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Semiclassical convergent calculations for the electron-impact broadening and shift of some lines of neutral helium in a hot plasma

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A theoretical formalism, which is the semiclassical analog of a unitarized Bethe-Born approximation, is used to calculate the broadening and shift, produced by electronic collisions, of some lines (7281, 7065, 6678, 5876, 5048, 5016, 4713, 4121, 3965, 3889, 3188, and 2945 Å) of neutral helium in a hot plasma. The effects of the ions are also taken into account by using the approach developed by Griem *et al.* Our theoretical predictions are compared with the experimental results of Wulff, Berg *et al.*, Kelleher, and Diatta.

I. INTRODUCTION

In a preceding paper, Bassalo and Cattani[1] have shown that their quantum-mechanical impact approach, developed to calculate the width and shift of spectral lines produced by electronic collisions, cannot explain satisfactorily the widths of neutral helium lines in plasmas with temperatures smaller than 50 000 K. As was shown by Griem, Baranger, Kolb, and Oertel,[2] the second Born approximation used by Bassalo and Cattani[1] is not suited, in this range of temperatures,[3,4] to calculating the widths which are caused mainly by inelastic collisions. Their formalism is satisfactory only to obtain the shifts.

We believe that for these cases, the broadening and shift of the spectral lines produced by electronic collisions can be better obtained by using a semiclassical formalism with convenient approximations to estimate the effects of the strong collisions, for which the perturbation theory breaks down.

As one can see in the literature,[5] we have, essentially, two slightly different semiclassical impact theories to evaluate the effect of the electronic collisions in plasmas: an impact-parameter "cutoff" theory and a "convergent" theory. The cutoff theory has been adopted by many authors[5] and has been used extensively by Griem and collaborators[2,5,6] and by Sahal-Brechot[7-9] to study the line shapes of neutral atoms and ions.

The convergent theory, developed by Vainshtein and Sobel'man[10] in a "two-level" approximation, was applied with some modifications by Dyne and O'Mara[11] to calculate the widths and shifts of some neutral helium lines. Their predictions have been compared with the experimental results of Wulff[12] and Berg *et al.*[13]

We must note that for the helium lines it should be necessary, in principle, to consider a "many-level"[2,5,7] instead of a two-level approximation.[11] So our intention in this paper is to apply the convergent method, in a many-level approximation, to study the helium lines, taking into account also the most recent experimental results of Kelleher[14] and Diatta.[15] To take into account the ion contribution we use the approach developed by Griem *et al.*[2] and Griem[6] (see also Griem[5]). Our theoretical predictions are compared, for many lines, with experimental results found in the literature.[12-15]

Although the convergent method requires a slight increase in computational effort compared with the cutoff method, its advantage is that there is no introduction of an estimated impact-parameter cutoff. However, we must note that the convergent theory is not necessarily superior to the cutoff theory to account for the strong collisions since both formalisms depend primarily on the S-matrix calculation that, in both methods, was taken only up to the second Born approximation.

II. CALCULATION OF $\Delta\nu$ AND S FOR HELIUM LINES

According to the convergent method, in a many-level approximation,[16,17] the half half-width $\Delta\nu_e$ and the shift S_e produced by electronic collisions, for an isolated Lorentzian line, measured in hertz, can be written as

$$\Delta\nu_e = N\int_0^\infty dv\, vF(v)\int_0^\infty db\, b\{1-\cos[\phi_{IF}(b,v)] \times \exp[-\tfrac{1}{2}\Gamma_{IF}(b,v)]\} \quad (1)$$

and

$$S_e = -N\int_0^\infty dv\, vF(v)\int_0^\infty db\, b\sin[\phi_{IF}(b,v)] \times \exp[-\tfrac{1}{2}\Gamma_{IF}(b,v)], \quad (2)$$

where the indices I and F refer to the initial and final states of the line, respectively, N is the density of perturbing electrons, v the electron velocity, $F(v)$ the Maxwell-Boltzmann velocity distribution function, b the impact parameter,

$$\Gamma_{IF}(b,v)=\Gamma_I(b,v)+\Gamma_F(b,v),$$

and

$$\phi_{IF}(b,v)=\phi_I(b,v)-\phi_F(b,v).$$

The functions $\Gamma_K(b,v)$ and $\phi_K(b,v)$, with $K=I$ or F, are given by[18]

$$\Gamma_K(b,v)=\frac{1}{\hbar^2}\sum_{M(M\neq K)}|\langle K|G(\omega_{KM})|M\rangle|^2_{\mathrm{Av}}$$

and

$$\phi_K(b,v)=\left(\frac{1}{2\pi\hbar^2}\right)\sum_{M(M\neq K)}P\int_{-\infty}^{+\infty}\frac{d\omega}{\omega_{KM}-\omega}|\langle K|G(\omega)|M\rangle|^2_{\mathrm{Av}},$$

where M are the intermediate states of the emitting atom, the symbol Av means an average over all possible values of the z component of the atomic angular momentum, $\hbar\omega_{KM}$ the energy difference between the states K and M,

$$G(\omega)=\int_{-\infty}^{+\infty}dt\,V(t)\exp(i\omega t),$$

and $V(t)$ the electron-atom interaction potential as

TABLE I. Comparison of measured and calculated half-widths for some neutral helium lines.

Wavelength (in Å)	Electron density (10^{+16} cm^{-3})	Temperature (10^3 K)	R	A	Half-widths (Å) Calculated No Debye shielding	Calculated Debye shielding	Measured
7281	1.03	20.9	0.29	0.076	0.80	0.80	0.88[a]
7065	1.03	20.9	0.29	0.062	0.46	0.46	0.47[a]
6678	1.03	20.9	0.29	0.190	0.78	0.78	0.98[a]
5876	16.0	49.0	0.30	0.162	4.50	4.50	5.5[b]
	13.0	43.0	0.31	0.152	3.68	3.68	4.9[b]
	4.1	20.0	0.37	0.104	1.22	1.22	
	2.0	18.0	0.35	0.088	0.58	0.58	
	1.03	20.9	0.29	0.076	0.28	0.28	0.39[a]
5048	3.2	30.0	0.29	0.173	5.22	5.22	4.6[c]
	2.0	18.0	0.35	0.157	3.10	3.10	3.4[d]
	1.03	20.9	0.29	0.132	1.58	1.58	1.68[a]
5016	3.2	30.0	0.29	0.257	2.48	2.44	1.9[c]
	17.0	24.0	0.43	0.409	14.90	13.36	13.0[b]
	4.1	20.0	0.37	0.262	3.36	3.24	3.8[d]
	2.0	18.0	0.35	0.213	1.60	1.58	1.8[d]
	1.03	20.9	0.29	0.184	0.78	0.78	0.86[a]
4713	3.2	30.0	0.29	0.138	2.98	2.98	2.9[c]
	13.0	20.0	0.45	0.202	12.06	12.06	14.0[b]
	4.1	20.0	0.37	0.151	3.66	3.66	4.6[d]
	2.0	18.0	0.35	0.128	1.72	1.72	2.05[d]
	1.03	20.9	0.29	0.107	0.90	0.90	0.95[a]
4121	3.2	30.0	0.29	0.189	8.12	8.12	6.2[c]
	2.9	18.0	0.37	0.190	6.98	6.96	7.0[d]
	1.03	20.9	0.29	0.145	2.42	2.42	2.22[a]
3965	1.4	18.0	0.33	0.395	3.34	3.14	4.1[d]
	1.03	20.9	0.29	0.353	2.38	2.28	2.30[a]
3889	3.2	30.0	0.29	0.103	0.70	0.70	0.73[c]
	15.0	26.0	0.41	0.151	3.46	3.46	4.5[b]
	4.1	20.0	0.37	0.109	0.92	0.92	1.25[d]
	2.0	18.0	0.35	0.093	0.42	0.42	0.55[d]
	1.03	20.9	0.29	0.078	0.22	0.22	0.24[a]
3188	15.0	29.0	0.38	0.289	11.74	11.32	13.4[b]
	4.1	20.0	0.37	0.202	3.00	2.98	3.0[d]
	1.7	18.0	0.34	0.161	1.20	1.20	1.35[d]
	1.03	20.9	0.29	0.143	0.72	0.72	0.78[a]
2945	1.03	20.9	0.29	0.220	1.98	1.98	2.0[a]

[a] Kelleher (Ref. 14).
[b] Berg *et al.* (Ref. 13).
[c] Wulff (Ref. 12).
[d] Diatta (Ref. 15).

a function of the time t.

Let us indicate by $|n_I^a l_I m_I\rangle$ and $|n_F^a l_F m_F\rangle$, where $a=1$ for para-helium and $a=3$ for ortho-helium, the initial and final states, respectively, of the analyzed transition. The final state will be chosen as the lowest energy level. In all cases analyzed in this paper the lowest energy levels are much less polarizable than the initial states. We verified also that their contributions to the broadening and to the shift are negligible compared with those of the initial states. So in our cases, Γ_{IF} and ϕ_{IF}, are given simply by $\Gamma_{IF}(b,v) \cong \Gamma_I(b,v)$ and $\phi_{IF}(b,v) \cong \phi_I(b,v)$, respectively.

Assuming that the electron describes a straight path, with constant velocity during the collision with the helium atom and that its interaction with this atom is dipolar, we can show that $\Gamma_I(b,v)$ and $\phi_I(b,v)$ can be written as,[2,5] omitting for simplicity the index I,

$$\Gamma(b,v)=\frac{4}{3}\left(\frac{e^2a_0}{\hbar bv}\right)^2\sum_{l'}|\langle n^a l||r||n^a l'\rangle|^2 A(Z_{n^a l,n^a l'}) \tag{3}$$

and

$$\phi(b,v)=\frac{2}{3}\left(\frac{e^2a_0}{\hbar bv}\right)^2\sum_{l'}|\langle n^a l||r||n^a l'\rangle|^2 B(Z_{n^a l,n^a l'}), \tag{4}$$

TABLE II. Comparison of measured and calculated shifts for some neutral helium lines.

Wavelength (in Å)	Electron density (10^{+16} cm^{-3})	Temperature (10^3 K)	R	A	Shifts (Å) Calculated: No Debye shielding	Shifts (Å) Calculated: Debye shielding	Shifts (Å) Measured
7281	1.03	20.9	0.29	0.076	+0.37	+0.36	+0.473 [a]
7065	1.03	20.9	0.29	0.062	+0.23	+0.23	+0.302 [a]
6678	1.03	20.9	0.29	0.190	+0.22	+0.19	+0.355 [a]
5876	16.0	49.0	0.30	0.162	−1.37	−1.22	+0.7 [b]
	13.0	43.0	0.31	0.152	−1.13	−1.02	0.0 [b]
	4.1	20.0	0.37	0.104	−0.41	−0.38	−0.30 [d]
	2.0	18.0	0.35	0.088	−0.20	−0.19	−0.10 [d]
	1.03	20.9	0.29	0.076	−0.097	−0.097	−0.074 [a]
5048	3.2	30.0	0.29	0.173	+2.19	+2.05	+2.0 [c]
	2.0	18.0	0.35	0.157	+1.43	+1.35	+0.90 [d]
	1.03	20.9	0.29	0.132	+0.71	+0.68	+0.891 [a]
5016	3.2	30.0	0.29	0.257	−0.83	−0.71	−0.55 [c]
	17.0	24.0	0.43	0.409	−5.14	−3.91	−4.8 [b]
	4.1	20.0	0.37	0.262	−1.14	−0.94	−0.85 [d]
	2.0	18.0	0.35	0.213	−0.54	−0.46	−0.40 [d]
	1.03	20.9	0.29	0.184	−0.25	−0.23	−0.283 [a]
4713	3.2	30.0	0.29	0.138	+1.34	+1.28	+1.4 [c]
	13.0	20.0	0.45	0.202	+5.98	+5.37	+6.0 [b]
	4.1	20.0	0.37	0.151	+1.81	+1.71	+2.3 [d]
	2.0	18.0	0.35	0.128	+0.87	+0.83	+1.0 [d]
	1.03	20.9	0.29	0.107	+0.44	+0.43	+0.538 [a]
4121	3.2	30.0	0.29	0.189	+3.61	+3.31	+2.8 [c]
	2.9	18.0	0.37	0.190	+3.43	+3.10	
	1.03	20.9	0.29	0.195	+1.15	+1.09	+1.124 [a]
3965	1.4	18.0	0.33	0.395	−1.19	−0.95	−0.73 [d]
	1.03	20.9	0.29	0.353	−0.83	−0.70	−0.771 [a]
3889	3.2	30.0	0.29	0.103	+0.14	+0.13	+0.3 [b]
	15.0	26.0	0.41	0.151	+0.77	+0.66	+1.2 [b]
	4.1	20.0	0.37	0.109	+0.21	+0.19	+0.25 [d]
	2.0	18.0	0.35	0.093	+0.10	+0.99	+0.10 [d]
	1.03	20.9	0.29	0.078	+0.048	+0.044	+0.080 [a]
3188	15.0	29.0	0.38	0.289	+3.13	+2.36	+4.1 [b]
	4.1	20.0	0.37	0.202	+0.80	+0.68	+0.9 [d]
	1.7	18.0	0.34	0.161	+0.31	+0.28	+0.30 [d]
	1.03	20.9	0.29	0.143	+0.18	+0.17	+0.258 [a]
2945	1.03	20.9	0.29	0.220	+0.46	+0.43	+0.683 [a]

[a] Kelleher (Ref. 14).
[b] Berg *et al.* (Ref. 13).
[c] Wulff (Ref. 12).
[d] Diatta (Ref. 15).

where $(n^a l||r||n^a l')$ are the reduced dipole matrix elements,

$$Z_{n^a l, n^a l'} = (b/v)\omega_{n^a l, n^a l'} ,$$

$$A(Z) = Z^2[K_0^2(|Z|) + K_1^2(|Z|)],$$

and

$$B(Z) = \pi Z^2[K_0(Z)I_0(Z) - K_1(Z)I_1(Z)].$$

The reduced matrix elements have been calculated using the oscillator strength values taken from the table reported by Wiese *et al.*[19] The energy differences $\hbar\omega_{n^a l, n^a l'}$ between the states $|n^a l)$ and $|n^a l')$ are given by Moore.[20]

According to Griem,[5] it seems that a better agreement between theory and experiment, for the widths and shifts of the helium lines, can be obtained if Debye shielding is neglected. We intend to investigate this point performing our calculations with and without the Debye shielding. In order to take into account, in our approach, the Debye screening effects, we integrate in Eqs. (1) and (2), the impact parameter b from 0 up to ρ_D, where ρ_D is the Debye radius.

Up to now we have evaluated the contribution of the electron impacts. To take into account the ion contribution we use the approach developed by Griem *et al.*[2] and Griem.[5] Following these authors, the total half-width $\Delta\nu$ and the total shift S are given, in terms of the parameters A and R, by

$$\Delta\nu = \Delta\nu_e + \Delta\nu_{ion} = \Delta\nu_e[1 + 1.75\,A(1 - 0.75\,R)], \quad (5)$$

and

$$S = S_e + S_{ion} = S_e \pm 2.0\,A(1 - 0.75\,R)\Delta\nu_e . \quad (6)$$

In Tables I and II the experimental results of Wulff,[12] Berg *et al.*,[13] Kelleher,[14] and Diatta[15] are compared with our theoretical predictions with and without the Debye shielding. We have also verified that, using the reduced dipole matrix elements calculated with hydrogenlike wave functions, our predictions for the widths and shifts are only slightly different from those showed in Tables I and II.

From Tables I and II, we may conclude, for the cases analyzed in this paper, the following.

(a) The linewidth calculations are practically independent of the Debye shielding.

(b) The Debye shielding affects, sometimes significantly, the shift calculations.

(c) A somewhat better agreement with experiment is found if the Debye screening effects are neglected.

We must note that, within the experimental errors, the agreement between theoretical and experimental results is good for the widths and only reasonable for the shifts.[21]

We have not included in Tables I and II, the predictions that could be made with the approach of Griem *et al.*[5] (many of them are given by Diatta[15]), as well as some predictions, reported by Diatta,[15] obtained with the approaches of Sahal-Brechot and Brissaud and Frisch. Comparing these and our predictions with the experimental results we observe that the cutoff and convergent methods are about equally successful descriptions of the data.

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