Do atomic electrons stay bound in changing plasma environment?

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We present a detailed theoretical study on the disappearance of bound states for two-electron atoms subject to electron-ion collisionless plasma. In contrast to many other recent theoretical works, our analysis leads to the conclusion that the two-electron Coulomb interaction between atomic electrons should not be modified by a long-range Coulomb screening similar to the one-electron screened Coulomb potential for the atomic electrons based on the Debye-Hückel model. Our quantitative estimates have also resolved the qualitative disparity on the disappearance of the bound states between the one- and two-electron atoms, which has been suggested implicitly by a series of recent theoretical studies. We also point out a number of interesting problems for further study and the potential impact on other high density plasma systems.

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Theoretical study of atomic processes in plasma environment has attracted considerable renewal interests recently [1-10] following a number of earlier works [11-13] based on the application of the Debye-Hückel model [14] for a classical electron-ion collisionless plasma under thermodynamical equilibrium. Quantitative atomic data have been compiled for the bound-bound transitions, the photoionization, and the electron-atom collision for one- and two-electron atoms [1-13]. Almost all the recent theoretical estimations [1-10] employ a screened Coulomb potential (or, the Yukawa potential) for an atomic electron subject to a one-electron Hamiltonian, i.e.,
\[
\hat{h}_o(r; D) = \frac{p^2}{2m} - \frac{Ze^2}{r}e^{-r/D},
\]
where \( p \) is the momentum operator of the atomic electron and \( Z \) is the nuclear charge. The screening parameter \( D \) is known as the Debye-Hückel length (or Debye length). It characterizes the screening of the nuclear charge experienced by the atomic electron due to the plasma in the outer region of an atom and given by (see, e.g., Eq. (2.5) of [13])
\[
D \text{ (in cm)} = 6.90 \left( \frac{T}{n} \right)^{1/2},
\]
where \( T \) and \( n \) are the plasma temperature (on Kelvin scale) and density (in \( cm^{-3} \)), respectively. The value of \( D \) ranges over many orders of magnitude, i.e., from \( 10^{-2} \) \( nm \) for the plasma in solar core to over \( 10^4 \) \( m \) for the ones in intergalactic medium. Since the plasma temperature usually varies only 3 to 4 orders in magnitude (e.g., from \( 10^2 \) \( °K \) to \( 10^6 \) \( °K \)), the value of \( D \) (or, the degree of penetration of the ion-electron gas into the atom) depends more on the variation of the plasma density.

For the low-density plasmas such as the ones in interstellar medium or even for those generated in low power gas discharge, the Debye length \( D \) may be a few orders of magnitude larger than the size of the atoms and should have little effect on the atomic processes. On the other hand, for the high density plasma system such as the ones in the Sun and Sun-like stars, the Debye length is of the order of \( 10^{-11} \) \( m \). Consequently, the effect of the screening could change significantly the atomic transitions for the astrophysical relevant elements. That, in turn, could have serious implication to the opacity data, which is of critical importance to the development of high quality equation of state for such systems [15]. For the laser-generated dense plasma at an electronic temperature of few hundred eV and a density of \( 10^{28} - 10^{36} \text{ m}^{-3} \) [16, 17], the Debye length would be comparable to the size of the atoms. Although the laser plasma is far from a thermodynamically equilibrium system, a detailed theoretical estimate based on the Debye-Hückel model may help to better understand qualitatively the physics behind the observed spectra.
For the one-electron atom, the most interesting feature of the screened Coulomb potential is the disappearance of the bound state as \( D \) becomes smaller than the corresponding critical screening length of that particular state (see, e.g., Tables III and IV of [11]). In other words, the potential can only attract a decreasingly finite number of bound states below the ionization threshold as \( D \) decreases [11-13]. For the multi-electron atoms (e.g., \( H^- \), \( He \) and \( Li \)), a number of recent works [2, 6-8] appear to suggest that many of the singly excited states remain bound even when \( D \) is smaller than the average size of an isolated atom in the same singly bound excited states. In particular, for the ground state of \( H^- \), it concludes that even when \( D \) is substantially smaller than the average size of the ground state of the isolated \( H^- \), its ground state remains bound [7]. Similar conclusion has also been reached based on the application of an exponential-cosine-screened Coulomb potential [18] for the ground state of \( He \) [8]. Such implication is intuitively and qualitatively different from the disappearance of the bound states for the hydrogen atoms in plasma environment. The main objective of this paper is to point out that such qualitative disparity between the disappearance of the bound states in one- and two-electron atoms results from an a priori application of the Debye screening to the two-electron interaction that is similar to the one for the one-electron orbit. It has perhaps unintentionally, but, effectively led to a potential for the atomic electrons that is significantly more attractive than it should be.

Following the Debye-Hückel original approximation, the potential \( V_o(r) \) due to an electron-ion plasma at a distance \( r \) far from a force center (e.g., an atomic nucleus) outside an inner Debye sphere of radius \( A \) can be derived from the Gauss’ law

\[
\nabla^2 V_o(r) = -\frac{\rho(r)}{\epsilon}, \quad r \geq A,
\]

where \( \epsilon \) is the dielectric constant of the electron-ion gas and \( \rho \) is its total charge density at \( r \). Assuming a charge density of \( \rho_o \) at \( r = \infty \) with a zero potential \( V_o(r = \infty) = 0 \) and following the Boltzmann distribution, the charge densities of the positive charge \( q \) and the negative charge \(-q\) at \( r \) could be expressed as \( \rho_+ (r) = \rho_o e^{-qV_o(r)/kT} \) and \( \rho_-(r) = \rho_o e^{+qV_o(r)/kT} \), respectively, where \( k \) is the Boltzmann constant and \( T \) the absolute temperature. The net total charge density at \( r \) is then given by

\[
\rho(r) = \rho_o(e^{-\frac{qV_o(r)}{kT}} - e^{\frac{qV_o(r)}{kT}}) = -2\rho_o \sinh \left( \frac{qV_o(r)}{kT} \right).
\]

Assuming, in addition, that the potential energy is relatively small comparing to the kinetic energy, Eq. (3) for the potential \( V_o(r) \) in the outer region of the Debye sphere.
could then be approximated by the *linear* Poisson-Boltzmann equation

\[ \nabla^2 V_o(r) = \left( \frac{1}{D^2} \right) V_o(r), \quad r \geq A, \]  

(5)

where \( D > A \) is the Debye length defined by the charge density \( n (\sim q \rho_o) \) and the temperature \( T \) outside the Debye sphere and given by Eq. (2). The potential inside the Debye sphere can also be derived from the Gauss’ law and takes the form of

\[ V_i(r) = -\frac{Ze}{r} + \text{Constant}, \quad r \leq A \]  

(6)

with a nucleus charge \( Z \) located at \( r = 0 \). By matching the two potentials \( V_o \) and \( V_i \) and their first-order derivatives at \( r = A \), one gets \([12, 13]\)

\[ V_D(r) = \begin{cases} V_i(r) = -Ze^2(\frac{1}{r} - \frac{1}{D+A}), & r \leq A \\ V_o(r) = -Ze^2(\frac{De^{A/D}}{D+A}) e^{-r/D}, & r \geq A. \end{cases} \]  

(7)

In the limit when \( A \to 0 \), Eq. (7) reduces approximately to the screened Coulomb potential employed in most of the recent theoretical atomic calculations. A more detailed atomic structure calculation should replace the one-electron Hamiltonian in Eq. (1) by the potential given by Eq. (7), i.e.,

\[ h_d(r; D) = \frac{p^2}{2m} + V_D(r), \]  

(8)

especially when \( D \) is comparable to the size of the atom (or, the radius \( A \) of the Debye sphere).

Following the Debye-Hückel model outlined above, the \( N \)-electron Hamiltonian for an atom in plasma environment can now be expressed in terms of \( h_d(r; D) \) given in Eq. (8) as

\[ H(r_i, r_j, \cdots; D) = \sum_{i=1,N} h_d(r_i; D) + \sum_{i>j} \frac{e^2}{r_{ij}}, \]  

(9)

where \( r_{ij} = | \vec{r}_i - \vec{r}_j | \) represents the separation between the atomic electrons \( i \) and \( j \). Qualitatively, the atomic processes are limited only to electrons which do not move freely far away from the nucleus. As a result, there is no compelling reason to modify the two-electron Coulomb interaction by the long-range Debye screening since the effect due to the plasma environment outside the Debye sphere is already accounted for by the potential \( V_D(r) \).
The numerical results presented below are calculated with the B-spline based methods which have been applied successfully to a large number of atomic structure properties [19-21]. The energies of the bound states and the oscillator strengths between various states are calculated typically with a basis set of atomic orbitals representing over 10,000 two-electron configurations. Our calculated results are in excellent agreement with the most accurate non-relativistic theoretical results [22, 23] in the absence of plasma environment, e.g., at $D = 10^{12}$ Bohr radius ($a_o$). For the excitation energies, the agreement is about $10^{-4}$ $Ry$ or better, the oscillator strengths to three to four digits, and the agreement between length and velocity results in oscillator strength at 0.1% or better.

As we pointed out earlier, the main objective of this work is to understand the qualitative disparity in the disappearance of bound states between the one- and two-electron atoms implied from the recent theoretical estimates and to clearly identify that such difference indeed results from the two-electron Debye screening included in those calculations for the two-electron atoms. To that end, we present in Fig. 1 the comparison between the calculations we have carried out with Hamiltonian given by Eq. (9) with $A = 0$ and the one by Eq. (1) of [6]. The threshold energies for $He^+$ (1s) shown in Fig. 1 are identical from both calculations as they should be. The energy for the $He$ 1s$^2$ 1S ground state from the present calculation intersects the threshold energy at a substantially larger $D$ (greater than 1.5 $a_o$) than a value of less than 0.5 $a_o$ (off the scale shown) from [6] which used a two-electron interaction term in the form of $e^{-r_{ij}/D}/r_{ij}$ in contrast to the $1/r_{ij}$ employed in the present calculation. In fact, even with a two-electron interaction modified with a $cos (r/D)$ factor [8, 18], i.e., which has the effect of a smaller reduction in the repulsive interaction between two atomic electrons than the strict two-electron screened Coulomb potential, the result given in [8] shows that the ground state remains bound at $D = 0.75$ $a_o$.

A more rigorous application of the Debye-Hückel model using the one-electron Hamiltonian given by Eq. (8) should lead to a more negative $He^+$ (1s) ground state energy since the one-particle attractive potential $V_D$ in the outer region with $r > A$ is substantially enhanced by the factor $e^{-L/D}/r_{ij}$ from the simple screened Coulomb potential. Fig. 2(a) shows a substantial change in the $He^+$ (1s) threshold energies with $A = 1.0$ $a_o$. Even with a much greater threshold energy, our calculations show clearly that the $He$ 1s$^2$ 1S ground state energy intersects the $He^+$ threshold at a value of $D$ around 1.0 $a_o$. This leads to a critical length approximately at 1.0 $a_o$ with a qualitative feature similar to the one-electron atoms. Again, Fig. 2(a) shows clearly that the estimated $He$ ground state energies and the $He^+$ threshold energies from [6] remain far apart at $D = 1.0$ $a_o$. In fact, as we pointed out earlier, the theoretical estimates from [6] and [8] imply that the ground state of $He$ will remain bound until the Debye lengths at $D = 0.45$ $a_o$ and
0.75 \ a_o, \ 
respectively, \ i.e., \ at \ a \ distance \ smaller \ than \ the \ average \ size \ of \ an \ isolated \ He \ atom \ in \ its \ ground \ state. \ Fig. \ 2(b) \ shows \ the \ results \ of \ the \ present \ calculation \ for \ H^- \ atom. \ Our \ estimated \ critical \ length \ is \ slightly \ greater \ than \ 17 \ a_o \ (close \ to \ the \ value \ of \ \ A) \ where \ the \ energy \ of \ the \ H^- \ 1S \ ground \ state \ intersects \ the \ H(1s) \ threshold \ energy. \ This \ suggests \ the \ disappearance \ of \ the \ H^- \ ground \ state \ at \ a \ value \ of \ D \ much \ greater \ than \ a \ value \ of \ D \ that \ is \ smaller \ than \ 1.4 \ a_o \ suggested \ by [7]. \ Again, \ this \ difference \ in \ theoretical \ estimates \ is \ due \ to \ the \ use \ of \ Debye \ screening \ for \ the \ two-electron \ interaction \ in \ the \ Hamiltonian \ for \ the \ two-electron \ atoms.

Fig. 3 presents the results of our calculation using the Hamiltonian given by Eq. (9) on the energy variation of the He \ n = 2 \ and \ 3 \ singly \ excited \ states \ as \ D \ changes. \ We \ have \ nominally \ chosen \ the \ radius \ of \ the \ Debye \ sphere \ A = n^2 a_o. \ For the \ n = 2 \ singly \ excited \ bound \ states, their \ disappearances \ occur \ at \ D \ values \ ranging \ from \ 7 \ a_o \ for \ the \ 1s2s \ 3S \ state \ to \ slightly \ less \ than \ 12 \ a_o \ for \ the \ 1s2p \ 1P \ state. \ In \ contrast, \ the \ results \ from [6] \ suggest \ that \ the \ n = 2 \ bound \ excited \ states \ remain \ bound \ even \ when \ D \ is \ as \ small \ as \ 1 \ a_o, \ i.e., \ at \ a \ D \ value \ substantially \ smaller \ than \ the \ estimated \ radius \ of \ the \ isolated \ He \ atom. \ The \ disappearance \ of \ the \ singly \ excited \ n = 3 \ states \ starts \ at \ D \ as \ large \ as \ 26 \ a_o \ for \ the \ 1s3p \ 1P \ state \ to \ around \ 19 \ a_o \ for \ the \ 1s3s \ 3S \ state. \ Clearly, \ based \ on \ the \ present \ calculation, \ there \ is \ no \ qualitative \ disparity \ between \ the \ disappearances \ of \ the \ bound \ states \ of \ the \ one- \ and \ two-electron \ atoms \ due \ to \ the \ plasma \ environment \ as \ suggested \ by \ the \ recent \ theoretical \ estimates.

As for the atomic transition, our calculation shows that there is indeed a decrease in the energy differences between the bound states and a small variation in the corresponding oscillator strength. For instance, the excitation energy for the transition from the He \ 1s^2 \ 1S \ ground \ state \ to \ the \ 1s2p \ 1P \ excited \ state \ decreases \ by \ about \ 6\% \ together \ with \ a \ small \ reduction \ (about \ 10\%) \ in \ the \ oscillator \ strength \ as \ D \ decreases \ to \ the \ limit \ when \ the \ 1s2p \ 1P \ state \ disappears. \ This \ is \ qualitatively \ consistent \ with \ the \ observed \ red \ shift \ in \ the \ emission \ spectra \ for \ the \ He-like \ atoms [2, 16, 17]. \ Although \ there \ is \ minor \ quantitative \ difference \ between \ the \ present \ calculation \ and \ other \ calculations \ with \ the \ screened \ two-electron \ interaction [5], \ there \ is \ little \ qualitative \ difference \ in \ the \ variation \ of \ the \ transition \ energy \ and \ oscillator \ strength \ as \ D \ decreases. \ More \ detailed \ quantitative \ results \ and \ comparison \ with \ the \ results \ from \ other \ calculations \ will \ be \ presented \ elsewhere.

The disappearance of the He singly excited bound states due to the plasma environment may also affect substantially the presence of the doubly excited resonances in the He ground state photoionization spectra. Since the spectra of such resonances, for isolated He atoms, are dictated primarily by the one-electron transitions from the 1sns
or $2pnp$ configurations mixed in the initial state to the doubly excited $2pns$, $2snp$, or $2pmd$ configurations in the final states, the transition amplitude leading to the doubly excited resonances would be greatly impacted by the disappearance of the corresponding $1sns^1S$ bound states as $D$ decreases. In addition, the lack of low-lying singly bound excited could also reduce substantially the dielectronic recombination rate. The other interesting question for further exploration is what happen to the $1s^2 \, ^1S \rightarrow 1snp \, ^1P$ transitions when the individual bound excited state is pushed into the continuum, if it indeed occurs, as $D$ decreases.

In conclusion, we present in this paper the Hamiltonian for a multi-electron atom subject to a thermodynamical equilibrium electron-ion collisionless plasma. It differs from the ones employed in other recent calculations. In particular, we have concluded that there is no theoretical ground to include a long-range Coulomb screening in the two-electron interaction between the atomic electrons. Our quantitative analysis has led to a more intuitively expected qualitative picture on the disappearance of the bound states as the penetration of the plasma gas increases. We have also pointed out a number of interesting problems for further investigations and the potential impact on the development of high quality equation of motion for high density solar plasma.

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References


Figure Captions

Figure 1: The energy variation of the $He^+$ (1s) threshold and the $He$ 1s$^2$ $^1S$ ground state as functions of $1/D$ with $A = 0$. The results from [6] are also presented for comparison.

Figure 2: (a) The energy variation of the $He^+$ (1s) threshold and the $He$ 1s$^2$ $^1S$ ground state as functions of $D$ with $A = 1a_o$. The results from [6] are also presented for comparison. (b) The energy variation of the $H^-$ (1s) threshold and the $H^- 1s^2$ $^1S$ ground state as functions of $D$ with $A = 17a_o$. The results from [8] are also presented for comparison.

Figure 3: The top plot presents the energy variation of the $He$ $(1s2p)^1P$, $(1s2p)^3P$, $(1s2s)^1S$, and $(1s2s)^3S$ states as functions of $D$ with $A = 4a_o$. The bottom plot presents the energy variation of the $He$ $(1s3p)^1P$, $(1s3p)^3P$, $(1s3s)^1S$, and $(1s3s)^3S$ states as functions of $D$ with $A = 9a_o$. 