Detachment energies for a negative hydrogen ion embedded in a variety of Debye plasmas

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Very accurate variational calculations have been performed to determine the ground state energy of the negative hydrogen ion when it is embedded in a variety of Debye plasmas. The results predict a high degree of stability even under strong plasma conditions. [S1063-651X(96)06105-3]

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I. INTRODUCTION

In the investigation of plasmas consisting of atomic ions and electrons a good understanding of the interaction potentials among those species is essential. Compared to the vacuum case the forces between the charges are modified due to short-range order and static and dynamical screening effects introduced by neighboring ions and fast electrons, respectively. These modifications effect one-electron properties (e.g., spectral lines which serve as key quantities in plasma diagnostics) as well as properties involving more than one electron (e.g., dielectronic recombination rates which lead to plasma losses). Extending the usual Debye-Hückel treatment of screening to encompass also dynamic screening effects due to ion motions, is an important research area in its own right. Such research is expected to be noticeably facilitated by the incorporation of the static screening effects into the calculation of the atomic properties and processes right from the beginning—in zeroth order, so to speak. Doing so, one can then formulate a procedure which allows the simultaneous evaluation of level broadening and of the lowering of the continuum threshold—both on the same footing.

In a recent study [1] the numerical pair function method [2] has been extended to incorporate the effect of electron-ion screening on the ground state energy of the negative hydrogen ion. In this investigation the attractive Coulomb potential between the electron and the nucleus has been replaced by a screened potential of the Debye type, as well as of the more general Debye-Laughton type. Varying the Debye length parameter D from infinity—which corresponds to no screening—to small values, different plasma conditions can be simulated. Since the Debye parameter is a function of both the electron density n_e and the electron temperature T_e, a particular value of D corresponds to a range of plasma conditions. It is, however, meaningful to associate smaller values of D with stronger screening. Furthermore, varying the parameter D in combination with an additional condition, such as the ratio of neutral to ionized species, it was possible to perform a systematic study of plasma effects. In this first study, the electron-electron interaction, however, has not been screened. Hence the calculated values of the binding energy of the negative hydrogen ion can only be taken as a first indication that the assumedly very fragile H^- ion is more stable under plasma conditions than initially assumed.

With the present study the screening has been extended to include also the effect on the electron-electron interaction. As expected, this modification results in a lowering of the ground state energy, corresponding to an increased stability of an H^- ion which is embedded in a Debye plasma. The magnitude of the effect, however, came as a surprise. Since screening in one form or the other is a fact in plasmas, the present results, based strictly on the validity of the Debye model, exhibit general, qualitative features but will have to be fine tuned when evidence exists that the Debye model is not a good approximation. This one would expect in plasmas which are far off from thermal equilibrium. Lacking such evidence for the general case, however, one may assume that the present results are representative for the main effects of screening on the binding energy. For an analysis of the ion population, on the other hand, the knowledge of very accurate ionization or, rather, detachment potentials is a critical issue because of their exponential magnification in Boltzmann factors.

II. CALCULATIONS

The nonrelativistic Hamiltonian

$$H=-\frac{1}{2}\nabla_1^2-\frac{1}{2}\nabla_2^2-\frac{\exp(-r_1/D)}{r_1}-\frac{\exp(-r_2/D)}{r_2}+\frac{\exp(-r_{12}/D)}{r_{12}}, \tag{1}$$

describing the negative hydrogen ion in a Debye plasma characterized by the parameter D, has been diagonalized in a basis of correlated functions of the following type:

$$\varphi_{klm}(r_1,r_2,r_{12})=N_{klm}(e^{-\alpha_k r_1}e^{-\beta_l r_2}\pm e^{-\beta_l r_1}e^{-\alpha_k r_2})e^{-\gamma_m r_{12}}. \tag{2}$$

Here the variables r_1 and r_2 are the radial coordinates of the two electrons and the variable r_{12} stands for the distance between them, while the quantity N_{klm} is a normalization factor. Expansions of this type have previously been shown to be very efficient in obtaining highly accurate variational wave functions for S states of two-electron atoms of [3]. The two signs correspond to singlet and triplet states, respectively. For the present study of the ground state binding energy of the system only the positive sign is relevant, because the ground state of the H^- ion has ^1S symmetry. The nonlinear parameters α_k, β_l, and γ_m have been preselected to approximate a definite integral optimally as described in the

TABLE I. The energy of the negative hydrogen ion (column 3) is compared to the ground state energy of the neutral hydrogen atom (column 2) as a function of the Debye parameter D (column 1). The detachment energy (column 4) is the difference of the entries in columns 2 and 3. All energy values are given in atomic energy units, while the Debye length is given in atomic length units.

Debye parameter in a.u.	Energy of neutral hydrogen	Energy of the negative ion	Detachment energy
0.875	−0.000 60	−0.000 62	0.000 024
0.9	−0.001 75	−0.001 89	0.000 137
0.95	−0.005 34	−0.005 72	0.000 378
1	−0.010 29	−0.010 95	0.000 655
2	−0.148 12	−0.157 83	0.009 706
4	−0.290 92	−0.310 74	0.019 816
6	−0.352 26	−0.375 68	0.023 417
8	−0.385 88	−0.410 92	0.025 035
10	−0.407 06	−0.432 95	0.025 892
15	−0.436 53	−0.463 38	0.026 848
20	−0.451 82	−0.479 04	0.027 215
30	−0.467 48	−0.494 99	0.027 505
50	−0.480 30	−0.507 95	0.027 654
100	−0.490 07	−0.517 80	0.027 731
200	−0.495 02	−0.522 76	0.027 743

earlier reference which introduced this particular type of integral transform wave functions. The linear parameters are determined in the usual variational procedure by solving the generalized secular equation

$$\mathrm{Det}(\mathbf{H}-\mathbf{S}E)=0. \tag{3}$$

Here $\mathbf{H}$ and $\mathbf{S}$ stand for the Hamiltonian and overlap matrices, respectively. Since the main goal of this study has been to accurately calculate the correlation energy of the H^- ion embedded in a pure Debye plasma without overestimating the effect, a comparatively large basis set of 120 functions of the type given in Eq. (2) has been used. For the same reason we have abandoned the previously used pair function approach, since this method is not variational and can, in principle, lead to energies that are lower than the true value although this has never happened before, at least not when the results were extrapolated to infinitely fine grid size.

The variational calculations have been performed with highly accurate integral transform wave functions which contain the interelectronic distance explicitly as a dynamical variable. The use of the correlated wave functions containing the interelectronic distance r_{12} as a dynamical variable in connection with the Debye potential is very convenient because all integrals can be expressed in closed form using the formulas given in [3]. No new integrals needed to be included.

Although an extension of the correlated wave function approach to atoms with more than two electrons may not be practical, the treatment of systems of particles interacting via Yukawa forces by an appropriate modification of more standard methods of quantum chemistry or atomic theory is possible. In fact, systems of particles interacting via Yukawa forces have been studied early on in nuclear physics, e.g., by Swiatecki [4]. This reference also contains the formulas for the interaction integrals of particles described by wave functions of a Gaussian type, i.e., $\exp(-\alpha r^2)$, and interacting via Yukawa forces. The adaptation to systems with both attractive and repulsive screened interactions and the interpretation of the results as meaningful for ions embedded in a plasma, however, is different and promises interesting results, in particular, for the further study of atomic processes in plasmas.

The results of the present calculations are presented in the third column of Table I. In column 2, the ground state energy of neutral hydrogen embedded in a Debye plasma is given for comparison. The fourth column, finally gives the detachment energies for various values of the Debye constant which is displayed in column 1. All calculations have been performed in extended precision on the CONVEX 120 computer system of the Chemical Physics program at the University of Nevada at Reno.

III. SUMMARY AND DISCUSSION

While in our previous work the screening effects were applied only to the electron-ion interaction, the present study extends Debye screening also to the electron-electron interaction. A variational calculation of the ground state energy of the negative hydrogen ion has been performed for various plasma conditions characterized by different values of the Debye parameter D. This results in a considerable increase in the stability of the ion as compared to the case of an unscreened interaction (i.e., with only the electron-ion potential screened). In fact, our findings indicate that the negative hydrogen ion survives increasing plasma conditions as safely as neutral hydrogen does and that both species lose their binding property simultaneously as a function of decreasing values of D. The smallest value for which binding of the two-electron system has been obtained (although with a tiny value of the detachment energy of 0.24×10^{-4} a.u.) is $D=0.875$ a.u. This value is so close to the value obtained by Rogers, Graboske, and Harwood [5] for the limit beyond which not even neutral hydrogen is able to support a bound state that it is safe to state as our main finding the fact that the two electrons are pressure ionized simultaneously as opposed to consecutively. As a function of decreasing values of D the detachment energy of H^- decreases initially very slowly from its vacuum value of 0.0277 a.u. and holds still a sizeable 0.0234 a.u. at $D=6$. From then on it drops rapidly.

As an example of related research, we refer to a study by Scheibner, Weisheit, and Lane [6] of plasma screening effects on proton-impact excitation of positive ions. In this work two screened ions interact via a Debye force.

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