Stability of the negative ion of hydrogen in nonideal classical plasmas

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The stability of the negative ion of hydrogen (H^-) embedded in nonideal classical plasma has been studied by computing the ground state energy of the ion quite accurately. The interactions among the charged particles in plasma have been modelled by a pseudopotential, derived from a solution of Bogolyubov's hierarchy equations. An extensive basis set is employed in Rayleigh-Ritz variational method to compute the ground state energy of H^- for various values of plasma parameters. Effects of nonideality of plasma on the stability of the ion have been investigated in detail for a wide range of nonideality. Particular emphasis is made to compute accurately the critical values of the plasma screening parameters.

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I. INTRODUCTION

The negative ion of hydrogen has long been the object of astronomical investigations [1–10]. The ion has huge impact on astrophysics. It is plentiful in several astrophysical environments, such as in late-type stars, stellar atmospheres, planetary nebulae, translucent clouds, etc. H^- is a major source of opacity of late-type stars, stellar atmosphere and other astrophysical environments [9]. It played an important role in the formation of early universe [10]. Structurally, the ion is composed of a proton and two electrons. The electron-electron interaction is as important as the electron-proton interaction in the formation of bound states. Large dipole polarizability of hydrogen atom is mostly responsible for the formation of H^-. An electron, slowly approaching a neutral hydrogen atom, induces dipole polarization to the hydrogen atom. The resulting attractive polarization potential leads to the formation of H^-. Moreover, the polarization interaction also leads to the continuous absorption which is a major source of opacity of various astrophysical environments [9]. This ion can break up through associative detachment to form H_2 which was essential for the formation of first stars [10].

In vacuum, the interaction between a pair of charged particles is governed by long-range Coulomb interaction. However, the interaction between a pair of charged particles embedded in a plasma environment gets screened. This screening depends on the temperature and density of the underlying plasma. In particular, two quantities that depend on temperature and density, namely the mean interparticle interaction and the mean kinetic energy of the thermal motion, play an important role in the characterization of classical plasmas and screening of interaction potentials. The ratio of these two quantities is known as the nonideal plasma parameter γ. If $\gamma = 0$, that is interparticle interactions vanish, plasma particles move with thermal velocity along straight lines, virtually without colliding with each other [11]. Such plasmas are called collisionless or ideal plasmas. In a strict sense, ideal plasma does not exist [12]. However, a low-density and high-temperature plasma (for which $\gamma \ll 1$) can be approximately considered as an ideal one [12]. For ideal plasmas, the screened interaction is generally modelled by the Debye-Huckel potential of the form

$$V_{\mathrm{DH}}(r) = \frac{e^{-r/\lambda}}{r}, \tag{1}$$

where λ is the Debye length. In atomic units (a.u.) it is given by $\lambda = (K_B T_e/4\pi n_e)^{1/2}$, where K_B, T_e, and n_e respectively denote the Boltzmann constant, temperature, and density. For an obvious reason, such plasmas are also known as Debye-type plasmas. Debye-Huckel potential adequately describes the effective potential in a plasma, when $\gamma \ll 1$.

With the increase in density (leading to the increase in nonideal parameter γ), inter-particle interactions comes into play. Under these circumstances, the Debye-Huckel model of screening cannot be used for the description of screened interactions in plasma [12]. For nonideal classical plasmas ($\gamma \neq 0$) having no degeneration quantum effects, the screened interaction between the charged particles (proton and electron) can be obtained from a sequential solution of the chain of Bogolyubov equations [13]. This screened interaction or the pseudopotential between a pair of charged particles (q_1, q_2), separated by a distance r, is given by (in a.u.) [13]

$$V(r) = \frac{q_1 q_2[10 + \gamma(e^{-\sqrt{\gamma}r/\lambda} - 1)(1 - e^{-2r/\lambda})]}{10[1 + c(\gamma)]}\frac{e^{-r/\lambda}}{r}, \tag{2}$$

where the nonideal plasma parameter $\gamma(=1/\lambda K_B T_e)$ characterizes the nonideality of the plasma, and $c(\gamma)$ is a function of γ, called the correction function. The values of the $c(\gamma)$ is known for a set of discrete values of γ in the range [0,4.5] [13]. The above pseudopotential takes into account the collective events and the screening effects in it, and correctly represents a pseudopotential model of particle interaction of a nonideal classical plasma (NICP) for $0 \leqslant \gamma \leqslant 4.0$. It is to be noted that this potential reduces to the Debye-Huckel potential in the form of Eq. (1) in the weak limit of nonideality ($\gamma \ll 1$). There are a good number of studies in which the pseudopotential in the form of Eq. (2) has been used to

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TABLE I. Ground state energies (in a.u.) of H^- in NICP with increasing N in the wave function (5).

κ (a_0^{-1})	γ	$-E_{H^-}(\sigma_{14})$ $N = 372$	$-E_{H^-}(\sigma_{15})$ $N = 444$	$-E_{H^-}(\sigma_{16})$ $N = 525$	$-E_{H^-}(\sigma_{17})$ $N = 615$	$-E_{H^-}(\sigma_{18})$ $N = 715$
0.00	0.1	0.487 935 46	0.487 935 47	0.487 935 47	0.487 935 48	0.487 935 48
0.10	0.1	0.396 927 25	0.396 927 26	0.396 927 26	0.396 927 26	0.396 927 27
0.25	0.1	0.280 296 91	0.280 296 93	0.280 296 93	0.280 296 94	0.280 296 94

represent the screening of NICPs [13–23]. Moreover, there are some studies in which quantum mechanical effects in nonideal plasmas have been considered [24–28].

In vacuum, the bound states of H^- have been studied extensively [29–33]. However, most of the astrophysical environments prevail in the state of plasma [34–38]. The screening of plasma significantly affects the stability of an atomic system. For example, the hydrogen atom has an infinite sequence of bound states in vacuum. As soon as it is embedded in plasma, the number of bound states is reduced to a finite number [23]. There are certain ranges of temperature and density of plasmas beyond which electron-proton system is unable to form a bound state. So far, some investigations have been made to study the stability of H^- in plasmas [39–41]. Those studies reveal that in Debye-type plasmas H^- exists when the Debye length approximately lies in the range $(\infty, 0.85]$ (in a_0) [39]. In other words, the plasma screening parameter $\kappa\,(=1/\lambda)$ approximately lies in the range [0, 1.17] (in a_0^{-1}). The value of κ beyond which there exists no bound states is called the critical screening parameter. As λ is related with temperature and density, we can estimate the ranges of temperature and density for which H^- exists in Debye plasma environments.

In this paper we shall pay our attention to investigate the bound states of H^- embedded in NICP in which interactions among the charged particles are governed by the pseudopotential in the form of Eq. (2). NICPs are found to exist in many natural and laboratory frameworks, such as in astrophysical objects and in plasmas produced by laser reduction of solid targets [13]. The center of the planets and stars are thought to consist of dense nonideal plasmas [24]. Our objective is to investigate the effects of nonideality of classical plasmas on the stability of H^-. We consider the temperature and density of the plasma to lie in the ranges $[1-10]\times 10^4$ K and $2.7\times(10^{23}\text{–}10^{26})$ m^{-3} respectively. This makes the nonideal plasma parameter γ lie in the range [0, 4]. We intend to make a detailed study on the properties of the ground sate of H^- for $0 \leqslant \gamma \leqslant 4.0$ within the framework of Rayleigh-Ritz variational principle. Particular emphasis would be given to determine the critical screening parameters quite accurately. In order to do these, we employ an extensive basis set in Rayleigh-Ritz variational principle. Here, it is worthwhile to mention that in electrolytic solutions, only the interactions among the ions are considered to be screened. But in plasma research, it is essential to replace all the Coulomb interactions by screened interactions [42]. This is particularly apparent in astrophysical hydrogen plasmas which, apart from electrons and protons, contain neutral hydrogen as well and even, as a rule, plenty of negative hydrogen ions [42]. It is to be noted that the pseudopotential (2) describes the interaction between two static charges and holds good if the relative velocity v of the interacting particles is less than the thermal velocity v_T. In Debye-type plasma environments, there exists a dynamical screening model in which the Debye length in Eq. (1) is replaced by $\lambda\sqrt{1+v^2/v_T}$ [43]. Atomic units (a.u.) will be used in the remaining part of this paper unless otherwise stated explicitly.

II. THEORY AND CALCULATIONS

We choose the origin of the coordinate system at the proton which is assumed to be at rest. Let $\vec{r}_1$, $\vec{r}_2$ be the coordinates of the electrons and $\vec{r}_{12}$ be the relative coordinate of the electrons. In this coordinate system, the nonrelativistic Hamiltonian of H^- embedded in NICP, characterized by the pseudopotential in the form of Eq. (2), is given by (in a.u.)

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - f(r_1;\gamma)\frac{e^{-r_1/\lambda}}{r_1} - f(r_2;\gamma)\frac{e^{-r_2/\lambda}}{r_2} + f(r_{12};\gamma)\frac{e^{-r_{12}/\lambda}}{r_{12}}, \quad (3)$$

where $f(r;\gamma) = [10+\gamma(e^{-\sqrt{\gamma}r/\lambda}-1)(1-e^{-2r/\lambda})]/[10\{1+c(\gamma)\}]$. We have considered 32 values of $c(\gamma)$ for $0 \leqslant \gamma \leqslant 4.5$

TABLE II. Comparison of the ground state energies of H^- and electron affinity of hydrogen embedded in Debye-type plasma ($\gamma = 0$).

κ (in a_0^{-1})	$-E_{H^-}$(in a.u.)	ϵ_H
0.00	0.527 751 012 422 14	0.027 751 012 422 14
	0.527 751 016 544 377 196 586 5[a]	
	0.527 751 016 544 377 196 503[b]	
	0.527 751 016 54[c]	0.027 751 016 54[c]
	0.527 751 01[d]	
0.05	0.479 034 780 252 19	0.027 218 351 727 68
	0.479 034 784 51[c]	0.027 218 355 98[c]
	0.479 04[e]	0.027 215[e]
0.10	0.432 952 194 650 02	0.025 894 164 036 62
	0.432 952 199 29[c]	0.025 894 168 68[c]
	0.432 95[e]	0.025 892[e]
0.25	0.310 735 811 689 67	0.019 816 224 168 47
	0.310 735 819 00[c]	0.019 816 231 48[c]
	0.310 74[e]	0.019816[e]
0.50	0.157 826 406 142 10	0.009 709 384 269 68
	0.157 826 419[c]	0.009 719 397[c]
	0.157 83[e]	0.009 706[e]

[a]See Frolov *et al.* [29].
[b]See Drake *et al.* [30].
[c]See Kar and Ho [39].
[d]See Ghoshal and Ho [40].
[e]See Winkler [41].

TABLE III. The ground state energies (in a.u.) of H^- and electron affinity of hydrogen (in a.u.) for various plasma temperatures and densities.

			$n_e = 2.7 \times 10^{23}$ m^{-3}		
T_e (in K)	10^4	2×10^4	5×10^4	8×10^4	10^5
γ	0.125 821 66	0.044 484 67	0.011 253 83	0.005 560 58	0.003 978 83
λ (in a_0)	250.970 411 60	354.925 759 84	561.186 900 68	709.851 519 68	793.638 125 97
$-E_{H^-}$	0.475 520 964 3	0.505 760 327 1	0.520 836 545 3	0.523 780 028 1	0.524 652 275 9
ϵ_H	0.025 200 035 9	0.026 737 953 5	0.027 479 807 1	0.027 615 561 8	0.027 653 779 2
			$n_e = 2.7 \times 10^{24}$ m^{-3}		
T_e (in K)	10^4	2×10^4	5×10^4	8×10^4	10^5
γ	0.397 883 02	0.140 672 89	0.035 587 74	0.017 584 11	0.012 582 17
λ (in a_0)	79.363 812 60	112.237 380 14	177.462 879 92	224.474 760 27	250.970 411 60
$-E_{H^-}$	0.388 810 346 7	0.466 149 161 4	0.506 609 319 6	0.515 391 808 2	0.518 059 640 4
ϵ_H	0.020 983 289 1	0.024 935 304 5	0.026 922 692 8	0.027 328 259 4	0.027 445 503 4
			$n_e = 2.7 \times 10^{25}$ m^{-3}		
T_e (in K)	10^4	2×10^4	5×10^4	8×10^4	10^5
γ	1.258 216 58	0.444 846 74	0.112 538 31	0.055 605 84	0.039 788 30
λ (in a_0)	25.097 041 16	35.492 575 98	56.118 690 07	70.985 151 97	79.363 812 60
$-E_{H^-}$	0.234 330 773 4	0.363 131 203 2	0.466 784 425 0	0.490 464 220 3	0.498 109 971 5
ϵ_H	0.013 503 726 9	0.020 178 560 3	0.025 360 672 3?	0.0264624502	0.0268022206
			$n_e = 2.7 \times 10^{26}$ m^{-3}		
T_e (in K)	10^4	2×10^4	5×10^4	8×10^4	10^5
γ	3.978 830 17	1.406 728 90	0.355 877 39	0.175 841 11	0.125 821 66
λ (in a_0)	7.936 381 26	11.223 738 01	17.746 287 99	22.447 476 03	25.097 041 16
$-E_{H^-}$	0.106 501 651 9	0.191 115 203 7	0.363 969 668 9	0.423 011 531 4	0.442 136 012 2
ϵ_H	0.006 785 662 6	0.011 796 779 7	0.021 044 546 8	0.023 967 177 2	0.024 860 689 4

as provided in Table I of Ref. [13]. The value of $c(\gamma)$ for a given γ in $[0, 4.0]$ is then determined by fitting a cubic polynomial with four values of γ in succession. In order to determine the bound state energies E_{H^-} and corresponding wave functions Ψ of H^-, we solve the Schrodinger equation $H\Psi = E_{H^-}\Psi$, $(E_{H^-} < 0)$. Solution of this Schrodinger equation with in the framework of Rayleigh-Ritz variational principle amounts to minimizing the Rayleigh quotient:

$$E_{H^-}[\Psi] = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{4}$$

by employing a trial wave function Ψ. In this paper, we have considered the following wave function to determine the $^1S^e$ state of H^- embedded in NICP:

$$\begin{aligned}\Psi(r_1, r_2, r_{12}) &= \sum_{i=1}^{N} C_i|\psi_i(r_1, r_2, r_{12}; a, l_i, m_i, n_i)\rangle\\ &= \sum_{i=1}^{N} C_{l_i m_i n_i}(1 + P_{12})e^{-a(r_1+r_2)} r_1^{l_i} r_2^{m_i} r_{12}^{n_i},\end{aligned} \tag{5}$$

where C_i's (or $C'_{l_i m_i n_i}$s) are expansion coefficients, a is nonlinear variational parameter and P_{12} is the exchange operator such that $P_{12}g(r_1, r_2) = g(r_2, r_1)$ for an arbitrary function g. The wave function (5) has been expanded by giving nonnegative integer values to l_i, m_i, and n_i such that $\sigma_i(= l_i + m_i + n_i) = 0, 1, 2, \ldots$. This means that σ_0 corresponds to $N = 1$, σ_1 corresponds to $N = 3$, σ_2 corresponds to $N = 7$, and so on. Substitution of Eq. (5) in the Rayleigh quotient (4) gives

$$E_{H^-}[\Psi] = \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} C_i^* C_j H_{ij}}{\sum_{i=1}^{N}\sum_{j=1}^{N} C_i^* C_j S_{ij}}, \tag{6}$$

where

$$\begin{aligned}H_{ij} &= \langle\psi_i(r_1, r_2, r_{12}; a, l_i, m_i, n_i)\\ &\quad \times |H|\psi_j(r_1, r_2, r_{12}; a, l_j, m_j, n_j)\rangle \text{ and}\\ S_{ij} &= \langle\psi_i(r_1, r_2, r_{12}; a, l_i, m_i, n_i)|\psi_j(r_1, r_2, r_{12}; a, l_j, m_j, n_j)\rangle\end{aligned} \tag{7}$$

are Hamiltonian matrix elements and overlap matrix elements respectively. After some algebraic calculations it can be shown that minimization of the Rayleigh quotient is equivalent to finding the least eigenvalue of the matrix $\tilde{S}^{-1}\tilde{H}$, where $\tilde{H} = [H_{ij}]$ and $\tilde{S} = [S_{ij}]$. The matrix eigenvalue problem has been solved by employing the *Q-R* algorithm after transforming the matrix to the Hessenberg form [44].

It is to be noted that we have used same screening parameters to describe the screened proton-electron and electron-electron interactions. In this connection, it is to be mentioned that screening in any form is a fact in plasma. So, the results in this paper, which are based on the validity of the screening model show general qualitative features. These have to be fine tuned when there exists evidences that the screening model is not a good approximation.

III. RESULTS AND DISCUSSION

In Table I, we put up the ground state energies of H^- embedded in NICP with an increase in the number of terms

TABLE IV. Critical values of κ (in a_0^{-1}) and γ.

κ_c	0.6	0.7	0.8	0.9	1.0	1.173 040
γ_c	2.943 723	1.810 911	1.161 095	0.690 811	0.416 252	0.0

in the wave function (5) for various values of the screening parameter κ and nonideal parameter γ. We have performed the computations in quadruple precision arithmetic. From Table I we can infer that convergent results of ground state energy up to eight decimal places can be obtained by using 715 terms (corresponds to σ_{18}) in the wave function (5). The accuracy of our results has been substantiated in Table II which includes some of most accurate results for vacuum and Debye-type plasma environment available in the literature. We notice that in all cases our results are in excellent agreement with those results of up to eight decimal places.

Table III shows the ground state energy of H^- for a number of plasma temperatures and densities lying in the ranges (1–10) $\times$ 10^4 K and $2.7 \times (10^{23}$–$10^{26})$ m^{-3} respectively. This table also shows the electron affinity of hydrogen. The ground state energies E_H of hydrogen have been calculated accurately by using the technique as described in our previous work [23]. From Table III we notice that for a given plasma density, the effect of increasing temperature is to lower the ground sate energy of H^-. On one hand, for a given temperature, the effect of increasing density is to increase the ground state energy of H^-. These facts are also true for hydrogen [23]. But, at a given density, ϵ_H increases with increasing temperature, whereas at a given temperature it decreases with increasing density. It is to be noted that the ion remains stable in the entire range of temperature and density considered here. The effect of increasing either κ or γ is to push the ground state energy towards the continuum. For a given Debye length, ground state energy is lifted towards continuum with the increase in nonideality (that is γ) leading to the instability of the ion. We have calculated the critical values of the parameters κ and γ. These are the values of κ and γ beyond which no bound state of the ion exists. From Table IV we note that for Debye-type plasmas ($\gamma = 0$), the critical value of κ is 1.173 040 (in a_0^{-1}) approximately. With an increase in the nonideality of plasma, the critical value of the screening parameter decreases.

In order to have a better understanding on the stability of the ion with respect to the parameters κ and γ, we plot the ground state energy of H^- as a function of γ for a number of values of κ. This is presented in Fig. 1. This imparts an idea of to what extent the potential (2) which explicitly depends on λ and γ is able to support the bound state of H^-. It is apparent that an increase of either κ or γ gradually leads to the instability of the ion. Dependence of electron affinity of hydrogen with the nonideality of plasma is shown in Fig. 2. As expected, we note that for a given Debye length, the electron affinity of hydrogen decreases with the increase in nonideality.

IV. CONCLUSIONS

To be succinct, we have made an attempt to study the effects of nonideal classical plasma on the ground state of the negative ion of hydrogen. Ground state energies for various values of plasma parameters have been calculated quite accurately by using an extensive basis set within the framework of the variational method. Our present study reveals that increasing nonideality of the plasma leads to the instability of the ion. The ion remains stable for the temperature and density of the plasma lying in the ranges (1–10) $\times$ 10^4 K and $2.7 \times (10^{23}$–$10^{26})$ m^{-3} respectively. We report the values of the Debye length and nonideal plasma parameter beyond which H^- does not exist. We believe that our present results will provide useful information in the understanding of kinetic properties of nonideal plasmas.

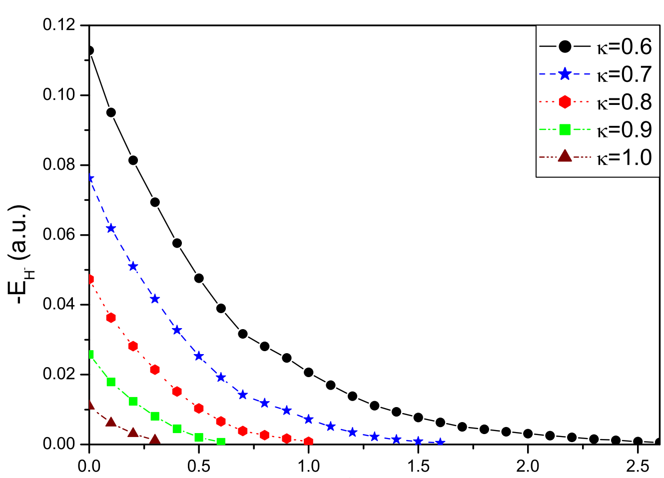

FIG. 1. Ground state energy of H^- as a function of γ for different values of κ (in a_0^{-1}).

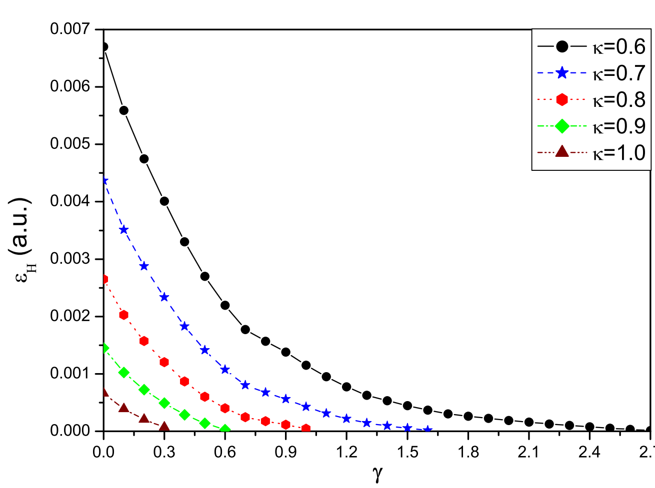

FIG. 2. Electron affinity of hydrogen as a function of γ for different values of κ (in a_0^{-1}).

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