Theory of interparticle correlations in dense, high-temperature plasmas. VII. Polarization shift of spectral lines

Xin-Zhong Yan and Setsuo Ichimaru
Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo 113, Japan
(Received 30 July 1985; revised manuscript received 29 April 1986)

The radial distribution functions between a charged radiator atom and plasma particles, investigated in the preceding paper, are applied to the calculation of shift of the spectral lines arising from average polarization of dense hydrogenic plasmas due to the Coulomb field of the radiator. Dependence of the line shift on the radiator charge, the plasma density, and temperature is numerically investigated and is compared with other theoretical predictions.

I. INTRODUCTION

In the preceding paper,[1] hereafter referred to as paper VI, we calculated the radial distribution functions between a charged radiator atom and dense hydrogenic plasmas on the basis of the hypernetted-chain (HNC) scheme developed in the earlier papers[2] of this series; the probability densities of various electric microfields at the radiatior were thereby evaluated. In the present paper we apply the numerical results obtained for the radial distribution functions to the calculation of the shift of spectral lines arising from the average polarization of the plasma due to the Coulomb field of the charged radiator.

The frequency shifts of spectral lines in plasmas have been investigated both experimentally[3–8] and theoretically[9–15] by many authors in the past. Both blue shifts and red shifts were observed in experiments, but a recent work[8] on the resonance lines of the hydrogenic ions C VI, N VII, and O VIII reported observation of virtually no significant plasma shifts at the electron densities 10^{21}–10^{23} cm^{-3} and the electron temperatures 70–100 eV.

The theoretical calculations of the plasma line shifts have been even more controversial. Several authors calculated the polarization shifts of the spectral lines by assuming that the effective potential at the radiator atom may be determined from the consideration of the time-averaged distributions of the plasma particles around it.[9,11,12,16,17] Others argued that the dynamic effects such as electron collisions and microscopic field fluctuations should be taken into account in the calculations of the spectal-line shifts.[10,13–15]

In the present paper, without delving into a difficult problem of resolving such a controversy, we confine ourselves only to the calculation of that part of the polarization shift arising from the time-averaged correlations between the radiator and the plasma particles. The interparticle correlations are calculated self-consistently by taking account of the strong Coulomb-coupling effect and quantum-mechanical interference effect between the charged particles. Since this work is a continuation of paper VI, we closely follow the notation and convention used in paper VI unless otherwise specified.

II. PLASMA POLARIZATION SHIFT

We consider a hydrogen plasma ($Z=1$) with number density n_E ($=n_I$) at temperature T, in which a radiator atom with electric charge $Z_R e$ is immersed. We assume that the radiator retains a single bound electron so that its nuclear charge is given by $(Z_R+1)e$. We are thus concerned with the hydrogenic energy levels of the electron in a bound state.

Setting the radiator at the origin of the coordinates, we express the average charge distribution $\rho_e(\mathbf{r})$ due to polarization as

$$\rho_e(\mathbf{r})=en_E[g_{RI}(\mathbf{r})-g_{RE}(\mathbf{r})]\ , \tag{1}$$

where $g_{RI(E)}(\mathbf{r})$ is the radial distribution function between the radiator and the ions (the electrons) in the plasma. The polarization potential to the electron is then given by

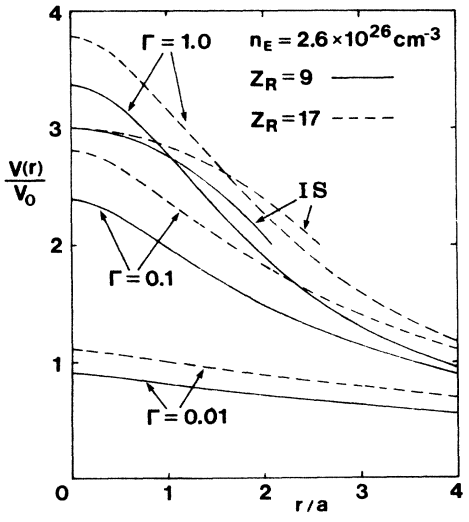

FIG. 1. Polarization potentials Eq. (2) at various Γ values and the ion-sphere (IS) model potential Eq. (9), both in units of V_0 given by Eq. (7), as functions of $r(4\pi n_E/3)^{1/3}$.

TABLE I. Energy level E_{nl} and its shift ΔE_{nl} (in atomic units of 27.21 eV) for $_{10}Ne^{9+}$ radiator atom in hydrogen plasmas with $n_E=2.6\times10^{26}$ cm^{-3}.

	T	1.7×10^6 K		1.7×10^7 K		1.7×10^8 K	
n	l	E_{nl}	ΔE_{nl}	E_{nl}	ΔE_{nl}	E_{nl}	ΔE_{nl}
1	0	−16.64	33.36	−26.00	24.00	−40.28	9.721
2	0	−1.277	11.22	−1.456	11.04	−5.303	7.197
2	1	−1.082	11.42	−1.092	11.41	−4.837	7.663
3	0	−1.042	4.514	−1.072	4.483	−1.356	4.200
3	1	−0.960	4.595	−0.972	4.583	−1.202	4.354
3	2	−0.987	4.569	−0.987	4.569	−1.000	4.556

$$V_P(r)=-e\int d\mathbf{r}'\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\ . \tag{2}$$

We shall use in Eq. (1) those radial distribution functions as calculated in the HNC scheme of paper VI. This procedure then amounts to assuming the radiator as a point charge of Z_Re, neglecting fine structures of its internal charge distribution. Skupsky[11] treated $g_{RI}(r)$ in the nonlinear Debye-Hückel approximation and $g_{RE}(r)$ in the finite-temperature Thomas-Fermi approximation, where he was able to take into account the internal charge distribution of the bound-state electron self-consistently. The self-consistency was enforced by following the steps of numerical iteration. We recall, however, that the numerical solution to the HNC equations also involves iteration. Since such a double iteration would impose a formidable task in numerical solution to the resulting equations, we were not able to incorporate Skupsky's self-consistent scheme in the present HNC formalism. The present method may be justified when $Z_R\gg1$.

The energy levels of the bound-state electron in the radiator are then determined from the solution to the Schrödinger equation,

$$H\psi_{nl}=E_{nl}\psi_{nl} \tag{3}$$

with the Hamiltonian

$$H=\frac{p^2}{2m}-\frac{(Z_R+1)e^2}{r}+V_P(r)\ , \tag{4}$$

where n and l are the principal and azimuthal quantum numbers. In the absence of $V_P(r)$, the energy levels are

$$E_{nl}^{(0)}=-m(Z_R+1)^2e^4/2\hbar^2n^2\ , \tag{5}$$

so that the plasma polarization shift of the energy levels is given by

$$\Delta E_{nl}=E_{nl}-E_{nl}^{(0)}\ . \tag{6}$$

III. NUMERICAL RESULTS AND DISCUSSION

Considering basically the same cases as treated numerically in paper VI, we take $_{10}Ne^{9+}$ ($Z_R=9$) and $_{18}Ar^{17+}$ ($Z_R=17$) as radiator atoms. The electron density of the hydrogen plasma is assumed to be 2.6×10^{26} cm^{-3}; the temperature, 1.7×10^6, 1.7×10^7, and 1.7×10^8 K. The Γ parameter [Eq. (39) in paper VI] then takes on 1, 0.1, and 0.01, respectively.

Figure 1 shows the polarization potentials, Eq. (2), calculated by substituting in Eq. (1) the values of the radial distribution functions as depicted in Figs. 1–3 of paper VI. Those potentials are plotted in units of

$$V_0=Z_Re^2/2R_0\ , \tag{7}$$

where

$$R_0=(3Z_R/4\pi n_E)^{1/3}\ . \tag{8}$$

As the temperature is raised, the correlation effects diminish, and we observe in Fig. 1 that $V_P(r)$ tends to decrease.

For comparison, we also plot in Fig. 1 the polarization potential in the constant-electron-density ion-sphere model:[11,17,18]

$$V_{IS}(r)=V_0\left[3-\left[\frac{r}{R_0}\right]^2\right]\quad(r\le R_0)\ . \tag{9}$$

TABLE II. The same as Table I, but for $_{18}Ar^{17+}$ radiator atom.

	T	1.7×10^6 K		1.7×10^7 K		1.7×10^8 K	
n	l	E_{nl}	ΔE_{nl}	E_{nl}	ΔE_{nl}	E_{nl}	ΔE_{nl}
1	0	−98.09	63.91	−114.4	47.62	−142.9	19.08
2	0	−2.62	37.88	−7.53	32.97	−24.28	16.22
2	1	−1.94	38.56	−5.05	35.45	−23.68	16.82
3	0	−1.96	16.04	−2.06	15.94	−5.81	12.19
3	1	−1.81	16.19	−1.93	16.07	−5.41	12.59
3	2	−1.83	16.17	−1.83	16.17	−4.55	13.45

TABLE III. The same as Table I, but with $n_E = 2.6 \times 10^{23}$ cm^{-3}.

	T	1.7×10^6 K		1.7×10^7 K		1.7×10^8 K	
n	l	E_{nl}	ΔE_{nl}	E_{nl}	ΔE_{nl}	E_{nl}	ΔE_{nl}
1	0	−46.69	3.31	−48.90	1.10	−49.68	0.32
2	0	−10.08	2.423	−11.47	1.026	−12.14	0.358
2	1	−9.910	2.590	−11.45	1.053	−12.14	0.362
3	0	−3.997	1.559	−4.695	0.861	−5.217	0.339
3	1	−3.913	1.642	−4.674	0.881	−5.214	0.341
3	2	−3.755	1.800	−4.635	0.921	−5.208	0.347

TABLE IV. The same as Table I, but for $_{18}Ar^{17+}$ radiator atom with $n_E = 2.6 \times 10^{23}$ cm^{-3}.

	T	1.7×10^6 K		1.7×10^7 K		1.7×10^8 K	
n	l	E_{nl}	ΔE_{nl}	E_{nl}	ΔE_{nl}	E_{nl}	ΔE_{nl}
1	0	−155.5	6.53	−159.9	2.14	−161.4	0.65
2	0	−35.29	5.21	−38.50	2.00	−39.84	0.66
2	1	−35.02	5.48	−38.45	2.05	−39.83	0.67
3	0	−14.25	3.75	−16.21	1.79	−17.35	0.65
3	1	−14.09	3.91	−16.18	1.82	−17.34	0.66
3	2	−13.78	4.22	−16.12	1.88	−17.33	0.67

TABLE V. Frequency shift (in units of eV) of the Lyman-α line for $_{10}Ne^{9+}$.

n_E (cm^{-3})	T (K)	$\hbar\Delta\omega$	$\hbar\Delta\omega_{IS}$	$\hbar\Delta\omega_{DH}$
2.6×10^{26}	1.7×10^6	−597	-5×10^2	-7.7×10^3
2.6×10^{26}	1.7×10^7	−343	-5×10^2	-7.7×10^2
2.6×10^{26}	1.7×10^8	−56	-5×10^2	−77
2.6×10^{23}	1.7×10^6	−20	−0.5	−7.7
2.6×10^{23}	1.7×10^7	−0	−0.5	−0.8
2.6×10^{23}	1.7×10^8	+0	−0.5	−0.1

TABLE VI. The same as Table V, but for $_{18}Ar^{17+}$.

n_E (cm^{-3})	T (K)	$\hbar\Delta\omega$	$\hbar\Delta\omega_{IS}$	$\hbar\Delta\omega_{DH}$
2.6×10^{26}	1.7×10^6	−690	-2×10^2	-8.1×10^3
2.6×10^{26}	1.7×10^7	−331	-2×10^2	-8.1×10^2
2.6×10^{26}	1.7×10^8	−61	-2×10^2	−81
2.6×10^{23}	1.7×10^6	−29	−0.2	−8.1
2.6×10^{23}	1.7×10^7	−2	−0.2	−0.8
2.6×10^{23}	1.7×10^8	+0	−0.2	−0.1

This ion-sphere model may be fairly accurate in describing the short-range radiator-ion correlations in the limit of strong Coulomb coupling.[18,19] As the model assumes $g_{RE}(r)=1$, however, it fails to account for the attractive nature [i.e., $g_{RE}(r)>1$] of the short-range radiator-electron correlations, which are manifested in Figs. 1–3 of paper VI. Consequently, $V_P(r)$ at $\Gamma=1$ exceeds $V_{IS}(r)$ in the short-range domain.

Substituting the polarization potentials of Fig. 1 in Eq. (4), we solve Eq. (3) numerically for the energy levels E_{nl}. The values of E_{nl} and ΔE_{nl} so computed are listed in Tables I and II, where the accuracy of the numerical solution is reflected in the significant digits.

For comparison we have additionally chosen the cases of the hydrogen plasma with $n_E=2.6\times10^{23}$ cm^{-3} and $T=1.7\times10^{6}$, 1.7×10^{7}, and 1.7×10^{8} K. Since the corresponding Γ values are 0.1, 0.01, and 0.001, much smaller than unity, we may use the Debye-Hückel approximation,

$$V_{DH}(r)=\frac{Z_R e^2}{r}\left[1-\exp\left[-\frac{r}{D}\right]\right], \tag{10}$$

with $D=(k_BT/8\pi e^2 n_E)^{1/2}$ for the expression of the polarization potential. The values listed in Tables III and IV are the results of numerical solution to Eq. (3), where Eq. (10) is substituted in place of $V_P(r)$ in Eq. (4). In Tables I–IV we clearly observe the general tendency in the increase of ΔE_{nl} as the density or Z_R is raised or as the temperature is lowered.

Finally we compute the frequency shift of the Lyman-α line

$$\hbar\Delta\omega=\Delta E_{21}-\Delta E_{10} \tag{11}$$

both for $_{10}Ne^{9+}$ and for $_{18}Ar^{17+}$, and list the results in Tables V and VI. Estimated errors involved in the computation of Eq. (11) are $\pm(1-2)$ eV, so that the computed values of $\hbar\Delta\omega$ less than these magnitudes are entered as zero with sign.

For comparison we also list in those tables the values of the shift in the constant-electron-density ion-sphere model,[4]

$$\hbar\Delta\omega_{IS}\simeq-2\times10^{-22}n_E/(Z_R+1)^2 \ \text{(eV)}, \tag{12}$$

and those in the linearized Debye-Hückel approximation,

$$\hbar\Delta\omega_{DH}=-\frac{Z_R e^2}{2D^2}\int dr\, r^3(\psi_{21}^2-\psi_{10}^2)$$

$$\simeq-5.6\times10^{-17}\frac{Z_R}{Z_R+1}\frac{n_E}{T} \ \text{(eV)}. \tag{13}$$

In Eqs. (12) and (13), n_E and T are in units of cm^{-3} and degree K. We observe substantial difference in the prediction of the frequency shift between various model calculations.

Among the particular calculations in the present theory, we note that the value of $\hbar\Delta\omega$ at $n_E=2.6\times10^{26}$ cm^{-3} and $T=1.7\times10^{7}$ K for $_{10}Ne^{9+}$ turns out greater, though slightly, than that for $_{18}Ar^{17+}$, a tendency opposite to other five cases of n_E-T combinations. We have reexamined the computational procedures carefully to make certain that errors do not enter the computation to cause this inversion. We remark that the calculations of frequency shift involve delicate interplay between correlation effects in the plasma and the wave-function spread of the electron in a bound state. The frequency shift is a monotonic function of n_E, T, and Z_R only in a simplified model calculation such as Eqs. (12) and (13). Because of the complex nature in the correlations between the radiator and the partially degenerate electrons as well as the classical ions, however, $\hbar\Delta\omega$ generally exhibits deviations from such a monotonicity; these features are illustrated in the results of the present and Skupsky's[11] calculations.

ACKNOWLEDGMENTS

The authors wish to thank Dr. Hiroshi Iyetomi, Dr. Takako Kato, Dr. Shigenori Tanaka, and Dr. Tsutomu Watanabe for useful discussions. This research was supported in part through Grant-in-Aid for Scientific Research No. 59380001, provided by the Japanese Ministry of Education, Science, and Culture.

[1]X.-Z. Yan and S. Ichimaru, preceding paper, Phys. Rev. A **34**, 2167 (1986).

[2]S. Ichimaru, S. Mitake, S. Tanaka, and X.-Z. Yan, Phys. Rev. A **32**, 1768 (1985) (paper I); S. Mitake, S. Tanaka, X.-Z. Yan, and S. Ichimaru, *ibid.* **32**, 1775 (1985) (paper II); S. Tanaka, S. Mitake, X.-Z. Yan, and S. Ichimaru, *ibid.* **32**, 1779 (1985) (paper III); X.-Z. Yan, S. Tanaka, S. Mitake, and S. Ichimaru, *ibid.* **32**, 1785 (1985) (paper IV); S. Ichimaru and S. Tanaka, *ibid.* **32**, 1790 (1985) (paper V).

[3]H. F. Berg, A. W. Ali, R. Lincke, and H. R. Griem, Phys. Rev. **125**, 199 (1962).

[4]J. R. Greig, H. R. Griem, L. A. Jones, and T. Oda, Phys. Rev. Lett. **24**, 3 (1970).

[5]T. L. Pittman, P. Voigt, and D. E. Kelleher, Phys. Rev. Lett. **45**, 723 (1980).

[6]S. Hashimoto, J. Phys. Soc. Jpn. **51**, 1613 (1982).

[7]J. C. Adcock, Jr. and H. R. Griem, Phys. Rev. Lett. **50**, 1369 (1983).

[8]S. Goldsmith and H. R. Griem, Phys. Rev. A **30**, 2775 (1984), and references cited therein.

[9]For a review on the plasma polarization-shift effect, see S. Volonté, J. Phys. D **11**, 1615 (1978).

[10]For a critical review on the line shifts, see D. E. Kelleher and J. Cooper, in *Spectral Line Shapes,* edited by F. Rostas (de Gruyter, Berlin, 1985), Vol. 3, p. 85.

[11]S. Skupsky, Phys. Rev. A **21**, 1316 (1980).

[12]U. Gupta and A. K. Rajagopal, J. Phys. B **14**, 2309 (1981).

[13]K. Yamamoto and H. Narumi, J. Phys. Soc. Jpn. **44**, 349 (1979); Phys. Lett. **86A**, 142 (1981).

[14]C. A. Iglesias, Phys. Rev. A **29**, 1366 (1984).

[15]D. B. Boercker and C. A. Iglesias, Phys. Rev. A **30**, 2771 (1984).

[16]J. C. Weisheit and B. F. Rozsnyai, J. Phys. B **9**, L63 (1976); B. F. Rozsnyai, J. Quant. Spectrosc. Radiat. Transfer **15**, 695 (1975).

[17]J. C. Stewart and K. D. Pyatt, Astrophys. J. **144**, 1203 (1966).

[18]E. E. Salpeter, Aust. J. Phys. **7**, 373 (1954).

[19]For discussion, see. e.g., S. Ichimaru, Rev. Mod. Phys. **54**, 1017 (1982).