening parameter.

II. VARIATIONAL CALCULATION

The Hamiltonian of a heliumlike atom in atomic units is

$$H = \tfrac{1}{2}\nabla_1^2 + \frac{Ze^{-\delta r_1}}{r_1} + \tfrac{1}{2}\nabla_2^2 + \frac{Ze^{-\delta r_2}}{r_2} - \frac{e^{-\delta r_{12}}}{r_{12}} \; , \tag{2}$$

where r_1 is the coordinate of the ith electron with respect to the nucleus of charge Ze and r_{12} is the distance between the two electrons. We shall use variational wave functions which are of the following form:

$$\psi = f(r_1) f(r_2) g(r_1, r_2, r_{12}) \; , \tag{3}$$

where $f(r_i)$ is a hydrogenlike wave function and $g(r_1,r_2,r_{12})$ is a correlation factor. This type of wave functions have been widely used for heliumlike systems, such as H^-, He, Li^+, etc.[13–15] We shall restrict ourselves to relatively simple forms of $g(r_1,r_2,r_{12})$. The wave functions (unnormalized) used by us are the following:

$$\psi = e^{-a(r_1+r_2)} \; , \tag{4}$$

$$\psi = e^{-a(r_1+r_2)}(1+br_{12})^{1/2} \; , \tag{5}$$

$$\psi = e^{-a(r_1+r_2)}(1+br_{12}) \; , \tag{6}$$

$$\psi = e^{-a(r_1+r_2)} e^{br_{12}} \; , \tag{7}$$

and

$$\psi = e^{-a(r_1+r_2)}[1+br_{12}+c(r_1-r_2)^2] \; . \tag{8}$$

Here a, b, and c are variational parameters. For the helium atom ($\delta=0$), wave function (8) is known to give better results than wave functions (4)–(7). However, when the screening is large, it was unclear what the situation might be. Therefore, the calculations were carried out for all the five wave functions. Equation (4) serves as a "zero" level for examining the role of correlation in the present problem. The energy is obtained from

$$E=\langle\psi\,|\,H\,|\,\psi\rangle/\langle\psi\,|\,\psi\rangle\ .$$

The energy associated with the kinetic-energy operator ∇_1^2 and the potential-energy operator $e^{-\delta r_i}/r_i$ can be integrated without much difficulty. The integration associated with the interaction between two electrons is carried out in a different way. The integrant $e^{-\delta r_{12}}/r_{12}$ has to be expanded in terms of the coordinates r_1 and r_2. To do this, we use the fact that

$$\frac{e^{ikr_{12}}}{r_{12}}=kj_0(kr_<)h_0^{(+)}(kr_>)$$
$$=k\frac{\sin(kr_<)}{kr_<}\frac{e^{ikr_>}}{kr_>}\ ,$$

where j_0 is the Bessel function and $h_0^{(+)}$ is the Hankel function of the first kind. $r_<$ stands for the smaller of the lengths r_1 and r_2, and $r_>$ stands for the larger of the lengths r_1 and r_2. If we write $k=i\delta$, it follows

$$\frac{e^{-\delta r_{12}}}{r_{12}}=-\frac{i}{\delta}\frac{\sin(i\delta r_<)}{r_<}\frac{e^{-\delta r_>}}{r_>}\ .$$

Because

$$\sin(i\delta r_<)=i\sinh(\delta r_<)=i\frac{e^{\delta r_<}-e^{-\delta r_<}}{2}\ ,$$

TABLE I. Energy eigenvalues of the screened helium atom from various trial wave functions.

Screening parameter δ	Eq. (4)	Eq. (5)	Energy Eq. (6)	Eq. (7)	Eq. (8)
0.0	2.847 66	2.871 59	2.891 12	2.889 62	2.902 43
0.0001	2.847 36	2.871 29	2.890 82	2.889 32	2.902 13
0.0002	2.847 06	2.870 99	2.890 52	2.889 02	2.901 83
0.0005	2.846 16	2.870 09	2.889 62	2.888 12	2.909 93
0.001	2.844 66	2.868 59	2.888 12	2.886 62	2.899 43
0.002	2.841 66	2.865 59	2.885 13	2.883 62	2.896 44
0.005	2.832 68	2.856 62	2.876 15	2.874 64	2.887 46
0.01	2.817 77	2.841 70	2.861 23	2.859 73	2.872 55
0.02	2.788 10	2.812 03	2.831 56	2.830 01	2.842 89
0.05	2.700 44	2.724 32	2.743 85	2.742 35	2.755 24
0.1	2.558 62	2.582 36	2.601 88	2.600 42	2.613 50
0.2	2.290 31	2.313 54	2.333 03	2.331 68	2.345 49
0.25	2.163 43	2.186 32	2.205 78	2.204 51	2.218 82
0.3	2.041 18	2.063 66	2.083 09	2.081 91	2.096 82
0.4	1.809 91	1.831 48	1.850 81	1.849 85	1.866 20
0.5	1.595 40	1.615 94	1.635 12	1.634 41	1.652 53
0.6	1.396 68	1.416 12	1.435 09	1.434 66	1.454 86
0.7	1.212 92	1.231 20	1.249 91	1.249 78	1.272 33
0.8	1.043 38	1.060 47	1.078 84	1.079 03	1.104 21
0.9	0.887 39	0.903 29	0.921 26	0.921 76	0.949 81
1.0	0.744 39	0.759 10	0.776 57	0.777 40	0.808 51
1.1	0.613 85	0.627 40	0.644 28	0.645 43	0.679 73
1.2	0.495 32	0.507 72	0.523 93	0.525 39	0.562 94
1.3	0.388 41	0.399 70	0.415 12	0.416 87	0.457 64
1.4	0.292 79	0.303 00	0.317 51	0.319 54	0.363 35
1.5	0.208 20	0.217 35	0.230 83	0.233 11	0.279 63
1.6	0.134 48	0.142 60	0.154 90	0.157 38	0.206 04
1.7	0.071 60	0.078 70	0.089 63	0.092 27	0.142 20
1.8	0.019 82	0.025 84	0.035 15	0.037 88	0.087 76
1.9	−0.019 91	−0.015 15	−0.007 92	−0.005 23	0.042 47
2.0					0.006 30
2.1					−0.020 10

TABLE II. Energy eigenvalues of screened He and screened He^+ atoms, and the ionization energy of the screened He atom.

Screening parameter δ	E(screened He)	E(screened He^+)	Ionization energy of the screened He atom
0.0	2.902 43	2.000 00	0.902 43
0.0001	2.902 13	1.999 80	0.902 33
0.0002	2.901 83	1.999 60	0.902 23
0.0005	2.900 93	1.999 00	0.901 93
0.001	2.899 43	1.998 00	0.901 43
0.002	2.896 44	1.996 00	0.900 44
0.005	2.887 46	1.990 02	0.897 44
0.01	2.872 55	1.980 07	0.892 48
0.02	2.842 89	1.960 30	0.882 59
0.05	2.755 24	1.901 85	0.853 39
0.10	2.613 50	1.807 27	0.806 23
0.20	2.345 49	1.628 23	0.717 26
0.30	2.096 82	1.461 84	0.634 98
0.40	1.866 20	1.307 23	0.558 97
0.50	1.652 53	1.163 68	0.488 85
0.60	1.454 86	1.030 55	0.424 31
0.70	1.272 33	0.907 32	0.365 01
0.80	1.104 21	0.793 50	0.310 71
0.90	0.949 81	0.688 68	0.261 13
1.00	0.808 51	0.592 47	0.216 04
1.10	0.679 73	0.504 53	0.175 20
1.20	0.562 94	0.424 54	0.138 40
1.30	0.457 64	0.352 23	0.105 41
1.40	0.363 35	0.287 33	0.076 02
1.50	0.279 63	0.229 60	0.050 03
1.60	0.206 04	0.178 82	0.027 22
1.70	0.142 20	0.134 77	0.007 43
1.80	0.087 76	0.097 26	−0.009 50

therefore

$$\frac{e^{-\delta r_{12}}}{r_{12}}=\frac{1}{2\delta}\frac{e^{\delta r_<}-e^{-\delta r_<}}{r_<}\frac{e^{-\delta r_>}}{r_>}\ .$$

III. RESULTS AND DISCUSSION

The energy expression for each of the five trial wave functions was minimized by varying the corresponding parameters. The resulting energy eigenvalues are shown in Table I for a number of values of δ.

It is of interest to examine the role of the correlation factor as δ increases. At $\delta=0.0001$, as compared to Eq. (4), the improvements obtained from Eqs. (5)–(8) are 0.83%, 1.5%, 1.45%, and 1.89%, respectively. The corresponding figures at $\delta=1.8$ are 23%, 44%, 48%, and 77%. This clearly shows that the factor $g(r_1,r_2,r_{12})$ becomes more important as δ increases.

The three-parameter trial wave function (8) gives the best results for the whole range of δ values. It is known that for the helium atom, this wave function gives fairly good results; the difference between the calculated and the experimental energy is only 0.046%. At low values of δ, we can expect the same sort of accuracy in the results presented here. At high values of δ, however, experience with the screened H atom[11] suggests that the accuracy is expected to diminish.

Among the three two-parameter wave functions that we have considered, Eq. (5) gives the poorest results. The energy from Eq. (6) is better than that from Eq. (7) for $\delta<0.74$, though only by a small margin (less than 0.1%). But this situation is reversed above $\delta\simeq0.74$, and by $\delta=1.8$, the energy from Eq. (7) is better than that from Eq. (6) by 7.8%. If one expands $e^{br_{12}}$ and retains the terms up to the first order of br_{12} in Eq. (7), Eq. (6) is readily obtained.

Table II shows the energies of screened He and screened He^+ atoms, and the difference between the two which is the ionization energy of the screened He atom. The tabulated results for the screened helium atom are from Eq. (8). The energy of screened He^+ atom was calculated using the wave function suggested in a previous paper[11] where it was shown to give very good results for the screened H atom. As the ionization energy is given by the difference between two numbers, in percentage terms, even small errors in those two numbers can get magnified in the resulting ionization energy. At $\delta=0$, the difference between the observed and the calculated value [Eq. (8)] of the ionization energy is 0.14%. It would be reasonable to expect the same sort of accuracy in the calculated value of the ionization energy when δ is small. As δ increases, the accuracy of both, E(screened He) and E(screened He^+), is expected to diminish, but as the errors will be in the same direction, there will be some cancellation. Overall it is reasonable to surmise that the accuracy of the ionization energy will also diminish with the increase of δ.

Our results indicate that the ionization energy of the screened helium atom becomes zero at about $\delta=1.74$, but as our results in this region may have poor accuracy, this value of δ can only be considered to be a lower limit for the critical screening parameter; the true value is expected to be a few percent larger.

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