Comparison between plasmon energy and binding energy of the last bound S state of the Debye-Hückel potential

F. A. Gutierrez
Departamento de Fisica, Universidad de Concepción, Casilla 3-C, Concepción, Chile
and Institute for Theoretical Physics, University of California, Santa Barbara, California 93106
(Received 5 February 1990)

It is shown that the ratio of the plasmon energy to the binding energy of the last bound S state of the Debye-Hückel potential is approximately independent of density and depends on temperature as $T^{1/2}$. A simple analytical condition for plasmon-induced free-bound transitions for the highest excited states of hydrogenic ions was obtained that is met by plasmas of interest.

In this Brief Report we analyze the ratio of the plasmon energy[1,2] $\hbar\omega_p = \hbar(4\pi n_e e^2/m_e)^{1/2}$ to the binding energy $W_{n,l}$ (n and l the principal and angular momentum quantum numbers, respectively) of the highest bound states of the Debye-Hückel potential (DHP),

$$V_{\rm DH} = -\frac{Ze^2}{r} e^{-r/\lambda_D} , \tag{1}$$

used to model the static screening[3] of the ion's field in plasmas within a range characterized by the Debye length[4] $\lambda_D = [k_B T/4\pi n_e e^2(Z+1)]^{1/2}$. We are considering here a hydrogenic plasma at (electron) temperature T, where m_e is the electron mass, n_e the electron density number, and Ze the ion's charge. Rewriting the plasmon energy in terms of the parameter $D \equiv Z\lambda_D/a_0$ (a_0 the Bohr radius) as

$$\hbar\omega_p = 0.384 \left[\frac{Z^2 k_B T}{Z+1} \right]^{1/2} \frac{1}{D} ; \tag{2}$$

in Ry (1 Ry=13.6 eV), with $k_B T$ given in eV, and using the data of Rogers, Graboske, and Harwood[5] for $W_{n,l}$ the ratio $R_{n,l}(D,T) \equiv \hbar\omega_p/W_{n,l}$ is obtained. It is plotted against D ($5 \le D \le 100$) for the case $Z=1$, $k_B T = 1$ eV, and for the states $n = g^*$, $l=0$ and 1, where g^* is the last bound principal quantum number for a given D. In Fig. 1 the dots represent $R_{g^*,0}$ while the $\times$'s represent $R_{g^*,1}$. Besides being larger than 2, $R_{g^*,0}$ seems to have a weak dependence on D implying (since T is fixed) a weak dependence on the electronic density n_e, an observation we shall presently verify. $R_{g^*,1}$ is also larger than 2 although it shows stronger fluctuations than $R_{g^*,0}$. One can easily show that this behavior is not present for $R_{g^*-1,0}$ which is, in general (although not always), smaller than 1 and strongly dependent on D. It should also be noted that for a fixed state (n,l) $R_{n,l}$ decays drastically with D since larger values of D (at fixed T) imply lower plasmon energy $\hbar\omega_p$, while $W_{n,l}$ becomes larger due to the weaker screening.

Consider now the analytical formula for the eigenvalues of the DHP in Ry, $E_{nl} = -W_{nl}$ with

$$W_{n,l} = \frac{Z^2}{n^2 D} \frac{[D - A_1(n+\sigma)^2 + A_2 n^2][D - A^{(l)}(n+\delta_l)^2]}{[D - A_2 n^2 + A^{(l)}(n+\delta_l)^2]} , \tag{3a}$$

where

$$A^{(l)} = S_0^{-2}(1+\gamma l + \Delta l^2)^{-2} ,$$
$$\delta_l = S_0 \sqrt{D_0}(1+\gamma l + \Delta l^2)(1+\alpha l + \beta l^2)^{1/2} - l - 1 . \tag{3b}$$

In these expressions $A_1 = 1.9875$, $A_2 = 1.2464$, $\sigma = 0.003\,95$, $S_0 = 1.1335$, $D_0 = 0.839\,908$, $\alpha = 2.739$, $\beta = 1.6242$, $\gamma = 0.019\,102$, and $\Delta = -0.001\,684$. Formula (3), valid for all the quantum numbers $n,l \lesssim 10$ over the entire range of Z and for all values of λ_D, was obtained by Green[6] by fitting the numerical data of Rogers, Graboske, and Harwood[5] to a 1% level of accuracy. Com-

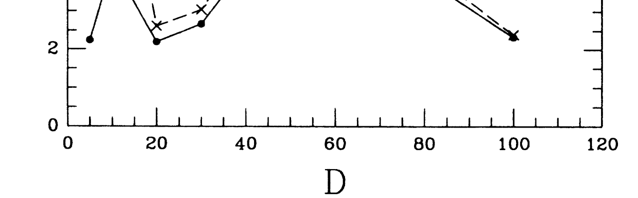

FIG. 1. The ratio $R_{n,l} = \hbar\omega_p/W_{n,l}$ vs $D = \lambda_D/a_0$ for the states $(n,l) = (g^*,0)$ and $(g^*,1)$ for $Z=1$. The dots represent the values of $R_{g^*,0}$ and the $\times$'s the values of $R_{g^*,1}$. The solid and the dashed lines are included only as an aid to the eye.

bining (2) and (3) we have

$$R_{n,l}=\frac{0.383\,57n^2}{D-A_1(n+\sigma)^2+A_2n^2}\times\left[1+\frac{A_2n^2}{D-A^{(l)}(n+\delta_l)^2}\right]\left[\frac{k_BT}{Z^2(Z+1)}\right]^{1/2}. \quad (4)$$

A general condition for real continuum-bound transitions is $R_{n,l}\geq 1$. For bound-bound transitions between states characterized by the set of quantum numbers (n,l) and (n',l') it is required that[2] $\hbar\omega_p\leq|W_{n,l}-W_{n',l'}|\leq\hbar\omega_p(1+\epsilon)$ or $1\leq|R_{n,l}^{-1}-R_{n',l'}^{-1}|\leq 1+\epsilon$ where $\epsilon\equiv\frac{1}{2}(\langle v^2\rangle/\omega_p^2)q_c^2\lesssim 1$. In what follows we particularize to the important case $n=g^*$, $l=0$, with[7]

$$(g^*)^2=cD\ , \quad (5)$$

where the value of c obtained from different studies in the literature[7] fluctuates between 0.804 and 1.2677. Since $g^*>1\gg\sigma$, δ_0 then we can in first approximation neglect σ and δ_0 in Eq. (4) (with $l=0$). Doing this and using (5) (with[8] $c=0.81$) it is straightforward to obtain the simple expression

$$R_{g^*,0}=2.9[k_BT/Z^2(Z+1)]^{1/2} \quad (6)$$

which verifies the above observation that R_{g^*0} is approximately independent of density. This is a quite remarkable result (considering that the plasma density varies over many orders of magnitude) which can be taken as a manifestation of a strong relationship between the highest bound atomic states of the DHP and the plasma oscillations. Indeed applying in (3) the same approximation that led to (6) gives for the binding energy of the last bound S state, $W_{g^*,0}=0.132(Z^2/D)$ Ry, which has the same dependence on D as the plasmon energy. A similar dependence appears in the energy shift contained in the Ecker-Weizel and related potentials for hydrogenic ions immersed in a plasma environment.[9,10] A simple argument to understand the strong relationship between the g^* states and the plasma oscillations is the following: It is well known that collective behavior in plasmas involves wavelengths $\lambda\gtrsim\lambda_D$, the waves with $q>q_c\sim\lambda_D^{-1}$ being strongly damped.[2] One also expects that the highest orbits have an average radius $\bar{r}\sim\lambda_D$ since at this distance the potential is shielded. Therefore there is an approximate matching between the minimum plasmon wavelength and the size of the last bound orbits which is valid at all densities. For inner orbits the electron is tightly bound to the ion and cannot respond to the collective modes, but for the highest orbits it is very loosely bound so that it strongly feels the long-range correlations with the other electrons; when the electron is at distances $d>\lambda_D$ from the ion it is more influenced by the whole system (collective behavior) than by the ion in such a way that it is no longer bound. The condition for plasmon-induced continuum-bound transition involving the g^* state is, with (6),

$$\frac{k_BT}{Z^2(Z+1)}\gtrsim 0.1\ , \quad (7)$$

which is well satisfied by plasmas under conditions ranging from those of stellar atmospheres ($Z=1$, $k_BT\sim 1$ eV, $D\sim 10$ at the base of the solar photosphere and $D\sim 100$ for white dwarf stars[11]), up to those relevant to recombination x-ray-laser experiments[12,13] ($Z=5$, $k_BT\sim 100$ eV, $D\sim 90$ for fully stripped C recombining to hydrogenic ions, and $Z=13$, $k_BT\sim 1$ keV, $D\sim 17$ for Al plasmas). For states with $n=g^*$ and $l\neq 0$ this collective mechanism is still allowed since $R_{g^*,l}$ gets larger at larger l. For bound-bound (collective) transitions with $n=n'=g^*$, $l=1$, and $l'=0$, it is readily seen that the corresponding condition is

$$100\lesssim\frac{Z^2(Z+1)}{k_BT}\lesssim 100(1+\epsilon)\ , \quad (8)$$

which is not satisfied by the above-mentioned system. The derivation of $R_{g^*,1}$ necessary to obtain (8) was done along the same lines followed to derive $R_{g^*,0}$ in (6) although the approximation of neglecting δ_1 compared to g^* is not as good as that of neglecting δ_0 since δ_1 is not much smaller than 1. However, for D not too small (say, $D\gtrsim 20$) the approximation is still good enough for the present purposes. Free-bound transitions involving states other than g^* states and bound-bound transitions between states with different principal quantum numbers are possible although no simple conditions can be obtained in those cases. It must be noted that since relation (3) is valid for $n,l\lesssim 10$, and since for $D\gg 100$ g^* will be larger than 10, then our conclusions should be in principle restricted to values of $D\lesssim D_0$ with D_0 of the order of 100. Fortunately in all the above-mentioned applications where collective mechanisms are expected to be important the values of D fall in this range.

In conclusion, we mention that recent calculations show that for H plasmas[9,14] with $k_BT\sim 1$ eV and $D\sim 100$, and for Al plasmas[15] with $k_BT\sim 100$ eV at metallic densities, plasmon-mediated recombination (to highly excited and perturbed atomic states) has larger cross sections than the usual radiative and three-body modes, respectively. These results could have strong implications for the basic theory of radiative equilibrium of partially ionized plasmas, and also in predicting and diagnosing the state of high-density laboratory systems.[15]

This research was supported in part by Fondo Nacional de Desarrollo Científico y Tecnológico de Chile under Project No. 90-0185, and also in part by the National Science Foundation under Grant No. PHY82-17853, supplemented by funds from the National Aeronautics and Space Administration, at the University of California at Santa Barbara. I should thank the Fundación Andes for the special grant that allowed me to participate in the program "Atoms and Ions in Strongly Coupled Plasmas" of the Institute for Theoretical Physics at the University of California, Santa Barbara, where part of this work was done. I am also indebted to Professor M. D. Girardeau for several useful conversations related to this work.

[1]D. Bohm and D. Pines, Phys. Rev. **92**, 609 (1953).

[2]Actually the energy of a plasmon of wave vector **q** is given by $\hbar\omega_{\mathbf{q}}=\hbar\omega_p[1+\frac{1}{2}(\langle v^2\rangle/\omega_p^2)q^2]$ with v the random thermal velocity of the electrons in the plasma. However, the constraint $q<q_c$, where q_c is the wave-vector cutoff above which the plasmons are not well-defined elementary excitations of the system because of a strong (Landau) damping, restrict the values of the plasmon energy to the narrow range $\hbar\omega_p<\hbar\omega_{\mathbf{q}}<\hbar\omega_p(1+\epsilon)$, $[\epsilon=\frac{1}{2}(\langle v^2\rangle/\omega_p^2)q_c^2]$, the higher limit being still of the order of $\hbar\omega_p$.

[3]For the highest bound states static screening is probably a good first approximation, something that is not true for tightly bound states which are affected by dynamical screening.

[4]S. Ichimaru, *Basic Principles of Plasma Physics: A Statistical Approach* (Benjamin, Reading, MA, 1973), p. 6ff.

[5]F. J. Rogers, H. C. Graboske, and D. J. Harwood, Phys. Rev. A **1**, 1577 (1970).

[6]A. E. S. Green, Phys. Rev. A **26**, 1759 (1982).

[7]See Rogers, Graboske, and Harwood, Ref. 5, and references therein.

[8]For $c>0.81$ one gets values of g^* larger than the true g^* (obtained from Table II of Ref. 5) especially at large D. In our case it is preferable to underestimate g^* not to overestimate $R_{g^*,l}$. Because of this we have chosen $c=0.81$, which gives values of g^* only slightly less than the true values.

[9]M. D. Girardeau and F. A. Gutierrez, Phys. Rev. A **38**, 1624 (1988).

[10]F. A. Gutierrez, Ph.D. dissertation, University of Oregon, 1988.

[11]J. C. Weisheit and B. W. Shore, Astrophys. J. **194**, 519 (1974).

[12]G. J. Pert, J. Phys. B **9**, 3301 (1976); G. J. Pert, Plasma Phys. and Controlled Fusion **27**, 1427 (1985).

[13]C. Chenais-Popovics *et al.*, Phys. Rev. Lett. **59**, 2161 (1987).

[14]F. A. Gutierrez and M. D. Girardeau, Phys. Rev. A **42**, 936 (1990).

[15]M. Rasolt and F. Perrot, Phys. Rev. Lett. **62**, 2273 (1989).