Autoionizing $^1S^e$ resonance of H^- in Debye plasma environments

Sabyasachi Kar and Y. K. Ho
Institute of Atomic and Molecular Sciences, Academia Sinica, P.O. Box 23-166, Taipei, Taiwan 106, Republic of China
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We have made an attempt to investigate atomic resonances in various Debye plasma environments. The $2s^2\ ^1S^e$ autoionization resonance for a two-electron system H^- is determined by calculating the density of resonance states using the stabilization method. Highly correlated Hylleraas-type wave functions are used to represent the correlation effects between the three charged particles. The calculated resonance energies and widths for the various Debye parameters ranging from infinity to a small value are reported.

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I. INTRODUCTION

The study of the atomic processes in the plasma environments has become an interesting topic in recent years. The investigations on the two-electron systems in the plasma networks play an important role because of the relative ease with which correlation effect can be identified. In such environments, the interaction between the core and the valence electrons with the atomic nucleus is screened. Several investigations on two electron systems have been performed in a variety of model plasmas. Winkler [1] and Zhang and Winkler [2] have studied the ground state energies of the negative hydrogen ion and helium embedded in a variety of Debye plasmas. In such environments, pair-function calculations for two-electron systems have been reported by Wang and Winkler [3]. In their pair function calculations, Wang and Winkler [3] have reported the stability of H^- and the energy splitting of several $1snp$ states of the He atom. Dai *et al.* [4] have reported a calculation of the properties of the screened He-like systems using correlated wave functions. The calculation of autoionizing states turns out to be more difficult and requires the development of an alternative technique. To our knowledge, no investigation on the *S*-wave autoionization states of H^- in Debye plasmas has been done in the literature. It is worthy of mention in this context that an investigation on resonances of model screened Coulomb potential was carried out by Wang and Winkler [5]. They have presented an analytic method for the calculation of shape resonances for a model problem. In the present work, we have investigated the lowest *S*-wave resonance using a model screened Coulomb potential [3] for the hydrogen negative ion. It should be mentioned in this regard that Roussel and O'Connell [6] have performed a variational calculation of the Schrödinger's equation for atomic hydrogen in static screened Coulomb potentials, and Rogers *et al.* [7] have investigated the bound states of H in static screened Coulomb potentials.

In the present work, an attempt has been made to investigate the $2s^2\ ^1S^e$ autoionization resonance for H^- in various model plasma environments. In this investigation, the attractive Coulomb potential between the electron and the nucleus has been replaced by a screened potential of Debye type $\exp(-r/D)/r$. The importance of the screened Coulomb potential in the modeling of atomic potential has been discussed in the work of Stein *et al.* [8]. It has already been mentioned that Wang and Winkler [5] have studied an analytic solution to the resonance problem of screened Coulomb potentials. In their study, Wang and Winkler [5] have used the four parameter Debye-Laughton potentials. We have not included explicitly the screening for the electron-electron interaction terms. Instead, we introduce a scaling factor b with the screened potential [to read $b\exp(-r/D)/r$], and adjust b to b' to reproduce the ground state energies of Winkler [1] where the electron-electron screening was explicitly included. Varying the Debye length D from infinity to small values, different resonance parameters (energy and width) have been obtained. A particular value of D corresponds to the range of plasma conditions, as the Debye parameter is a function of electron density and the electron temperature. The smaller values of D are associated with the stronger screening. A parameterized screening potential approximated the effects of the plasma charges on the interaction between the bound electron and the atomic nuclei. We have used the stabilization method proposed by Mendelshtam *et al.* [9] to calculate the resonance energy E_r and the width Γ of the $2s^2\ ^1S^e$ autoionizing resonant state of H^- embedded in a variety of model plasmas. The latest development of this method [9–11] to calculate resonance positions and widths requires only L^2 functions. The details of this simple and powerful method are available in the works of Ho and coworkers [11].

II. CALCULATIONS

The nonrelativistic Hamiltonian (in Rydbergs) describing the negative hydrogen ion in Debye plasma characterized by the parameter D is given by [1]

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

where r_1 and r_2 are the radial coordinates of the two electrons and r_{12} is their relative distance. In the present calculation, we have considered no explicit screening on r_{12}. For this, we have set the Hamiltonian (in Rydbergs) as

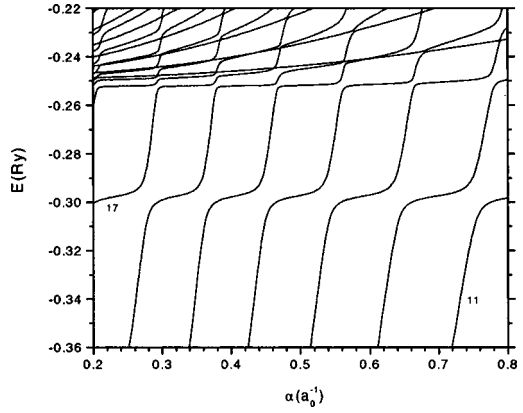

FIG. 1. Energy eigenvalues vs α parameters for the $2s^2\ ^1S^e$ states of H^-.

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

where the scaling factor b is adjusted to reproduce the ground state energy of H^-, as reported by Winkler [1] for various Debye parameters in which the electron-electron screening was also included.

For the singlet S-wave doubly excited states of H^-, we have used the Hylleraas-type wave functions

$$\Psi = \sum_{k+m+n\leqslant\omega} C_{kmn} r_{12}^n (r_1^k r_2^m + r_1^m r_2^k)\exp[-\alpha(r_1+r_2)], \tag{3}$$

with k,m,n, and ω being the positive integer or zero, $k \geqslant m,\omega$ will determine the basis size N in the basis expansion of Eq. (3).

We have used the stabilization method to extract resonance energies and widths by calculating the density of resonance states. After diagonalization of the Hamiltonian (2) with the Hylleraas-type basis function (3), we obtained the energy levels $E(\alpha)$ which leads to a stabilization plot. The scaling parameter α in the wave function [Eq. (3)] can be considered as the reciprocal range of a "soft" wall [11]. Detailed discussions are available in the recent work of Kar and Ho [11].

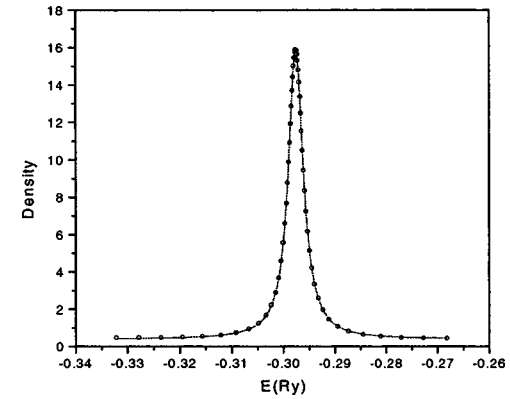

FIG. 2. Calculated density (circles) and the fitted Lorentzian (solid line) for the $2s^2\ ^1S^e$ resonance states of H^-.

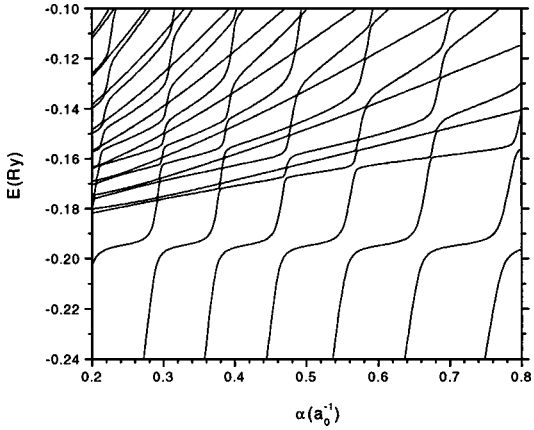

FIG. 3. Stabilization plot for the $2s^2\ ^1S^e$ states of H^- in model Debye plasma environments for $D=30$ and $b=b'$.

To extract the resonance energy E_r and the resonance width Γ, we have calculated the density of the resonance states for a single energy level with the help of the following formula:

$$\rho_n(E) = \left|\frac{E_n(\alpha_{i+1}) - E_n(\alpha_{i-1})}{\alpha_{i+1} - \alpha_{i-1}}\right|^{-1}_{E_n(\alpha_i)=E}, \tag{4}$$

where the index i is the ith value for α and the index n is for the nth resonance. After calculating the density of resonance states $\rho_n(E)$ with the above formula (4), we fit it to the following Lorentzian form that yields resonance energy E_r and total width Γ, with

$$\rho_n(E) = y_0 + \frac{A}{\pi}\frac{\frac{\Gamma}{2}}{(E-E_r)^2 + \left(\frac{\Gamma}{2}\right)^2}, \tag{5}$$

where y_0 is the baseline offset, A is the total area under the curve from the baseline, E_r is the center of the peak, and Γ denotes the full width of the peak of the curve at half height.

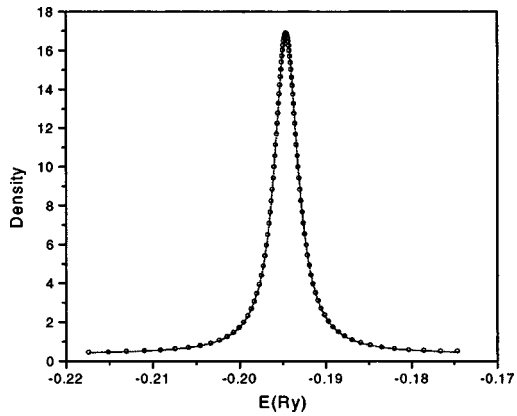

FIG. 4. Calculated density (circles) and the fitted Lorentzian (solid line) for the $2s^2\ ^1S^e$ resonance states for $D=30$ and $b=b'$.

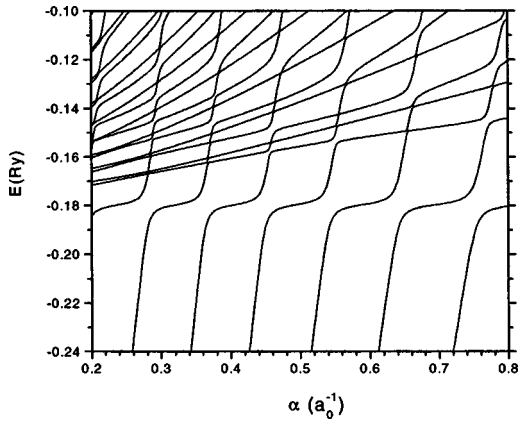

FIG. 5. Stabilization plot for the $2s^2\ ^1S^e$ states of H^- in model Debye plasma environments for $D=30$ and $b=1$.

To construct the stabilization plot, we have used expansion length of $N=715$ ($\omega=18$) in the basis function (3). Considering Debye length tends to infinity which corresponds to no screening, we have successfully reproduced the results of Tan and Ho [11] for $N=525$ and 715. Reproduced results of Tan and Ho [11] for the $2s^2\ ^1S^e$ resonant states of e^--H scattering are presented in Figs. 1 and 2 using $N=715$. We use 301 points to cover the range of α from 0.2 to 0.8. The stabilization plot in Fig. 1 shows the stabilization character near $E=-0.3$ Ry. We have calculated the density of resonance states for the individual energy levels from 11th to 17th in the range 0.2–0.8, with one energy level at a time. The calculated density of resonance states from the single energy eigenvalue is then fitted to Eq. (5), and the one that gives the best fit (with the least chi-square) to the Lorentzian form is considered as the desired results for that particular resonance. Figure 2 shows the fitting of the density of the resonance states for the 16th eigenvalue of the stabilization plot. From the fit, we obtain the resonance energy $E_r=-0.297\,55$ Ry and the corresponding width as $\Gamma=-0.003\,47$ Ry. The circles are the results of the actual calculations of the density of the resonance states using formula (4) and the solid line is the fitted Lorentzian form of the corresponding $\rho_n(E)$. The result for the $2s^2\ ^1S^e$ resonant states of e^--H scattering is comparable with the reported results of Ho *et al.* [12]. During their study on the precision calculation of the lowest $^1S^e$ resonance in e^--H scattering, they have reported the resonance energy $E_r=-0.297\,553\pm0.000\,004$ Ry and the corresponding width as $\Gamma=-0.003\,462\pm0.000\,008$ Ry which are nicely comparable to our results $E_r=-0.297\,55$ Ry and the corresponding width as $\Gamma=-0.003\,47$ Ry.

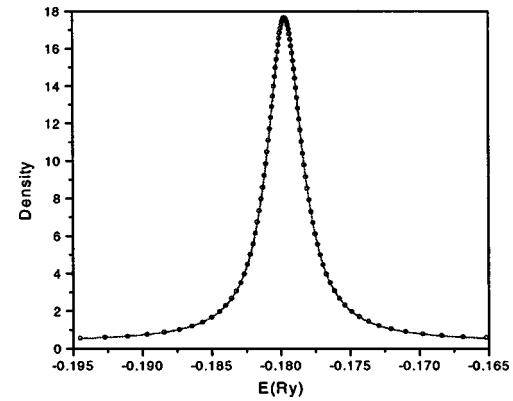

FIG. 6. Calculated density (circles) and the fitted Lorentzian (solid line) for the $2s^2\ ^1S^e$ resonance states for $D=30$ and $b=1$.

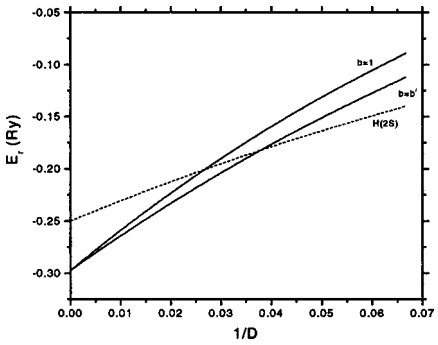

FIG. 7. The $2s^2\ ^1S^e$ resonance energy E_r as a function of $1/D$. Dashed line denotes the H(2*S*) threshold energy.

When the density of the resonance states $\rho_n(E)$ is fitted to the Lorentzian form, it has been observed that the value of χ^2 for each fitting is much less than 0.1. All the results shown in Figs. 1–10 and Table I are obtained using the 715-term wave functions. It is mentioned earlier that we have not included explicitly the screening for the electron-electron correlation terms. It is therefore worthwhile to include the electron-electron screening explicitly in future investigations.

The $2s^2\ ^1S^e$ resonance energies and widths for $D=15$, 20, 30, 50, and 100 Ry have been calculated by considering $b=1$ and $b=b'$ separately. The values of b' corresponding to different values of the Debye parameter D are quoted in Table I. Figures 3 and 7 show the stabilization plot for $D=30$ and $b=b'$. Figures 5 and 9 are the similar plot for $D=30, b=1$ in the range 0.2–0.8 with mesh point 0.0005. Ultimately we use 1201 points to cover range 0.2–0.8 for $D=15$, 20, 30, 50, and 100. Figures 4 and 6 show the fitting of the density of resonance states with help of Eq. (5) corresponding to the 16th eigenvalues in the stabilization plots 3 and 5. The results obtained from the fit are given in Table I. The resonance energies reported in Table I are associated with the $N=2$ hydrogen threshold.

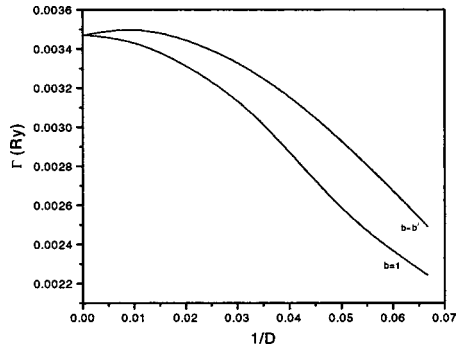

FIG. 8. Resonance width Γ corresponding to the resonance energy in Fig. 7 as a function of $1/D$.

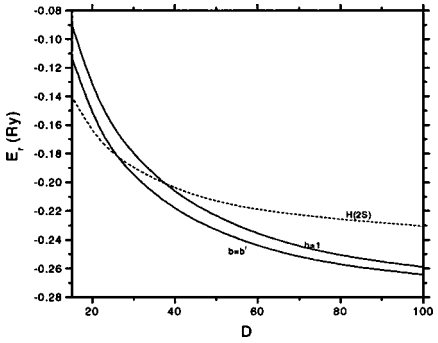

FIG. 9. The $2s^2\ ^1S^e$ resonance energy E_r for the different values of the Debye parameter D. Dashed line denotes H(2) threshold energy.

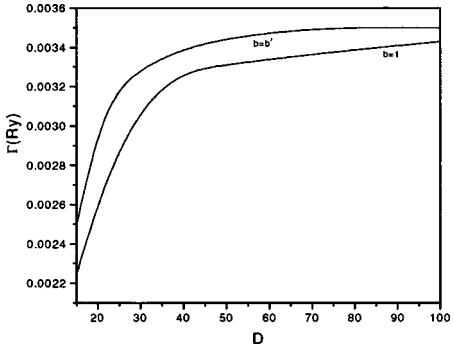

FIG. 10. Resonance width Γ corresponding to the resonance energy in Fig. 9 for the different values of the Debye parameter D.

Our calculated resonance energies associated with the $N=2$ hydrogen threshold for $b=1$ and $b=b'$ are plotted in Figs. 7 and 9 along with the H($2S$) threshold energies for the different values of $1/D$ and D, respectively, with corresponding widths plotted in Figs. 8 and 10. We have also tabulated in Table I the H($2S$) threshold values for various Debye parameters as obtained in Refs. [6,7]. Also from Table I, it is clear that the difference in the resonance energies is about 0.02 for $b=b'$ with $b=1$, and that is about 0.0002 for the corresponding widths.

From Fig. 9 and Table I, it is observed that, for $b=b'$, the resonances obtained below the H($2S$) threshold, which occur for the values of D greater than 25 approximately, correspond to Feshbach resonances (below threshold) and that obtained above the H($2S$) threshold for the values of D less than 25 are corresponding to shape resonances (above threshold). The cutoff value of the Debye parameter D is approximately 25 for the appearance of Feshbach to shape resonances. For $b=1$, that cutoff value of D is nearly 38.

From Fig. 10, it is seen that the resonance width Γ decreases with decreasing value of D. The situation can be explained in the following way: The $2s^2\ ^1S^e$ state in H^- is a "+" state, and the two electrons are located on opposite sides of the nucleus. The movements of the two electrons are moving toward the nucleus "in phase." The autoionization of such a state is through the momentum transfer, as one of the electrons is "knocked out" by the other via the nucleus. Apparently, when the electron-ion screening is increased (decreasing D, increasing $1/D$), the movement of the electrons will be slowed down. As a result, the lifetime of the autoionization process will be prolonged, leading to the narrowing of the resonance width, a consequence of the uncertainty principle.

It should be mentioned here that we have not found any resonance for $D=10$. To obtain resonance for $D=15$ we have extended the range of α up to 1.2. For $D=10$, the resonance, if existing, would be located quite far above the H($2S$) threshold. Usually, it is more difficult to locate a shape resonance far above the threshold, as more extensive basis sets are needed. Such a calculation is beyond the scope of our present investigation.

III. SUMMARY AND CONCLUSIONS

This work presents a first attempt to calculate the $2s^2\ ^1S^e$ autoionization resonance for H^- embedded in various model plasma environments. The $2s^2\ ^1S^e$ states resonance energies and widths for the various Debye parameters ranging from infinity to small value (up to 15) have been reported. The screening effects have been applied to electron-ion interaction. At the present stage, we have not included explicitly the screening for the electron-electron interaction. For this, we have introduced a scaling factor in the electron-ion interaction terms to reproduce the reported ground state energies as obtained by Winkler [1] with which the electron-electron screening was included. We reported the results with and without inclusion of the scaling factor. We have also found the values of the Debye parameter from which the occurrence of Feshbach resonances to shape resonances could be identified. The stabilization method is used to extract reso-

TABLE I. Calculated $2s^2\ ^1S^e$ resonance energies and widths for the varous Debye parameters obtained for the scaling factor $b=b'$ and $b=1$ along with the excited $2S$ hydrogen threshold. All the results are in Rydbergs.

	$b=b'$			$b=1$		
D	b'	E_r	Γ	E_r	Γ	The H($2S$) threshold [6,7]
15	1.045 50	−0.112 22	0.002 49	−0.089 27	0.002 24	−0.1400
20	1.034 64	−0.151 01	0.002 93	−0.131 25	0.002 59	−0.1635
30	1.023 45	−0.194 56	0.003 28	−0.179 66	0.003 06	−0.1895
50	1.014 28	−0.233 07	0.003 44	−0.223 27	0.003 31	−0.2123
100	1.007 225	−0.264 21	0.003 50	−0.258 99	0.003 43	−0.2306
∞	1.0	−0.297 55	0.003 47	−0.297 55	0.003 47	−0.2500

nance energy and width. This method is a practical method to calculate resonance parameters (E_r, Γ). Our present work will provide useful information to the plasma physics research community.

ACKNOWLEDGMENT

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