Influence of a dense plasma on the fine-structure levels of a hydrogenic ion

Debasis Ray*
Condensed Matter Physics Group, Saha Institute of Nuclear Physics, Sector-I, Block-AF, Bidhannagar, Calcutta 700 064, India
(Received 21 March 2000)

We discuss the effects of plasma electron polarization surrounding a multiply charged hydrogenic impurity in a high density plasma on the fine-structure levels of the impurity ion. Calculations performed using the ion sphere model suggest that the magnitude of the fine-structure correction smoothly increases with increasing plasma electron density. The other features of the dense plasma effects include the removal of the k degeneracy of the Dirac levels, and a breakdown of the Z^4 scaling of the fine-structure correction along the hydrogenic sequence of ions. The resultant outcome is a complete modification of the fine-structure multiplets in terms of the ordering and spacing between the multiplet components.

PACS number(s): 52.25.Vy, 32.10.Fn

Theoretical simulation of the screening effects of a surrounding plasma medium on the nonrelativistic bound energy levels of plasma-embedded one- [1–6] and two-electron [7–10] atomic systems has evoked considerable interests over the years. Experimentally observed dense plasma effects, such as the lowering of the ionization potential [11–13] and the redshift of x-ray emission lines [14–16] of plasma-embedded atomic ions, may now be explained at a qualitative level, at least. In contrast to these, the influence of a dense plasma on more subtle aspects, e.g., the fine structures of atomic levels that arise from a relativistic treatment of the atomic system within a plasma, has received little attention. We should note that the fine structures are an integral part of an atomic spectra. Besides, the fine-structure effects on atomic levels that are very subtle in low-Z one-electron ions become quite accentuated in high-Z species due to Z^4 dependence of the fine-structure correction along the hydrogen isoelectronic series. Earlier theoretical investigations [17–19] considered the role of plasma screening on proton impact-induced fine-structure transitions ($2s_{1/2}$-$2p_{1/2}$, $2s_{1/2}$-$2p_{3/2}$, and $2p_{1/2}$-$2p_{3/2}$) between $n=2$ fine-structure levels of excited hydrogenic ions. The plasma effects were simulated in these calculations by means of two static potential models, e.g., the ion sphere model [20] and the Debye-Hückel model [21], which are appropriate in the limiting cases of low-temperature, high-density and high-temperature, low-density plasmas, respectively. Investigation of the plasma-induced modifications in the collisional characteristics, such as the excitation cross sections and the rate coefficients, was the principal objective of these studies, and the influence of the plasma on the fine-structure corrections and the multiplet level structures had remained somewhat implicit there. The present paper attempts to bring out the essential features of the effects of a dense plasma on the fine structures in plasma-embedded hydrogenic ions, treating them within the framework of the ion sphere model.

The ion sphere (or, alternatively called the ''Wigner-Seitz sphere'') model is a reasonable approximation for describing the effects of static screening within a dense, strongly coupled plasma. It makes qualitatively correct predictions at high densities and has been widely used to investigate atomic processes in such plasmas [22]. In this model, a hydrogenic ion with nuclear charge Z and $n_b(=1)$ number of bound electrons is surrounded by a sphere of radius $R_0=[3(Z-1)/4\pi n_e]^{1/3}$ containing exactly $n_f(=Z-1)$ number of uniformly distributed free plasma electrons to neutralize the charge of the ion, where n_e is the plasma electron density. Under these assumptions, the electrostatic potential energy (in a.u.) seen by the bound electron is given by

$$V(r;R_0)=-(Z/r)+(Z-1/2R_0)[3-(r/R_0)^2], \quad r<R_0. \tag{1}$$

The total potential and its first derivative vanish at the ion sphere radius $r=R_0$. Beyond the ion sphere boundary the distribution of the positive charge is assumed to neutralize exactly the negative electron distribution, thereby producing an electrically neutral background.

Now, the fine-structure correction E_{nlj}^{FINE} to a nonrelativistic level (n,l) with energy E_{nl}^{NR} of a hydrogenic ion subject to the central potential $V(r;R_0)$ in Eq. (1) (that is *not* Coulombic) is expressed as

$$E_{nlj}^{\mathrm{FINE}}=E_{nk}^{\mathrm{DIRAC}}-E_{nl}^{\mathrm{NR}}. \tag{2}$$

E_{nl}^{NR} is obtained by solving the radial Schrödinger equation (in a.u.) [23]:

$$[-\tfrac{1}{2}d^2/dr^2+l(l+1)/2r^2+V(r;R_0)]P_{nl}(r;R_0)$$
$$=E_{nl}^{\mathrm{NR}}(R_0)P_{nl}(r;R_0) \tag{3}$$

and E_{nk}^{DIRAC} is an eigenvalue of the radial Dirac equations (in a.u.) [24–26]:

$$(d/dr)P_{nk}(r;R_0)=-(k/r)P_{nk}(r;R_0)-(1/c)[E_{nk}^{\mathrm{DIRAC}}(R_0)-V(r;R_0)+2c^2]Q_{nk}(r;R_0), \tag{4a}$$

$$(d/dr)Q_{nk}(r;R_0)=(k/r)Q_{nk}(r;R_0)+(1/c)[E_{nk}^{\mathrm{DIRAC}}(R_0)-V(r;R_0)]P_{nk}(r;R_0). \tag{4b}$$

In Eqs. (4a) and (4b), E_{nk}^{DIRAC} is the energy excluding the rest-mass energy, i.e., the total energy including the rest-mass energy would be $E_{nk}^{\mathrm{DIRAC}}+c^2$ (in a.u.). The relativistic

*Email address: debasis@cmp.saha.ernet.in

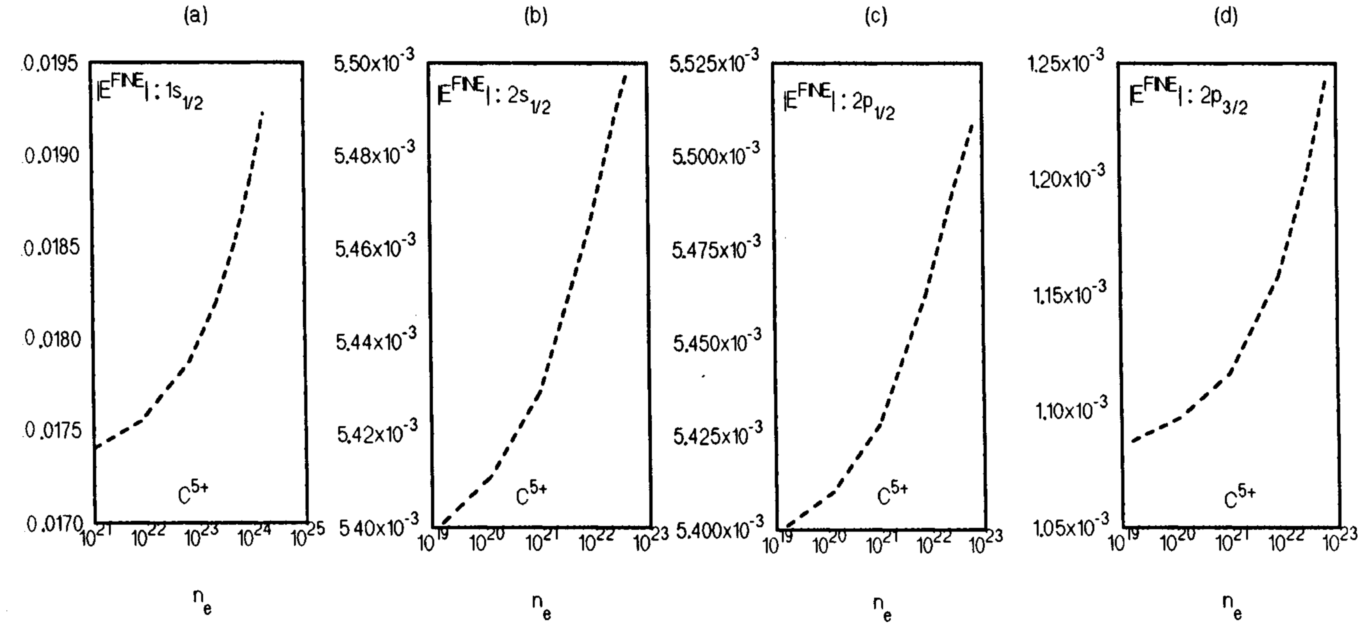

FIG. 1. Variation of the magnitude of the fine-structure correction ($|E^{\mathrm{FINE}}|$, in rydberg units) in C^{5+} ion with plasma electron density (n_e, in cm^{-3}) for (a) $n=1$ level ($1s_{1/2}$), and (b)–(d) $n=2$ levels ($2s_{1/2}$, $2p_{1/2}$, and $2p_{3/2}$), respectively.

angular momentum quantum number k, the total angular momentum j, and the orbital angular momentum l are connected through the following relations:

$$k=(l-j)(2j+1)=-(j+\tfrac{1}{2})\sigma,$$

$$\sigma\equiv-\operatorname{sgn}(k)=-|k|/k,$$

$$j=|k|-\tfrac{1}{2}=l+\tfrac{1}{2}\sigma, \tag{5}$$

$$l=j-\tfrac{1}{2}\sigma=|k|-\tfrac{1}{2}(1+\sigma),$$

$$l(l+1)=k(k+1).$$

It should be noted that, for the particular case of a Coulomb potential, $E_{nl}^{\mathrm{NR}}=E_{n}^{\mathrm{NR}}$ (l degenerate), $E_{n,\pm k}^{\mathrm{DIRAC}}=E_{n|k|}^{\mathrm{DIRAC}}$ (k degenerate), and $E_{nlj}^{\mathrm{FINE}}=E_{nj}^{\mathrm{FINE}}$ (l degenerate). These degeneracies are removed for a general central potential as indicated in Eqs. (2)–(4). So far we have used generalized a.u.: the reduced Planck constant $\hbar$, the electronic charge e, and the mass m of the considered particle are taken as unity. All distances (r,R_0) are measured in atomic length units of the Bohr radius $a_0=(\hbar^2/me^2)=0.529\,177$ Å, all energies are expressed in atomic energy units (hartrees) of $E_0=(\hbar^2/ma_0^2)=(e^2/a_0)=(me^4/\hbar^2)=27.2114\,\mathrm{eV}$, and the angular momenta in units of $\hbar$. Using these units, the speed of light c in vacuum is 137.036, i.e., the inverse of the dimensionless fine structure constant $\alpha=(e^2/c\hbar)=(\hbar/mca_0)$ that controls the order of magnitudes of the fine-structure corrections.

The trend of variation of the magnitude $|E^{\mathrm{FINE}}|$ of the fine-structure correction (E^{FINE} is always negative) against plasma electron density n_e is depicted in (a)–(d) of Fig. 1, for the levels $1s_{1/2}$, $2s_{1/2}$, $2p_{1/2}$, and $2p_{3/2}$, respectively, in the hydrogenlike ion C^{5+} as a typical representative case. The free-ion ($n_e=0$) magnitudes of the correction (given in rydbergs, where 1 Ry$=\frac{1}{2}$ a.u. of energy) for these levels are 0.017 25, 0.005 392, 0.005 392, and 0.001 078, respectively. In all the cases under consideration, a gradual increase in the fine-structure magnitude is observed in the high-density regime. For the ground state $1s_{1/2}$, the magnitude remains almost at the free-ion value up to a density $10^{21}/\mathrm{cm}^3$. This is followed by a continuous growth of about 11% up to a density $1.74\times10^{24}/\mathrm{cm}^3$, which is the maximum density under consideration for the C^{5+} ion in the present study. For the fine-structure levels belonging to the $n=2$ excited state, the correction magnitudes exhibit a noticeable upward trend from a relatively low density threshold of $\sim10^{19}/\mathrm{cm}^3$. But, up to $n_e=6.44\times10^{22}/\mathrm{cm}^3$ the correction magnitudes for the $2s_{1/2}$ and $2p_{1/2}$ levels have only ~2.0% gain over the free-ion values, while that for the level $2p_{3/2}$ rises by about 15%.

It should be of interest to have an idea about electron density dependence of the individual contributing terms that the fine-structure correction to a particular level is made up of (up to order v^2/c^2), because these contributions are separately accessible through theoretical considerations only. Therefore, we study (1) the *mass-velocity* term, (2) the *spin-orbit* term and, (3) the *Darwin* term, each of which can be estimated separately as a function of the plasma electron density as the expectation value of the corresponding relativistic operator [27] in the unperturbed nonrelativistic eigenstate P_{nl} of Eq. (3), using first-order perturbation theory. For the $l=0$ levels $1s_{1/2}$ and $2s_{1/2}$, the spin-orbit correction E_{SO} is zero, the mass-velocity E_{MV} (always negative in sign), and the Darwin (E_D, always positive) corrections exist. As displayed in Fig. 2(a) and 2(b), the magnitudes of these two terms for the level $1s_{1/2}$ exhibit counteracting patterns of variation with increasing plasma electron density. For the $2s_{1/2}$ level, the observations are similar and therefore, are omitted from Fig. 2. On the other hand, for the $2p$ levels $(l\neq0)$, $E_D=0$ but E_{MV} and E_{SO} contribute. E_{MV} is identical for $2p_{1/2}$ and $2p_{3/2}$ levels with a negative sign, while E_{SO} is different in magnitude for these two levels and negative for the $2p_{1/2}$ and positive for the $2p_{3/2}$ level. Their variations

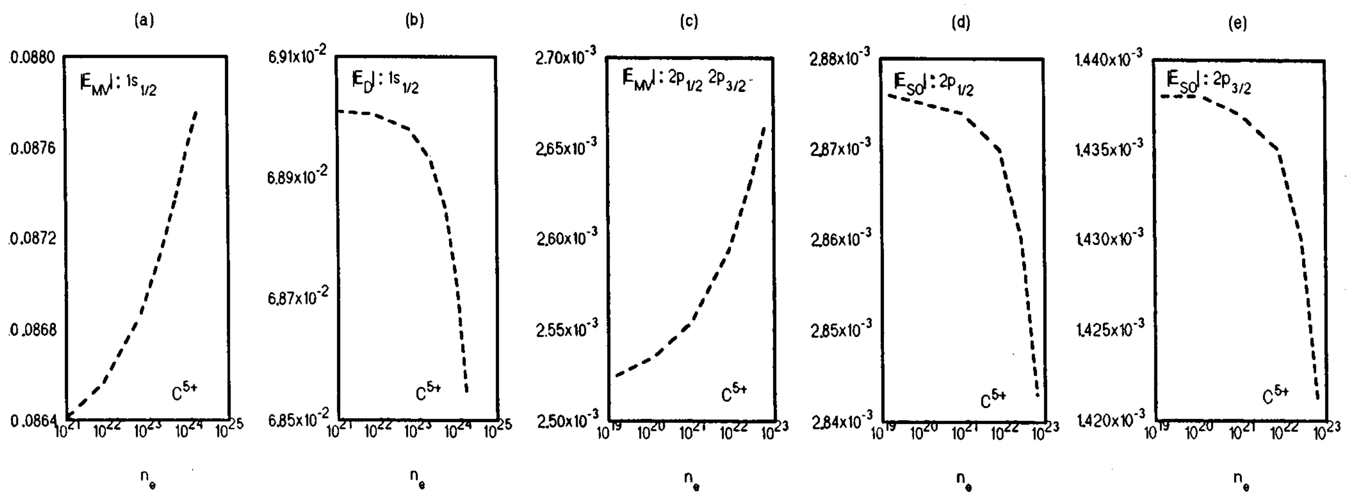

FIG. 2. Magnitudes of the different terms (in Rydberg units) contributing to the fine-structure corrections in C^{5+} ion, as a function of plasma electron density (n_e, in cm^{-3}): (a) Mass-velocity term ($|E_{MV}|$) for $1s_{1/2}$ level, (b) Darwin term ($|E_D|$) for $1s_{1/2}$ level, (c) mass-velocity term ($|E_{MV}|$) for $2p_{1/2}$ and $2p_{3/2}$ levels, (d) spin-orbit term ($|E_{SO}|$) for the $2p_{1/2}$ level, (e) spin-orbit term ($|E_{SO}|$) for the $2p_{3/2}$ level.

with n_e are presented in Figs. 2(c)–2(e), respectively. It is seen that $|E_{MV}|$ and $|E_{SO}|$ change in an opposite manner with plasma electron density n_e.

The k degeneracy (e.g., for two levels with the quantum numbers $\{n,+k\}$ and $\{n,-k\}$, $E_{nk}^{\rm DIRAC}$ is the same and depends on $|k|$ only) of the Dirac levels in an isolated ($n_e=0$) hydrogenic ion is lifted within a plasma in the presence of a non-Coulomb central potential when $n_e \neq 0$. In Fig. 3, we present plasma electron density-dependent removal of the degeneracy between the $2p_{1/2}$ ($k=+1$) and $2s_{1/2}$ ($k=-1$) levels of C^{5+}. As can be seen from Fig. 3, the onset of the splitting occurs at $n_e \sim 10^{20}\,{\rm cm}^{-3}$. Then the separation grows monotonically with increasing electron density and rises sharply between $n_e=10^{22}$–$10^{23}\,{\rm cm}^{-3}$, attaining a magnitude of $0.013\,{\rm Ry} \approx 0.177\,{\rm eV}$ at $n_e=6.0\times 10^{22}\,{\rm cm}^{-3}$. It is observed that the dominant contribution to the splitting comes from the density-dependent nonrelativistic energy difference between $2p$ and $2s$ levels. The separate (i.e., l dependent within a plasma) fine-structure corrections for these two levels contribute a negligible amount (for this, we refer to Fig. 5).

It is well known that for free one-electron ions, the fine-structure correction for a particular (nlj) level scales as Z^4 [27]. This simple form of Z dependence does not hold well any longer when the ions are immersed in dense plasmas. Increased breakdown of the scaling law with increasing plasma electron density is demonstrated in Fig. 4, with reference to the $1s_{1/2}$ level in the ions C^{5+}, O^{7+}, Ne^{9+}, Al^{12+}, Ar^{17+}, and Fe^{25+} within the segment $Z=6$–26. In Fig. 4, we have plotted the ratio $|E^{\rm FINE}|/Z^4$ against Z. For isolated ions, $|E^{\rm FINE}| \propto Z^4$; so at $n_e=0$ the ratio should be a constant, independent of Z. This is indicated by the straight line parallel to the abscissa in Fig. 4. For $n_e \neq 0$, the ratio is *not* independent of Z—it depends on (Z,n_e) both and exhibits a nonlinear but, smooth and regular behavior. Growing nonlinearity is obtained with increasing plasma electron density. For a particular ion with nuclear charge Z, the deviation from the straight line increases with larger screening effects induced by higher electron densities; and, at a particular density, the

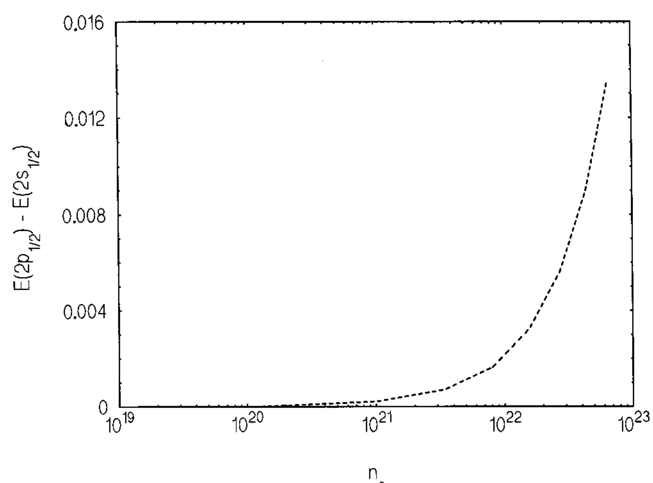

FIG. 3. Dependence of the energy separation (in rydberg units) between the levels $2p_{1/2}$ and $2s_{1/2}$ in C^{5+} ion on plasma electron density (n_e, in cm^{-3}).

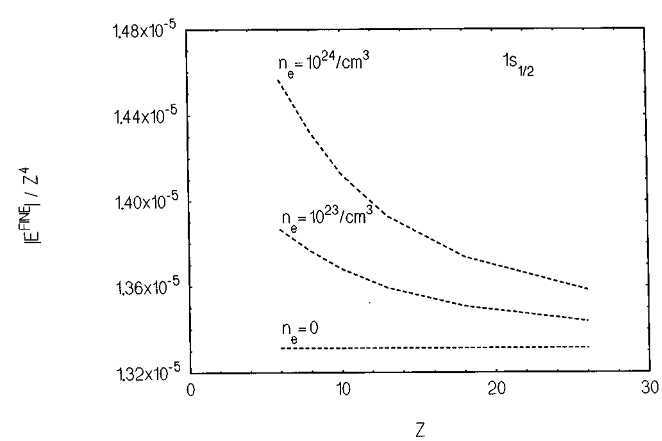

FIG. 4. Departure of the fine-structure correction ($E^{\rm FINE}$) for the $1s_{1/2}$ level from its Z^4 scaling for free ($n_e=0$) hydrogenlike ions in the cases of plasma-embedded ions at plasma electron densities $n_e=10^{23}$ and $10^{24}\,{\rm cm}^{-3}$.

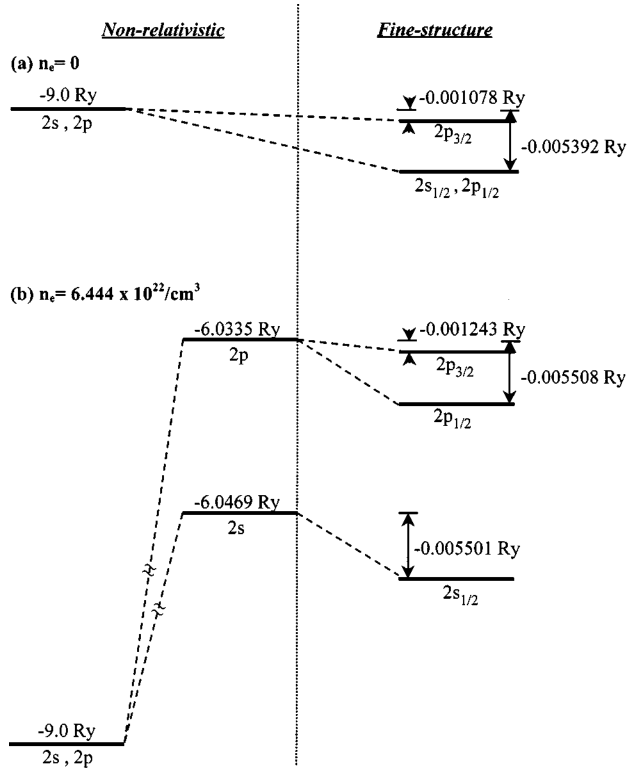

FIG. 5. The modification of the $n=2$ fine-structure multiplet of C^{5+} ion within a dense plasma: (a) normal multiplet structure for an isolated ion ($n_e=0$); (b) deformed multiplet structure for a plasma-embedded ion ($n_c=6.444\times10^{22}\,\mathrm{cm}^{-3}$) (the diagrams are only schematic, and are *not to scale*).

departure is more prominent for a low-Z ion because its bound electron is less strongly attached to the nucleus—hence, more susceptible to density-induced perturbations than in relatively indifferent higher-Z cases.

The deformation of the atomic multiplet structure within a dense plasma is highlighted graphically in the diagrams of Fig. 5, for the fine-structure levels pertaining to the $n=2$ state of the C^{5+} ion. For an isolated ion at $n_e=0$, the $n=2$ multiplet is composed of two components—the degenerate ($2s_{1/2}$,$2p_{1/2}$) levels and the $2p_{3/2}$ level, with the multiplet width or spread (the energy difference between the two extreme members) of 0.004 314 Ry$\sim$0.0587 eV. For a plasma-embedded species the $2s_{1/2}$ and $2p_{1/2}$ levels stand apart even before the consideration of the Lamb shift $-2s_{1/2}$ being lower in energy, so the $n=2$ multiplet has three members and an increased spread of 0.017 66 Ry$\sim$0.24 eV, at an electron density $n_e=6.444\times10^{22}\,\mathrm{cm}^{-3}$. The magnitudes and directions of the Lamb shift within a dense plasma have to be calculated separately for these three components for a more precise specification of their positions. However, since the Lamb shifts are smaller than the fine-structure corrections by an order of magnitude or more, it might be presumed that the post-Lamb shift ordering of the multiplet members within a dense plasma will remain as $E[2s_{1/2}]<E[2p_{1/2}]<E[2p_{3/2}]$, in contrast to the ordering $E[2p_{1/2}]<E[2s_{1/2}]<E[2p_{3/2}]$ in a free ion. Thus, a distortion in the multiplet structure both in terms of the spacing and the ordering might be anticipated within a dense plasma.

Finally, before we conclude our discussion it would be appropriate to comment upon the possible spectroscopic implications that emerge from this theoretical calculation of the plasma density effects on hydrogenic fine structures. For this purpose we consider the Lyman-α emission doublet arising from the transitions ($2p_{1/2}\rightarrow1s_{1/2}$ and $2p_{3/2}\rightarrow1s_{1/2}$) in a relatively high-$Z$ ion like Fe^{25+} ($Z=26$), in which the fine-structure effects would be more prominent than in C^{5+} ($Z=6$), so that the chances of detection of the plasma-induced changes in the fine structure of spectral emission lines would be somewhat more. With increasing plasma electron density, the shift of the Lyman-α doublet lines to the low-energy side of the spectrum is an obvious observation in this calculation. But, since this is essentially equivalent to the redshift of the $2p\rightarrow1s$ emission line (i.e., of the center of gravity of the doublet) as had been pointed out in earlier nonrelativistic calculations, we exclude it from our discussion. On the other hand, the observation related to the doublet spread (separation between the two emission lines), albeit extremely small, might generate some experimental interests. To quote the results of a test calculation as an example, in a free ($n_e=0$) Fe^{25+} ion the magnitude of doublet spread is 1.5209 Ry, that is just the difference between the fine structure corrections to the $2p_{3/2}$ (-0.3802 Ry) and $2p_{1/2}$ (-1.9011 Ry) levels. At a plasma electron density $n_e=8.7\times10^{24}/\mathrm{cm}^3$, the fine-structure corrections for these two levels become -0.4484 and -1.9622 Ry, respectively. So, the modified separation between the emission doublet members becomes 1.5138 Ry. This means a reduction in the spread of the doublet by 0.0071 Ry$\approx$0.1 eV, that attains the threshold of measurability, so to speak (similar reduction in the spread has been obtained in the calculations repeated at this density for all other low-Z ions; the magnitude of reduction is smaller, and hence, less detectable for lower-Z ions). However, it is to be noted that, in practice, the line-broadening mechanisms operative within high density plasmas would tend to obscure such highly subtle fine-structure-related plasma density effects. This, together with the inherent difficulties associated with precise x-ray measurements of the fine structure, would make the spectroscopic observation of the plasma density effects on atomic fine structures a highly challenging undertaking.

The author thanks Professor R. K. Moitra, Professor A. Mukhopadhyay, and Professor B. K. Chakrabarti for their hospitality.

[1] F. J. Rogers, H. C. Graboske, Jr., and D. J. Harwood, Phys. Rev. A **1**, 1577 (1970).
[2] S. Skupsky, Phys. Rev. A **21**, 1316 (1980).
[3] J. Davis and M. Blaha, J. Quant. Spectrosc. Radiat. Transf. **27**, 307 (1982).
[4] H. Nguyen, M. Koenig, D. Benderjen, M. Caby, and C. Couland, Phys. Rev. A **33**, 1279 (1986).
[5] H. R. Griem, Phys. Rev. A **38**, 2943 (1988).

[6] J. Seidel, S. Arndt, and W. D. Kraeft, Phys. Rev. E **52**, 5387 (1995).
[7] C. S. Lam and Y. P. Varshni, Phys. Rev. A **27**, 418 (1983).
[8] Z. Wang and P. Winkler, Phys. Rev. A **52**, 216 (1995).
[9] P. Winkler, Phys. Rev. E **53**, 5517 (1996).
[10] D. Ray and P. K. Mukherjee, Eur. Phys. J. D **2**, 89 (1998); J. Phys. B **31**, 3479 (1998).
[11] D. K. Bradley, J. Kilkenny, S. J. Rose, and J. D. Hares, Phys. Rev. Lett. **59**, 2995 (1987).
[12] D. Riley, O. Willi, S. J. Rose, and T. Afshar-Rad, Europhys. Lett. **10**, 135 (1989).
[13] W. Schwanda and K. Eidmann, Phys. Rev. Lett. **69**, 3507 (1992).
[14] G. Jamelot, P. Jaegle, P. Lemaire, and A. Carillon, J. Quant. Spectrosc. Radiat. Transf. **44**, 71 (1990).
[15] St. Boeddeker, S. Guenter, A. Koenies, L. Hitzschke, and H.-J. Kunze, Phys. Rev. E **47**, 2785 (1993).
[16] A. Saemann, K. Eidmann, I. E. Golovkin, R. C. Mancini, E. Andersson, E. Foerster, and K. Witte, Phys. Rev. Lett. **82**, 4843 (1999).
[17] K. Scheibner, J. C. Weisheit, and N. F. Lane, Phys. Rev. A **35**, 1252 (1987).
[18] B. Zygelman and A. Dalgarno, Phys. Rev. A **35**, 4085 (1987).
[19] B. Zygelman and A. Dalgarno, Phys. Rev. A **37**, 2693 (1988).
[20] J. C. Weisheit, Adv. At. Mol. Phys. **25**, 101 (1988).
[21] S. Ichimaru, *Basic Principles of Plasma Physics* (Benjamin, Reading, MA, 1973), pp. 5–8.
[22] Y. D. Jung, Eur. Phys. J. D **7**, 249 (1999), and references therein.
[23] L. I. Schiff, *Quantum Mechanics*, 3rd ed. (McGraw-Hill, New York, 1968).
[24] D. W. Walker, Adv. Phys. **20**, 257 (1971).
[25] I. P. Grant, Proc. R. Soc. London, Ser. A **262**, 555 (1961); Adv. Phys. **19**, 747 (1970).
[26] F. Salvat and R. Mayol, Comput. Phys. Commun. **62**, 65 (1991).
[27] B. H. Bransden and C. J. Joachain, *Physics of Atoms and Molecules* (Longman, New York, 1983), Sec. 5.1.