# Shifts of one-electron ions lines from  $\Delta n = 0$  interactions with electrons in hot and dense plasma

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Abstract. This paper is concerned with lineshifts of hydrogen-like ions due to electron collisions in dense and hot plasmas. These collisions are treated by including all effects due to monopole, dipole, and quadrupole interactions between radiator and electron perturbers. The latter follow exact hyperbolic trajectories with a possible penetrating part inside atomic orbits. A simple closed form for the line shift has been derived. Comparison between our semi-classical results and the quantum mechanical ones shows good agreement for a large range of high electron densities and temperatures.

**PACS.** 32.70.Jz Line shapes, widths, and shifts  $-32.70$ .n Intensities and shapes of atomic spectral lines

# 1 Introduction

Stark-broadened spectral lines emitted or absorbed by dense and hot plasmas are currently used in density and temperature diagnostics, and radiative transfer measurements, especially for X-ray Laser research.

Spectral lines emitted by hydrogenic ions have been reported to be shifted when they are excited in dense plasma [1–5]. Since the standard Stark-broadening theories [6] when applied to hydrogen-like ions do not predict line shifts, the observed effect was first related to the formation of a time-averaged negative charge which overlaps the bound electron orbits, and produces shifts of energy levels. This "plasma polarization shift" has been considered in several theoretical advances. There are two equivalent methods of calculation: the first one is based on the ensemble average of atomic properties, such as the Debye-Hückel theory, average atom method [7] and the self-consistent-field for confined atom model [8]; the second one corresponds to the time average of these properties using quantum mechanical impact theory [8–10].

The purpose of this paper is to use the semi-classical approximation for treating the effect of electronic collisions in the shift of hydrogenic lines. In particular, the penetrating collisions in the atomic orbitals, which were analyzed by the quantum mechanical theory in the literature as mentioned previously, are treated here by the semi-classical approximation. The monopole, dipole and quadrupole terms are used in the ion-electron interaction and the hyperbolic trajectory effects of electron collision are included. Accordingly, a simple analytical formula will be established to evaluate the electronic shift. The results deduced from this method for electronic shift are in agreement with those obtained from the quantum mechanical impact theory in the Coulomb-Born-Oppenheimer (CBO) approximation [8].

# 2 Method of calculation

In the framework of impact theory [6,11], the electron width  $w$  and shift  $d$  of a spectral line, are given by:

$$
w + id = \int d\gamma \langle i, f | 1 - S_i \otimes S_f^* | i, f \rangle.
$$
 (1)

Here,  $\int d\gamma$  denotes the thermal average and the subscripts  $i$  and  $\hat{f}$  of the S-matrix allow the specification of the initial and final states of the optical transition.  $S = T(+\infty, -\infty)$ is deduced from the time dependent Schrödinger equation:

$$
i\hbar \frac{d}{dt}T(t,0) = V(t)T(t,0)
$$
 and  $T(0,0) = 1$  (2)

where,  $T(t, 0)$  is the time development operator and  $V(t)$ is the binary electron-radiator interaction which intervene in the line broadening. In equation (2), transitions between states with different principal quantum number  $n$ are neglected (non-quenching approximation),  $T(t)$  and  $V(t)$  correspond to one level i or f. The symbols **r** and  **denote the operator position of bound electron and** vector position of perturbing electron respectively. In the semi-classical description, the potential  $V(t)$  and the hyperbolic trajectory are deduced from the total interaction  $V_{tot}(t)$  by the following relations:

$$
V_{tot}(t) = -\frac{Ze^2}{r} - \frac{Ze^2}{R(t)} + \frac{e^2}{|\mathbf{R}(t) - \mathbf{r}|}
$$
  
= 
$$
-\frac{Ze^2}{r} - \frac{(Z - 1)e^2}{R(t)} + e^2 \Big[ \frac{1}{|\mathbf{R}(t) - \mathbf{r}|} - \frac{1}{R(t)} \Big].
$$
(3a)

The potential  $V(t)$  is given by,

$$
V(t) = e^{2} \left[ \frac{1}{|\mathbf{R}(t) - \mathbf{r}|} - \frac{1}{R(t)} \right] = V^{(0)} + \sum_{p=1}^{+\infty} V^{(p)}(t)
$$

$$
V^{(0)}(t) = -e^{2} \left[ \frac{1}{R(t)} - \frac{1}{r} \right] E(R(t) < r)
$$

$$
V^{(p)}(t) = e^{2} \frac{P_{p}(\cos \alpha)}{R^{2}} \left[ \frac{r^{p}}{R^{p-1}} E(R(t) > r) \right]
$$
(3b)

$$
+\frac{R^{p+2}}{r^{p+1}}E(R(t) < r)\Big] \quad \text{for} \quad p \ge 1; \alpha = (\widehat{\mathbf{r}, \mathbf{R}(t)})
$$

where,  $V^{(0)}, V^{(p)}$  and  $P_p$  are the monopolar, the 2<sup>p</sup>-polar potential and the Legendre polynomal of degree p, respectively. To separate the penetrating interactions  $(R(t) < r)$ and the external interactions  $(R(t) > r)$  one uses the Heaviside function  $E$  (...).

The term  $\frac{(Z-1)e^2}{R(t)}$  in (3a) gives the equation-trajectory of the perturber, which is in the form,

$$
R(t) = \frac{\rho \sqrt{\epsilon^2 - 1}}{1 + \epsilon \cos \theta(t)}, \quad \epsilon = \left(1 + \frac{\rho^2}{\rho_0^2}\right)^{1/2};
$$

$$
\rho_0 = \frac{(Z - 1)e^2}{mv^2} \quad \text{and} \quad R^2 \frac{d\theta}{dt} = \rho v \tag{4}
$$

where the symbols  $\rho, v, \theta$  and Z denote the impact parameter, the velocity, the polar angle of perturber and nuclear charge of radiator, respectively.

The diffusion-matrix  $S$  is given by,

$$
S = T(+\infty, -\infty) = \Theta \exp(-i\Phi)
$$
  
where  $\Phi = \frac{1}{\hbar} \int_{-\infty}^{+\infty} V(t)dt$ . (5)

Since  $V(t)$ , restricted to level i or f, does not commute with itself at different instants generally, the S-matrix must be expressed with the ordering-time operator  $\Theta$ . However, the electronic lineshift depends essentially on the monopole. Indeed, this spherical operator commutes with itself at different instants.

In order to prove the aforesaid statement, we study high and low temperature regimes.

#### 2.1 Case of high temperatures

At the limit of high temperatures, the phase-shift  $\Phi$  nearly vanishes. Therefore, the corresponding S-matrix can be studied within the second order perturbation theory. Accordingly, we have

$$
S = 1 - \frac{i}{\hbar} \int_{-\infty}^{+\infty} V(t)dt - \frac{1}{\hbar^2} \int_{-\infty}^{+\infty} dt \int_{-\infty}^{t} V(t)V(t')dt'.
$$
\n(6)

The lineshift which is given by the imaginary part of the electron broadening operator expressed in equation (1), becomes,

$$
\hbar d = \int d\gamma \int_{-\infty}^{+\infty} dt (V_i(t) - V_f^*(t)). \tag{7}
$$

The angular average of the integrand in (7) contributes only for monopole. The effects of dipole and multipole terms vanishes. Therefore, the lineshift depends only on the monopolar potential and becomes,

$$
\hbar d = \left\langle \int_{-\infty}^{+\infty} dt (V_i^{(0)}(t) - V_f^{(0)}(t) \right\rangle_{av}
$$
 (8)

where, the symbol  $\langle \cdots \rangle_{av}$  indicates the average over the impact-parameter and the velocity of the perturber.

### 2.2 Case of low temperatures

In this region, we show that the interactions inside the atomic orbital, that are the first causes of lineshift, contribute essentially via the monopole term. In fact, we show in the appendix, that the matrix-elements of multipoles are modified by a factor namely the "reduction factor", which truncates the multipolar effects inside the atomic orbital. This factor is given by,

$$
\langle n l m | V^{(p)}(R) | n l' m' \rangle
$$
  
= 
$$
\frac{e^2}{R^{p+1}} \langle n l m | r^p P_p(\cos \alpha) n l' m' \rangle \Delta_p(X)
$$
 (9)

where,

$$
\Delta_0(X) \approx \begin{cases} 1 - \frac{X}{X_{nl}} = 1 - \frac{R}{r_{nl}} & \text{for} \quad R < r_{nl} \\ 0 & \text{for} \quad R > r_{nl} \end{cases} \tag{10}
$$

$$
\Delta_p(X) \approx \begin{Bmatrix} 0 & \text{for } R < R_p^{(1)} \\ A_p(X - X_p^{(0)}) + B_p & \text{for } R_p^{(1)} < R < R_p^{(2)} \\ 1 & \text{for } R > R_p^{(2)} \end{Bmatrix} \tag{11}
$$

 $X = ZR/a_0, r_{nl}$  is in the order of the atomic rayon, which will be determined later. The quantities expressed in  $(11)$ are given in the appendix.

The analytical forms of "reduction factors" shows that the internal orbital interactions contributes essentially by the monopole.

### 3 Lineshift induced by electron collisions

The lineshift is given by the imaginary part of the electron broadening operator, equation (1). Where the scatteringmatrix  $S$  is in the form,

$$
S = \exp(-i\phi_0)
$$
 where  $\phi_0 = \frac{1}{\hbar} \int_{-\infty}^{+\infty} V^{(0)}(t) dt.$  (12)

The line shift  $d_{nl\rightarrow 1s}$  for Lyman serie, caused by  $N_e$  where electrons/cm<sup>3</sup> of velocity  $\nu$ , is given by:

$$
d_{nl \to 1s} = 2\pi N_e v \int_0^{\rho max} \rho \sin[\langle n, 1 | \phi_0 | n, 1 \rangle
$$

$$
- \langle 1s | \phi_0 | 1s \rangle] d\rho.
$$
(13)

### 3.1 Matrix elements of the monopolar phase-shift  $\Phi_0$

$$
\langle n l m | \Phi_0 | n l' m' \rangle = \frac{1}{\hbar} \int_{-\infty}^{+\infty} \langle n l m | V^{(0)}(t) | n l' m' \rangle dt
$$

$$
\langle n l m | \Phi_0 | n l' m' \rangle =
$$
  

$$
- \frac{e^2}{\hbar \rho v} \int_{-\theta_{max}}^{+\theta_{max}} R(\theta) \Big( 1 - \frac{R(\theta)}{r_{nl}} \Big) E(R(\theta) < r_{nl}) d\theta \delta_{ll'} \delta_{mm'}.
$$
  
(14)

The condition  $R < r_{nl}$  is equivalent to  $R_{min} < r_{nl}$  and  $\theta < \theta_{max}$ , where,

$$
R_{min} = \rho \sqrt{\frac{\epsilon - 1}{\epsilon + 1}}
$$
 and  $\cos \theta_{max} = \frac{1}{\epsilon} \left[ \frac{\rho \sqrt{\epsilon^2 - 1}}{r_{nl}} - 1 \right].$ 

Note that if  $R(\theta)$  is explicited in (14), the following integrals appear as,

$$
I_1 = \int \frac{d\theta}{1 + \epsilon \cos \theta} = \left[\epsilon^2 - 1\right]^{-\frac{1}{2}} \log\left[\frac{1 + s}{1 - s}\right];
$$

$$
s = \left[\frac{\epsilon - 1}{\epsilon + 1}\right]^{\frac{1}{2}} \tan \frac{\theta}{2}
$$
(15)

$$
I_2 = \int \frac{d\theta}{(1 + \epsilon \cos \theta)^2} = \frac{1}{\epsilon^2 - 1} \Big[ \frac{\epsilon \sin \theta}{1 + \epsilon \cos \theta} - I_1 \Big] \tag{16}
$$

then the matrix element of the monopolar phase shift becomes,

$$
\langle n l m | \Phi_0 | n l' m' \rangle = -\frac{e^2}{\hbar \nu} (1 + u_0) \left[ \log \frac{1 + x}{1 - x} - 2x \right]
$$

$$
\times E(R_{min} < r_{nl}) \delta_{ll'} \delta_{mm'} \tag{17}
$$

where  $u = \frac{\rho}{r_{nl}}$ ,  $u_0 = \frac{\rho_0}{r_{nl}}$  and  $x = \left[1 - \frac{u^2 + u_0^2}{(1 + u_0)}\right]$  $\frac{u^2+u_0^2}{(1+u_0)^2}$  $\frac{1}{2}$ . It is easy to show that this matrix element is lower than 1, in fact:

$$
\frac{e^2}{\hbar v} = \left[\frac{13.605}{kT_e(eV)}\right]^{1/2}, u_0 \approx \frac{Z(Z-1)}{n^2} \left(\frac{13.605}{kT_e(eV)}\right)
$$

where  $T_e$  is the electronic temperature.

(i) For the high temperatures

$$
\frac{e^2}{\hbar\nu}\ll 1 \Rightarrow |\langle n l m| \phi_0 | n l m \rangle| < 1.
$$

(ii) For the low temperatures  $(u_0 \gg 1)$ ,

$$
0 \le R_{min} \le r \Leftrightarrow 0 \le u \le \sqrt{1+2u_0} \Leftrightarrow x_0 \ge x \ge 0,
$$

$$
x_0 = \frac{\sqrt{1+2u_0}}{1+u_0} u_0 \gg 1 \Rightarrow x_0 \ll 1 \Rightarrow x \ll 1
$$
  

$$
\Rightarrow \log \frac{1+x}{1-x} - 2x = \frac{2}{3}x^3(1 + \frac{3}{5}x^2 + \cdots) \approx \frac{2}{3}x^3
$$
  

$$
\Rightarrow |\langle n|m|\Phi_0|nlm\rangle| \approx \frac{e^2}{\hbar v}(1 + u_0)\frac{2}{3}x^3 \le \frac{e^2}{\hbar v}(1 + u_0)\frac{2}{3}x_0^3
$$
  

$$
\approx \frac{4}{3}\frac{e^2}{\hbar v}\sqrt{\frac{2}{u_0}} = \xi
$$

where, 
$$
\xi = \frac{4\sqrt{2}}{3} \left[ \frac{r_{nl}}{(Z-1)a_0} \right]^{1/2} \approx \frac{4\sqrt{2}}{3} \frac{n}{\sqrt{Z(Z-1)}}.
$$

If  $Z \geq 5$  and  $n \leq 4$  then  $|\langle n l m | \Phi_0 | n l m \rangle \leq 1$ . Consequently, the monopolar phase shift is less than unity for all temperatures, and we can replace sinx by  $x$  in equation (13).

#### 3.2 Analytical expression of the line-shift

The thermal average in equation (13) is performed as follows,

$$
\rho d\rho = -r_{nl}^2 (1 + u_0)^2 x dx,
$$
  
\n
$$
(\rho = 0 \Rightarrow x = x_0),
$$
  
\n
$$
(\rho = \rho_{max} = r_{nl}\sqrt{1 + 2u_0} \Rightarrow x = 0)
$$
  
\n
$$
2\pi N_e v \int_0^{\rho_{max}} \rho d\rho \langle n l m | \phi_0 | n l m \rangle
$$
  
\n
$$
= -\frac{e^2}{\hbar} 2\pi N_e (r_{nl})^2 (1 + u_0)^3 \int_0^{x_0} x \, dx \langle n l m | \phi_0 | n l m \rangle
$$
  
\n
$$
= -\frac{2\pi N_e e^2}{3\hbar} (r_{nl})^2 f_{nl}(u_0) \qquad (18)
$$

$$
(19)
$$

where,

$$
f_{nl}(u_0) = 3(1+u_0)^3 \left[ x_0 - \frac{1}{2} (1-x_0^2) \log \frac{1+x_0}{1-x_0} - \frac{2}{3} x_0^3 \right].
$$
\n(20)

At high temperature  $(u_0 \rightarrow 0, x_0 \rightarrow 1 \text{ and } f_{nl}(u_0 \rightarrow 1),$ we obtain the results of the uniform electron-gas model [9], where the expression of  $r_{nl}$  is given by,

$$
(r_{nl})^2 = \langle nl|r^2|nl\rangle
$$
  
=  $\frac{a_0}{Z} \left[ \frac{n^2}{2} (5n^2 + 1 - 3l(l+1)) \right]^{1/2}$ . (21)

**Table 1.** Temperature dependence of the Lyman  $\alpha$ ,  $\beta$  and  $\gamma$  line-shift factor  $D(n, l, T)$  according to equations (21, 22).

$T_e({\rm eV})/Z^2$	D(2s)	D(2p)	D(3s)	D(3p)	D(3d)	D(4s)	D(4p)	D(4d)	D(4f)
$\mathbf{1}$	12.39	8.27	47.06	40.66	27.86	118.75	109.80	91.91	65.08
$\overline{2}$	9.05	6.06	35.40	30.60	20.99	92.31	85.37	71.48	50.65
3	7.62	5.11	30.54	26.41	18.13	81.63	75.49	63.23	44.82
$\overline{4}$	6.80	4.56	27.80	24.04	16.52	75.73	70.04	58.67	41.61
$\overline{5}$	6.25	4.20	26.02	22.50	15.47	71.96	66.56	55.76	39.56
6	5.86	3.94	24.76	21.42	14.74	69.33	64.13	53.73	38.14
7	5.56	3.74	23.82	20.61	14.19	67.39	62.34	52.24	37.09
8	5.33	3.59	23.09	19.98	13.76	65.90	60.97	51.09	36.28
9	5.14	3.47	22.51	19.48	13.42	64.72	$59.88\,$	50.18	35.64
10	4.98	3.36	22.03	19.07	13.14	63.76	58.99	49.44	35.12
11	4.85	3.28	21.63	18.73	12.91	62.97	58.26	48.83	34.69
12	4.74	3.20	21.30	18.44	12.72	62.30	57.64	48.32	34.33
13	4.64	3.14	21.01	18.19	12.55	61.73	57.11	47.87	34.02
14	4.56	3.09	20.76	17.97	12.40	61.23	56.65	47.49	33.76
15	4.48	3.04	20.54	17.78	12.28	60.80	56.25	47.16	33.52
16	4.42	2.99	20.34	17.62	12.16	60.42	55.90	46.87	33.32
17	4.36	2.96	20.17	17.47	12.06	60.08	55.59	46.61	33.14
18	4.30	2.92	20.02	17.34	11.98	59.78	55.31	46.38	32.98
19	4.25	2.89	19.88	17.22	11.90	59.51	55.06	46.17	32.83
20	4.21	2.86	19.75	17.11	11.82	59.27	54.84	45.98	32.70

Finally, the lineshift takes the following form,

$$
\hbar d_{nl \to 1s} = -\frac{2\pi N_e \langle nl|r^2|nl\rangle}{3} [f_{nl}(u_0) - f_{1s}(u_0)]. \tag{22}
$$

In order to compare with quantum mechanical results [8], we rewrite equation (21) as

$$
\hbar d_{nl \to 1s} = -\frac{10^{-22} N_e \, (\text{cm}^{-3})}{Z^2} D(n, l, T) \, (\text{eV}) \tag{23}
$$

and calculate  $D(n, l, T)$  for different n, l, temperature T, and  $Z \geq 5$ . The examination of numerical results reported in Table 1, shows the following:

- (i)  $D(n, l, T)$  decreases smoothly with increasing l and varies approximately as the fourth power of  $n$ .
- (ii)  $D(n, l, T)$  decreases sharply when the temperature increases until the value  $T \approx 5Z^2$  (eV). Beyond this temperature,  $D(n, l, T)$  decreases smoothly and tends towards a finite limit  $D(n, l, \infty)$  for extremely high temperatures.

## 4 Comparisons results and conclusion

The shift of hydrogenic lines induced by electronic collisions in dense plasmas are calculated by using the semiclassical approximation. This approximation has been extended to treat the penetrating collision in atomic orbitals where the hyperbolic path and the multipolar effects are included.

Accordingly, a simple analytical formula has been derived for the electronic line shift. The results obtained for this, as illustrated by Table 1, are compared with those given by the quantum mechanical calculations in the CBO approximation (see Tab. 6 of Ref. [8]).This comparison reveals that, if the penetrating collisions are treated carefully by the semi-classical approximation, the discrepancy between semi-classical and quantum results is very small in a large range of plasmas conditions. In fact it disappears completely at high temperature  $(T (\text{eV}) \gg Z^2)$  where the exchange effect is negligible.

### Appendix

In this appendix, we give the expressions of the "reduction factors" of the interaction.

### Reduction factor of the monopole

$$
V^{(0)}(t) = -e^2 \left[ \frac{1}{R(t)} - \frac{1}{r} \right] E(R(t) < r)
$$

$$
\langle n l m | V^{(0)}(t) | n l' m' \rangle = -\frac{e^2}{R(t)} \delta_{l,l'} \delta_{m,m'} \Delta_0(X)
$$

$$
\Delta_0(X) = \int_X^{\infty} \left( 1 - \frac{X}{y} \right) R_{nl}^2(y) y^2 dy
$$

$$
= e^{-\frac{2X}{n}} F_{nl} \left( \frac{2X}{n} \right);
$$

$$
X = \frac{Z R(t)}{a_0}, y = \frac{Zr}{a_0} \qquad (A.1)
$$



Fig. 1. Dependence of reduction factor on  $R$  of monopole  $(n = 3, \ell = 1)$ , dipole  $(n = 3, \ell = 1, \ell' = 2)$  and quadripole  $(n = 3, \ell = 1, \ell' = 1).$ 

Here  $R_{nl}$  is the radial hydrogenic wave function and  $F_{nl}$  is a polynomial of degree  $2n - 1$ . The examination of the reduced factor  $\Delta_0(X)$ , represented in Figure 1, for different values of n, l, and l' shows that it can be approximated by

$$
\Delta_0(X) \approx
$$
\n
$$
\begin{cases}\n1 - \frac{X}{X_{nl}} = 1 - \frac{R}{r_{nl}} & \text{if } R < r_{nl}, \ X_{nl} = \frac{Zr_{nl}}{a_0} \\
0 & \text{if } R > r_{nl}\n\end{cases}
$$
\n(A.2)

where  $r_{nl}$  is in the order of the atomic rayon. We can choose this quantity by imposing the condition at  $\Delta_0(X)$ , and its approach form to have the same moment of degree k,

$$
\int_0^{x_{nl}} X^k \left( 1 - \frac{X}{X_{nl}} \right) dX = \int_0^{+\infty} X^k \Delta_0(X) dX
$$

$$
\frac{(x_{nl})^{k+1}}{(k+1)(k+2)} = \int_0^{+\infty} X^k dX \qquad (A.3)
$$

$$
\times \int_X^{+\infty} \left( 1 - \frac{X}{y} \right) R_{nl}^2(y) y^2 dy.
$$

After integration of the second member of (A.3), we obtain the following relation:

$$
(r_{nl})^{k+1} = \langle n l m | r^{k+1} | n l m \rangle.
$$
 (A.4)

It was shown (see Eq. (20)) that  $k = 1$ .

#### Reduction factor of the multipole

$$
V^{(p)}(t) = e^{2} \frac{P_{p}(\cos \alpha)}{R^{2}} \left[ \frac{r^{p}}{R^{p-1}} E(R(t) > r) + \frac{R^{p+2}}{r^{p+1}} E(R(t) < r) \right]
$$

for 
$$
p \ge 1
$$
;  $\alpha = (\mathbf{r}, \mathbf{R}(t))$ ;  
\n
$$
\langle nlm|V^{(p)}(R)|nl'm'\rangle = \frac{e^2}{R^{p+1}} \langle nlm|r^p P_p(\cos \alpha)
$$
\n
$$
\times |nl'm'\rangle \Delta_p(X)
$$
\n
$$
\Delta_p(X) = \left[\int_0^X y^{p+2} R_{nl}(y) R_{nl'}(y) dy + X^{2p+1} \right]
$$
\n
$$
\times \int_X^{+\infty} \frac{1}{y^{p-1}} R_{nl}(y) R_{nl'}(y) dy \right] [\langle nl|y^p|nl\rangle]^{-1}
$$
\n
$$
= 1 - \frac{\int_X^{+\infty} \left(1 - \frac{X^{2p+1}}{y^{2p+1}}\right) y^{p+2} R_{nl}(y) R_{nl'}(y) dy}{\langle nl|y^p|nl'\rangle}
$$
\n
$$
= 1 - e^{-\frac{2X}{n}} F_p(n, l, l', X); \quad X = \frac{Z}{a_0} y = \frac{Zr}{a_0}
$$
\n(A.5)

where,  $F_p(n, l', X)$  is a polynomial of degree  $2n$ , which depends on the parameters  $n, l, l',$  and  $p$ . The examination of the reduced factor  $\Delta_p(X)$ , represented in Figure 1, for different values of  $n, l$ , and l' shows that it can be approximated by

$$
\Delta_p(X) \approx \begin{cases}\n0 & \text{for } R < R_p^{(1)} \\
A_p(X - X_p^{(0)}) + B_p & \text{for } R_p^{(1)} < R < R_p^{(2)} \\
1 & \text{for } R > R_p^{(2)}\n\end{cases}
$$
\n
$$
R_p^{(i)} = \frac{a_0 X_p^{(i)}}{Z} \tag{A.6}
$$

Where the quantity  $A_p$ ,  $B_p$ ,  $X_p^{(0)}$ ,  $X_p^{(1)}$ , and  $X_p^{(2)}$  are determined by

$$
\left[\frac{d^2}{dX^2}(\Delta_p(X))\right]_{X=X_p^{(0)}} = 0;
$$
  

$$
A_p = \left[\frac{d}{dX}(\Delta_p(X))\right]_{X=X_p^{(0)}}; \quad B_p = \Delta_p(X_p^{(0)});
$$
  

$$
X_p^{(1)} = X_p^{(0)} - \frac{B_p}{A_p} \quad \text{and} \quad X_p^{(2)} = X_p^{(0)} + \frac{1 - B_p}{A_p}.
$$

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