

# Influence of an intense magnetic field on transition arrays

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The effect of an intense magnetic field on transition arrays is investigated. Explicit formulas for the first moments of the array are given in the weak- and strong-field limits. The result related to the strong-field case is particularly simple: the transition array splits into three components located at the relative positions  $-\mu_B H, 0, \mu_B H$ , each component having the same variance as the array without magnetic field. The changes in the opacity of aluminum and neon at low density are then computed for a range of magnetic fields relevant to Z-pinch experiments [S1050-2947(96)07106-5]

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## I. INTRODUCTION

The magnetic fields obtained in Z-pinch experiments are so strong (of the order of  $10^3$  T) that they may affect radiative transport in the surrounding plasma. A small change in the transition arrays, for instance, could cause the Rosseland mean opacity to vary significantly. However, the effect of a magnetic field on the bound-bound transition spectrum has been investigated only in the case where Coulombic electron-electron interactions are neglected [1]. Since the latter effect can be important, this assumption limits the use of these results.

In this paper we first show that the overall increase of variance due to the magnetic field is equal to the variance obtained when neglecting the Coulombic terms, averaged over the possible polarizations of the absorbed photon. Hence the formulas given in [1] can be directly used to calculate the overall variance in  $jj$  coupling. In the strong-field limit, the transitions must be described in intermediate coupling. The effect of the field is then particularly simple: it splits the transition array into three components located at the relative positions  $-\mu_B H, 0, \mu_B H$ . The variance of each of these components is equal to the variance of the transition array in the absence of magnetic field. Note that the term variance for a transition array is used in its usual statistical sense as the mean square measure of the spread of the intensity-weighted frequencies of the individual spectral lines in the array, calculated relative to the intensity-weighted mean transition frequency of the individual lines in the array.

In the first section we give some orders of magnitude and a qualitative analysis of the effect of a magnetic field on bound-bound transitions. In Sec. II we present calculations of the transition arrays in  $jj$  and intermediate coupling. A numerical application is carried out in the last section. The influence of the field on the Rosseland mean opacity is computed in aluminum and neon at 20 eV for various densities.

## II. ORDERS OF MAGNITUDE AND GENERAL BACKGROUND

The coupling with the magnetic field is given by ([2], Chap. XV, paragraph 113)

$$\mu_B \mathbf{H} \cdot (\hat{\mathbf{L}} + 2\hat{\mathbf{S}}) + \frac{e^2}{8mc^2} \sum_a (\mathbf{H} \times \mathbf{r}_a).$$

The second term (diamagnetic) is usually neglected in the weak-field limit. Following [3], the ratio of the second term over the first is approximately  $\mu_B H \bar{r}^2 m / \hbar^2$ . This ratio is found to be small in most situations when the field is not greater than  $10^3$  T, and when the ionic density is larger than  $10^{-4}$  g/cm<sup>3</sup>. We therefore neglect the diamagnetic term. Finally, the field that makes the magnetic term of the order of  $10^{-2}$  hartree is  $5 \times 10^3$  T. Hence the magnetic term is generally smaller than the electrostatic interactions.

As is well known, only two situations are easily dealt with.

(1) The Zeeman effect is relevant to the weak-field limit. The electronic state is then described using the quantum numbers  $(\dots, J, M_J)$ , and the perturbation due to the field is

$$\Delta E = \mu_B H g_J M_J, \quad (1)$$

where the coefficient  $g_J$  is the Landé factor.

(2) The Paschen-Back effect applies to the strong-field limit. The electronic state must then be described using the quantum numbers  $(\dots, L, S, M_L, M_S)$ . The perturbation due to the field is

$$\Delta E = \mu_B H (M_L + 2M_S) \quad (2)$$

to which the perturbation due to the spin-orbit coupling is added:

$$+ A M_L M_S. \quad (3)$$

In hydrogen, the critical field for which the magnetic interaction is equal to the spin-orbit is 7800 G [3]. Because the spin-orbit coupling is of order  $(Z_{\text{eff}} e^2 / \hbar c)^2 m e^4 / \hbar^2$  [2], we obtain estimates of this critical field for various effective charges (cf. Table I). Except for a few core electrons, the screening effect makes the effective charge significantly smaller than the atomic number. Hence, given the large values of the magnetic field obtained in Z pinch, the Paschen-Back (PB) effect generally applies to outer electrons, whereas core electrons may necessitate a Zeeman (Z) description.

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TABLE I. Order of magnitude of the critical field for which the magnetic interaction is equal to the spin orbit, as a function of the effective charge.

$Z_{\text{eff}}$	Critical field (teslas)
1	0.78
4	13
6	28
13	130
29	650
47	1700
79	4900

Three types of transitions should therefore be considered, according to the effect (PB or Z) that applies to the initial and final states.

(1) Weak-field limit:  $Z \rightarrow Z$ . According to (1) the change in the transition energy due to the magnetic field is

$$\begin{aligned} \Delta E(H) &= \mu_B H (g_{J'} M_{J'} - g_J M_J) \\ &= \mu_B H [(g_{J'} - g_J) M_{J'} + g_J (M_{J'} - M_J)], \end{aligned} \quad (4)$$

where  $|\Delta M_J| \leq 1$  and  $|J-1| \leq J' \leq |J+1|$ . Two modifications of the spectrum are therefore expected. The first is a decomposition of the line into three components, according to the value of  $\Delta M_J$ , which arises from the term  $g_J (M_{J'} - M_J)$ . Each component corresponds to a polarization of the absorbed photon, which is related to  $\Delta M_J = 0, \pm 1$ . The second is an increase of the variance of each component, which originates from the variations of the Landé factor [term  $(g_{J'} - g_J) M_{J'}$ ]. The increase of variance can be calculated exactly following [4,5] (see Sec. III). However, when the magnetic field is large, the calculated variance does not represent a continuous broadening of each component, but a decomposition in subcomponents which corresponds to the new description required for the final state.

(2) Intermediate field:  $Z \rightarrow \text{PB}$ . The initial state, which is correctly described using the quantum numbers  $(\dots, J, M_J)$ , is a linear combination of states such as  $(\dots, L', S', M_{L'}, M_{S'})$ . The transition to a state  $(\dots, L, S, M_L, M_S)$  may then be calculated. Practical use of this description is difficult, since the electrons of the same atom must be calculated differently. Moreover, the resulting analysis would be incomplete because the Zeeman and Paschen-Back effects are simplifications which are not necessarily valid for intermediate fields.

(3) strong-field limit:  $\text{PB} \rightarrow \text{PB}$ . In that case, the initial and final states are described using the quantum numbers  $(\dots, L, S, M_L, M_S)$ . The electronic transitions are subject to the selection rules  $|L-1| \leq L' \leq |L+1|$ ,  $|\Delta M_L| \leq 1$ ,  $\Delta S = 0$ , and  $|\Delta M_S| = 0$ . The change in the transition energy is then

$$\Delta E(H) = \mu_B H \Delta M_L. \quad (5)$$

Provided that the three causes of broadening (electrostatic, spin orbit, magnetic) can be calculated independently (this will be seen in Sec. III), the effect of the field is a decomposition in three subcomponents (according to  $\Delta M_L$ ).

The effect of a magnetic field on an absorption spectrum will be described in the weak- and strong-field limits,  $Z \rightarrow Z$  and  $\text{PB} \rightarrow \text{PB}$ , using transition arrays [4,5]. We first recall how the moments of the transition arrays are calculated in the absence of magnetic field.

Following [4–6], we denote by  $H_0$  the average central potential,  $G$  the electrostatic interaction between electrons, and  $\Lambda$  the spin-orbit coupling. An *orbital* is the group of one-electron states which are degenerate in a one-electron description. For example, if the one-electron basis used is diagonal with respect to  $H_0 + \Lambda$  (case of  $jj$  coupling), then a transition is first described as a transition from an orbital  $(n, l, j)$  to an orbital  $(n', l', j')$  (which defines a single absorption line). The electron-electron interaction, however, is not diagonalized in this description. Its diagonalization transforms the unique line  $(n, l, j) \rightarrow (n', l', j')$  into a distribution of lines called a transition array. Following [7,4], the first two moments of this distribution can be calculated exactly. The transition array may then be represented using a Gaussian profile having these moments in the place of the true distribution (unresolved transition arrays, super transition arrays [8,9]). Because the moments can be expressed as a trace [see [4], Eq. (6), for instance], they can be calculated in the basis we choose. Since  $G$  is a two-electron operator, we may use a two-electron basis, and this is the origin of Moszkowski's approximation [5,10]. Finally, it is sufficient to calculate the moments related to the transition from a configuration with one electron in orbital  $K$  and one in orbital  $I$ , to a configuration with one electron in orbital  $K$  and one in orbital  $F$ . The two-electron basis required for a calculation in  $jj$  coupling is then characterized by the quantum numbers  $|AKJM\rangle$ , where  $A$  represents either  $I$  or  $F$ . The moments are

$$\begin{aligned} \langle E_{FK} - E_{IK} \rangle_{jj} &= \sum_{J, J'} P_{IF}^K(JJ') [E_{FKJ'} - E_{IKJ}], \\ \langle (E_{FK} - E_{IK})^2 \rangle_{jj} &= \sum_{J, J'} P_{IF}^K(JJ') [E_{FKJ'} - E_{IKJ}]^2, \end{aligned} \quad (6)$$

where  $P_{IF}^K(JJ')$  is the probability that a photon induces a transition from a state with momentum  $J$  to a state with momentum  $J'$ , and where

$$E_{AKJ} = \langle AKJM | H_0 + \Lambda + G | AKJM \rangle.$$

The two-electron variance is  $\sigma^2(IK \rightarrow FK) = \langle (E_{FK} - E_{IK})^2 \rangle_{jj} - \langle E_{FK} - E_{IK} \rangle_{jj}^2$ .

When  $\Lambda$  is treated on the same footing as  $G$ , we have a situation of intermediate coupling in which the lines are best described as broadened  $(n, l) \rightarrow (n', l')$  transitions. As is well known [4], the crossed terms  $\Lambda G$  that appear in calculating the variance then have a zero contribution. Hence the variance of the transition array is simply the sum of the variance due to  $G$  and of that due to  $\Lambda$ .

### III. CALCULATION OF THE TRANSITION ARRAYS

Let  $\Gamma = \mu_B H (\hat{L}_z + 2\hat{S}_z)$  be the coupling with the magnetic field, and  $q$  represent the polarization of the incident photon. In the following, we consider a specific polarization, and we

compute the weighted moments (6).

The energies  $E_{AKJ}$  in Eq. (6) are the expectation values of the Hamiltonian  $H_0 + \Lambda + G$  in a two-electron state  $|\dots, J, M_J\rangle$ . In the presence of a magnetic field, these energies are changed into  $E_{AKJM_J} = E_{AKJ} + \mu_B g_J H M_J$ . If we part the transitions according to  $q = M_{J'} - M_J (=0, \pm 1)$  and denote  $\tilde{P}_{IF}^K(JM_J, J'q)$  the probability of a transition from  $(J, M_J)$  to  $(J', M_J + q)$ , then the angular part in  $\tilde{P}_{IF}^K(JM_J, J'q)$  may be factorized as (see [11])

$$\tilde{P}_{IF}^K(JM_J, J'q) = \begin{pmatrix} J & 1 & J' \\ -M_J & -q & M_J + q \end{pmatrix}^2 P_{IF}^K(JJ').$$

Well-known sum rules on the 3- $j$  symbols yield  $\sum_{M_J} \tilde{P}_{IF}^K(JM_J, J'q) = P_{IF}^K(JJ')P(q)$ , where  $P(q) = \frac{1}{3}$  is the probability of a given polarization. In the following, we denote

$$P_{IF}^K(JM_J, J'q) = \frac{\tilde{P}_{IF}^K(JM_J, J'q)}{P(q)}. \quad (7)$$

Supposing  $q$  is given, the first moment of the transition is

$$\begin{aligned} \langle E_{FK} - E_{IK}; q \rangle_{jj} &= \sum_{J, J', M_J} P_{IF}^K(JM_J, J'q) \\ &\times \{E_{FKJ'} - E_{IKJ} + \mu_B H (g_{J'} M_{J'} - g_J M_J)\}. \end{aligned}$$

In this expression, we write the magnetic term using

$$\begin{aligned} g_{J'} M_{J'} - g_J M_J &= (g_{J'} - g_J)(a_{JJ'} M_J + b_{JJ'} M_{J'}) \\ &+ (a_{JJ'} g_{J'} + b_{JJ'} g_J)(M_{J'} - M_J), \end{aligned}$$

where  $a_{JJ'} + b_{JJ'} = 1$ . The first moment is then

$$\begin{aligned} \langle E_{FK} - E_{IK}; q \rangle_{jj} &= \langle E_{FK} - E_{IK} \rangle_{jj,0} + \mu_B H q \sum_{J, J'} P_{IF}^K(JJ') \\ &\times (a_{JJ'} g_{J'} + b_{JJ'} g_J) \\ &+ \mu_B H \sum_{J, J'} \frac{P_{IF}^K(JJ')}{P(q)} (g_{J'} - g_J) \\ &\times \sum_{M, M'} (a_{JJ'} M + b_{JJ'} M') \\ &\times \begin{pmatrix} J & 1 & J' \\ -M & -q & M' \end{pmatrix}^2, \end{aligned}$$

where  $\langle E_{FK} - E_{IK} \rangle_{jj,0}$  is the first moment in the absence of magnetic field, and where the expression (7) of  $P_{IF}^K(JM_J, J'q)$  has been used. If  $q = 0$ , then

$$\sum_{M, M'} M \begin{pmatrix} J & 1 & J' \\ -M & -q & M' \end{pmatrix}^2 = \sum_M M \begin{pmatrix} J & 1 & J' \\ -M & 0 & M \end{pmatrix}^2 = 0.$$

The first moment reduces to

$$\langle E_{FK} - E_{IK}; q = 0 \rangle_{jj} = \langle E_{FK} - E_{IK} \rangle_{jj,0}. \quad (8)$$

If  $q \neq 0$ , then

$$\begin{aligned} \sum_{M, M'} (M' - M) \begin{pmatrix} J & 1 & J' \\ -M & -q & M' \end{pmatrix}^2 \\ = q \sum_{M, M'} \begin{pmatrix} J & 1 & J' \\ -M & -q & M' \end{pmatrix}^2 = q/3. \end{aligned} \quad (9)$$

Choosing

$$a_{JJ'} = \frac{3}{q} \sum_{M, M'} M' \begin{pmatrix} J & 1 & J' \\ -M & -q & M' \end{pmatrix}^2, \quad (10)$$

$$b_{JJ'} = \frac{-3}{q} \sum_{M, M'} M \begin{pmatrix} J & 1 & J' \\ -M & -q & M' \end{pmatrix}^2,$$

then  $a_{JJ'} + b_{JJ'} = 1$ , and the first moment simplifies into

$$\begin{aligned} \langle E_{FK} - E_{IK}; q \rangle_{jj} &= \langle E_{FK} - E_{IK} \rangle_{jj,0} + \mu_B H q \sum_{J, J'} P_{IF}^K(JJ') \\ &\times (a_{JJ'} g_{J'} + b_{JJ'} g_J). \end{aligned} \quad (11)$$

The second moment is

$$\begin{aligned} \langle (E_{FK} - E_{IK})^2; q \rangle_{jj} &= \sum_{J, J', M_J} P_{IF}^K(JM_J, J'q) \{ (E_{FKJ'} - E_{IKJ})^2 \\ &+ 2\mu_B H (E_{FKJ'} - E_{IKJ})(g_{J'} M_{J'} - g_J M_J) \\ &+ [\mu_B H (g_{J'} M_{J'} - g_J M_J)]^2 \}. \end{aligned}$$

Since the energies  $E_{AKJ}$  do not depend on  $M_J$ , the technique detailed above can be used to simplify the crossed terms which are linear with respect to  $M_J$ . We obtain

$$\begin{aligned} \langle (E_{FK} - E_{IK})^2; q \rangle_{jj} &= \langle (E_{FK} - E_{IK})^2 \rangle_{jj,0} \\ &+ 2\mu_B H q \sum_{J, J'} P_{IF}^K(JJ') (E_{FKJ'} - E_{IKJ}) \\ &\times (a_{JJ'} g_{J'} + b_{JJ'} g_J) \\ &+ (\mu_B H)^2 \sum_{J, J'} \frac{P_{IF}^K(JJ')}{P(q)} (g_{J'} - g_J)^2 \\ &\times \sum_{M_J} (a_{JJ'} M_J + b_{JJ'} M_{J'})^2 \\ &\times \begin{pmatrix} J & 1 & J' \\ -M_J & -q & M_{J'} \end{pmatrix}^2 \\ &+ (\mu_B H q)^2 \sum_{J, J'} P_{IF}^K(JJ') \\ &\times (a_{JJ'} g_{J'} + b_{JJ'} g_J)^2. \end{aligned} \quad (12)$$

Taking into account the expression (11) of the first moment, the variance is

$$\begin{aligned}
\sigma^2(IK \rightarrow FK; q)_{jj} = & \langle (E_{FK} - E_{IK})^2 \rangle_{jj,0} - \langle E_{FK} - E_{IK} \rangle_{jj,0}^2 \\
& + 2\mu_B H q \sum_{J,J'} P_{IF}^K(JJ') (a_{JJ'} g_{J'} + b_{JJ'} g_J) (E_{FKJ'} - E_{IKJ} - \langle E_{FK} - E_{IK} \rangle_{jj,0}) \\
& + (\mu_B H)^2 \sum_{J,J'} \frac{P_{IF}^K(JJ')}{P(q)} (g_{J'} - g_J)^2 \sum_{M_J} (a_{JJ'} M_J + b_{JJ'} M_{J'})^2 \begin{pmatrix} J & 1 & J' \\ -M_J & -q & M_{J'} \end{pmatrix}^2 \\
& + (\mu_B H q)^2 \left[ \sum_{J,J'} P_{IF}^K(JJ') (a_{JJ'} g_{J'} + b_{JJ'} g_J)^2 - \left( \sum_{J,J'} P_{IF}^K(JJ') (a_{JJ'} g_{J'} + b_{JJ'} g_J) \right)^2 \right]. \quad (13)
\end{aligned}$$

The above expression comprises the following.

(1) The variance without magnetic field (first line).

(2) A term which is linear in  $H$  (second line). This term originates from the correlations between  $G$  and  $\Gamma$  and does not appear in [1], since electron-electron interaction was neglected in that work.

(3) Terms that are proportional to  $H$  squared. These terms are independent of the electron-electron interaction. They are calculated in [1] using a one-electron framework.

In order to simplify these results, we may use a simpler description of the effect of the field. We may, for instance, calculate the moments irrespective of the polarization of the photon. This strategy is supported by the possibility that the term  $(g_{J'} - g_J)M_{J'}$ , that appears in the transition energy (4),

$$\Delta E(H) = \mu_B H [(g_{J'} - g_J)M_{J'} + g_J(M_{J'} - M_J)],$$

is larger than  $g_J(M_{J'} - M_J)$ , which corresponds to the Zeeman effect. The three components would then be merged in one broad line.

The first moment of the total distribution is equal to zero from Eqs. (8) and (11):

$$\langle E_{FK} - E_{IK} \rangle_{jj} = \sum_q P(q) \langle E_{FK} - E_{IK}; q \rangle_{jj} = 0.$$

The overall variance is

$$\begin{aligned}
\sigma^2(IK \rightarrow FK)_{jj} = & \sum_q P(q) \langle E_{FK} - E_{IK}; q \rangle_{jj}^2 \\
& + \sum_q P(q) \sigma^2(IK \rightarrow FK; q)_{jj}.
\end{aligned}$$

This may be expressed as

$$\sigma^2(IK \rightarrow FK)_{jj} = \sigma_{jj,0}^2 + \sigma_{jj,1}^2 + \overline{\sigma_{jj}^2}, \quad (14)$$

where

$$\sigma_{jj,0}^2 = \langle (E_{FK} - E_{IK})^2 \rangle_{jj,0} - \langle E_{FK} - E_{IK} \rangle_{jj,0}^2$$

is the variance without magnetic field

$$\begin{aligned}
\sigma_{jj,1}^2 = & \sum_q P(q) \langle E_{FK} - E_{IK}; q \rangle_{jj}^2 \\
= & \frac{2}{3} \left( \mu_B H q \sum_{J,J'} P_{IF}^K(JJ') (a_{JJ'} g_{J'} + b_{JJ'} g_J) \right)^2 \quad (15)
\end{aligned}$$

is the variance due to the Zeeman splitting, and where

$$\begin{aligned}
\overline{\sigma_{jj}^2} = & (\mu_B H)^2 \left\{ \sum_{J,J'} P_{IF}^K(JJ') (g_{J'} - g_J)^2 \sum_{q, M_J} P(q) \right. \\
& \times (a_{JJ'} M_J + b_{JJ'} M_{J'})^2 \begin{pmatrix} J & 1 & J' \\ -M_J & -q & M_{J'} \end{pmatrix}^2 \\
& + \frac{2}{3} \left[ \sum_{J,J'} P_{IF}^K(JJ') (a_{JJ'} g_{J'} + b_{JJ'} g_J)^2 \right. \\
& \left. \left. - \left( \sum_{J,J'} P_{IF}^K(JJ') (a_{JJ'} g_{J'} + b_{JJ'} g_J) \right)^2 \right] \right\} \quad (16)
\end{aligned}$$

is the variance of each component (13), averaged over  $q$ . In the above expression, the crossed terms of Eq. (13):

$$\begin{aligned}
& 2\mu_B H q \sum_{J,J'} P_{IF}^K(JJ') (a_{JJ'} g_{J'} + b_{JJ'} g_J) \\
& \times (E_{FKJ'} - E_{IKJ} - \langle E_{FK} - E_{IK} \rangle_{jj,0})
\end{aligned}$$

have disappeared because they are odd with respect to  $q$ . Hence the increase in variance caused by the magnetic field ( $\sigma_{jj,1}^2 + \overline{\sigma_{jj}^2}$ ) is independent of the correlations between  $G$  and  $\Gamma$ . It can then be calculated in a one-delectron basis, and the work of Bauche and Oreg [1] can be directly used to obtain  $\sigma_{jj,1}^2 + \overline{\sigma_{jj}^2}$  when the transitions are described in  $jj$  coupling (weak-field limit).

We have seen that the correlations between  $G$  and  $\Gamma$  do not contribute to the total variance in  $jj$  coupling. It is shown in the Appendix that the contributions of the correlation between  $G$  and  $\Gamma$ , and those between  $\Lambda$  and  $\Gamma$  to the total variance, are also equal to zero in intermediate coupling. The moments are then obtained from the formulas in  $jj$  coupling

TABLE II. Rosseland mean opacity in  $\text{cm}^2/\text{g}$  for aluminum at 20 eV and various densities. Calculation performed using the OPAP code.

$H$ (teslas)	Rosseland mean opacity ( $\text{cm}^2/\text{g}$ )		
	$10^{-4} \text{ g/cm}^3$	$10^{-3} \text{ g/cm}^3$	$10^{-2} \text{ g/cm}^3$
0	203.8	1001	4715
500	233.2	1076	4821
1500	234.4	1102	4844
3000	234.0	1117	4888
5000	233.8	1123	4940

by replacing  $J$  with  $L$ , and  $g_J$  with 1. Applying this rule to Eq. (15) and (16) yields the results in intermediate coupling:

$$\sigma_{\text{int},1}^2 = \frac{2}{3}(\mu_B H)^2, \quad (17)$$

$$\overline{\sigma_{\text{int}}^2} = 0.$$

Moreover, the difference of variance between the left and right polarizations arises from the crossed terms (Coulombic plus spin orbit) multiplied by magnetic, as is seen in Eq. (13) and in the Appendix. The expectation value of the Hamiltonian  $H_0 + G + \Lambda + \Gamma$  in a two-electron state  $|\eta\rangle = |A, K, L, M_L, M_S\rangle$  is

$$E_{AKLM_L M_S} = \langle \eta | H_0 + G + \Lambda | \eta \rangle + \mu_B H (M_L + 2M_S).$$

From this and the selection rules, the first two moments of the transition are

$$\begin{aligned} \langle E_{FK} - E_{IK}; q \rangle_{\text{int}} &= \sum_{L_I, L_F, M_{L_I}, M_{S_I}} P_{IF}^K(L_I M_{L_I} L_F q) \\ &\times \{ \langle \eta_F | H_0 + G + \Lambda | \eta_F \rangle \\ &- \langle \eta_I | H_0 + G + \Lambda | \eta_I \rangle + \mu_B H q \}, \end{aligned}$$

$$\begin{aligned} \langle (E_{FK} - E_{IK})^2; q \rangle_{\text{int}} &= \sum_{L_I, L_F, M_{L_I}, M_{S_I}} P_{IF}^K(L_I M_{L_I} L_F q) \\ &\times \{ \langle \eta_F | H_0 + G + \Lambda | \eta_F \rangle \\ &- \langle \eta_I | H_0 + G + \Lambda | \eta_I \rangle + \mu_B H q \}^2 \end{aligned}$$

from which the crossed (Coulombic plus spin orbit) multiplied by magnetic terms in the variance are reckoned as

$$\begin{aligned} \sum_{L, L', M_L, M_S} 2P_{IF}^K(L M_L L' q) \mu_B H q \{ \langle \eta_F | H_0 + G + \Lambda | \eta_F \rangle \\ - \langle \eta_I | H_0 + G + \Lambda | \eta_I \rangle - \langle E_{FK} - E_{IK} \rangle_{\text{int},0} \} = 0. \end{aligned}$$

Hence the first moment and the variance related to a given polarization are simply

$$\langle E_{FK} - E_{IK}; q \rangle_{\text{int}} = \langle E_{FK} - E_{IK} \rangle_{\text{int},0} + \mu_B H q, \quad (18)$$

$$\sigma^2(IK \rightarrow FK; q)_{\text{int}} = \sigma_{\text{int},0}^2,$$

where  $\langle E_{FK} - E_{IK} \rangle_{\text{int},0}$  and  $\sigma_{\text{int},0}^2$  are the first moment and variance without magnetic field (including spin-orbit) calculated in intermediate coupling. The effect of a magnetic field on a transition array described in intermediate coupling is therefore to split the array into three identical components located at the relative positions  $-\mu_B H, 0, \mu_B H$ . This result was confirmed by a detailed calculation of a ( $s^2 \rightarrow sp$ ) transition [12].

#### IV. NUMERICAL APPLICATION

The above effect is expected to be significant (change the Rosseland mean opacity) in situations where (1) the transition arrays play an important role, and (2)  $\mu_B H$  is not negligible when compared to other causes of broadening. This can be the case when the density and the temperature are relatively low. As examples of application, we calculated the absorption spectra and mean Rosseland opacity for aluminum and neon at a temperature of 20 eV. The effect can be observed when  $\mu_B H$  is larger than the interval of frequency used to calculate the absorption spectrum. In our calculations, this was the case for fields larger than 300 T. According to Table I, the field must then be accounted for in the Paschen-Back limit for both aluminum and neon.

We used the OPAP code, developed in Limeil, to calculate the opacity. The magnetic field was taken into account by modifying the calculations of the transition arrays in intermediate coupling according to (18). The results are reproduced in Tables II and III. Figure 1 shows the influence of a field of 500 T on the absorption spectrum of aluminum at 20 eV and  $10^{-4} \text{ g/cm}^3$ . Because of the continuous broadening of each line (due to Stark effect, natural life time, etc.), the magnetic field results in a broadening of the rays, thus increasing their overlap. Hence the magnetic field contributes to smoothing the absorption spectrum, and this causes the Rosseland mean opacity to increase.

#### V. CONCLUSION

The effect of a magnetic field on transition arrays has been investigated. Simple formulas are proposed to account for the effect of magnetic field on transition arrays in both the weak- and strong-field limits. It is found that the very strong magnetic fields obtained in Z-pinch experiments can change the Rosseland mean opacity of the plasma. This effect may be significant at low temperatures and low densities. Calculations in aluminum and neon at 20 eV and  $10^{-4} \text{ g/cm}^3$  under a field of 500 T have shown a 20% increase in the Rosseland mean opacity.

TABLE III. Rosseland mean opacity in  $\text{cm}^2/\text{g}$  for neon at 20 eV and various densities. Calculation performed using the OPAP code.

$H$ (teslas)	Rosseland mean opacity		
	$10^{-4} \text{ g/cm}^3$	$10^{-3} \text{ g/cm}^3$	$10^{-2} \text{ g/cm}^3$
0	524.3	4112	21 130
500	629.6	4466	21 420
1500	640.6	4527	21 680
3000	660.7	4635	22 020
5000	690.5	4753	22 540

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### APPENDIX: CONTRIBUTIONS OF CROSSED TERMS TO THE VARIANCE

We suppose that the magnetic field is polarized along  $z$ . The coupling with the field is then

$$\Gamma = \mu_B H (\hat{L}_z + 2\hat{S}_z).$$

We consider the contribution of crossed terms to the variance in intermediate coupling.

*Crossed terms between  $G$  and  $\Gamma$ .* The two-electron states are described as  $|a\rangle = |A, K, L, M_L, M_S\rangle$ , where  $A$  is either  $I = (n_I, l_I)$  or  $F = (n_F, l_F)$ , and where  $K$  is the orbital of the spectator electron. We define a two-electron *orbital* as the space  $[AK]$  generated by the states  $|A, K, L, M_L, M_S\rangle$  for various  $L, M_L, M_S$ . The contribution of  $G\Gamma$  to the variance can be expressed as the trace of certain operators (see [4]). We sort these operators according to the polarization of the photon. (1) If the polarization is parallel to  $z$ , they are such as

$$P_{[IK]} z P_{[FK]} z P_{[IK]} G P_{[AK]} \Gamma, \quad (\text{A1})$$

where, for example,

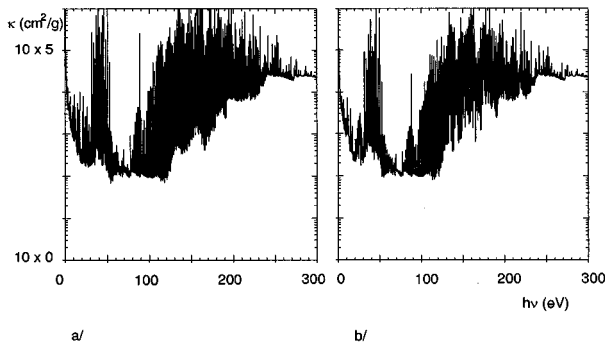


FIG. 1. Spectral cross section  $\kappa$  of aluminum at  $T=20$  eV and density  $10^{-4} \text{ g/cm}^3$ , without magnetic field (a) and under 500 T (b). The Rosseland mean opacities are, respectively, equal to  $\kappa_R = 203.8$  and  $233.2 \text{ cm}^2/\text{g}$ .

$$P_{[IK]} = \sum_{i \in [IK]} |i\rangle\langle i|$$

is the projector on the two-electron orbital  $[IK]$ , and where  $[AK]$  is either  $[IK]$  or  $[FK]$ .

(2) If the polarization is circular right or left, they are such as

$$P_{[IK]}(x \pm iy) P_{[FK]}(x \mp iy) P_{[IK]} G P_{[AK]} \Gamma.$$

In expression (A1),  $P_{[IK]} z P_{[FK]} z P_{[IK]}$  arises from the transition matrix element, whereas  $G P_{[AK]} \Gamma$  is the cross product of the terms of the Hamiltonian. We now consider the operator  $T$ , defined in the space  $[IK] \oplus [FK]$  by

$$T|A, K, L, M_L M_S\rangle = |A, K, L, -M_L - M_S\rangle,$$

where  $A$  is either  $I$  or  $F$ . The following may be seen.

- (1)  $T$  is nilpotent:  $T^2 = T$ .
- (2)  $T$  is self-adjoint:  $T^\dagger = T$ .
- (3)  $T$  commutes with both  $P_{[IK]}$  and  $P_{[FK]}$ .
- (4)  $T|i\rangle\langle i|z|f\rangle\langle f| = \pm|i\rangle\langle i|z|f\rangle\langle f|T$  according to the evenness of  $L_i + L_f$ .
- (5)  $T|i\rangle\langle i|x|f\rangle\langle f| = |i\rangle\langle i|x|f\rangle\langle f|T$  and  $T|i\rangle\langle i|y|f\rangle\langle f| = -|i\rangle\langle i|y|f\rangle\langle f|T$  (or inversely, according to the evenness of  $L_i + L_f$ ).
- (6)  $T$  commutes with  $G$ , because  $G$  depends on distances.
- (7)  $T$  commutes with

$$O_z = P_{[IK]} z P_{[FK]} z P_{[FK]} z P_{[IK]} G P_{[AK]}.$$

(8) Denoting

$$O_\pm = P_{[IK]}(x \pm iy) P_{[FK]}(x \mp iy) P_{[IK]} G P_{[AK]},$$

we have  $TO_\pm = O_\mp T$ .

(9)  $T$  anticommutes with  $\Gamma$ .

From the above properties, we see that

$$\begin{aligned} \text{Tr}(O_+ \Gamma) &= \text{Tr}(O_+ T^2 \Gamma) = -\text{Tr}(O_+ T \Gamma T) = -\text{Tr}(TO_+ T \Gamma) \\ &= -\text{Tr}(O_- \Gamma). \end{aligned} \quad (\text{A2})$$

A similar calculation shows that  $\text{Tr}(O_z \Gamma) = -\text{Tr}(O_z \Gamma)$  and therefore  $\text{Tr}(O_z \Gamma) = 0$ . When we average over polarizations, we find the overall contribution of the crossed terms to the variance:

$$[\text{Tr}(O_- \Gamma) + \text{Tr}(O_z \Gamma) + \text{Tr}(O_+ \Gamma)]/3 = 0.$$

It is equal to zero from Eq. (A2). This result was obtained in Sec. III, together with an explicit expression for  $\text{Tr}(O_+ \Gamma)$  (which reduces to zero in intermediate coupling).

*Crossed terms between  $\Lambda$  and  $\Gamma$ .* With obvious notations, we decompose  $\Gamma$  as  $\Gamma_L + \Gamma_S$ , and examine their contributions separately. Because both  $\Lambda$  and  $\Gamma$  are one-electron operators, the contribution to the variance can be calculated in a one-electron basis  $|a\rangle = |A, M_{l_a}, M_{s_a}\rangle$ . The two bases (obtained using  $a=i$  and  $a=f$ ) generate the one-electron orbitals  $[I]$  and  $[F]$ . Again, we introduce  $P_{[I]}$  and  $P_{[F]}$ , the projectors on the electronic orbitals between which the transition occurs. We now consider the operator  $R$ , defined in the space  $[I] \oplus [F]$  by

$$R|A, M_{l_a}, M_{s_a}\rangle = |A, M_{l_a}, -M_{s_a}\rangle.$$

Then (1)  $R$  is nilpotent:  $R^2 = R$ ; (2)  $R$  is self-adjoint:  $R^+ = R$ ; (3)  $R$  commutes with  $P_{[I]}, P_{[F]}, P_{[I]}, P_{[F]}, (x \pm iy)P_{[F]}$ , and  $\Gamma_L$ ; (4) hence,  $R$  commutes with both  $O_z^{\Gamma_L} = P_{[I]}zP_{[F]}zP_{[I]}\Gamma_L P_{[A]}$  and  $O_{\pm}^{\Gamma_L} = P_{[I]}(x \pm iy)P_{[F]} \times (x \mp iy)P_{[I]}\Gamma_L P_{[A]}$ ; (5)  $R$  anticommutes with  $\Lambda$ ; and we have

$$\begin{aligned} \text{Tr}(O\Lambda) &= \text{Tr}(OR^2\Lambda) = -\text{Tr}(OR\Lambda R) = -\text{Tr}(ROR\Lambda) \\ &= -\text{Tr}(O\Lambda), \end{aligned}$$

where  $O$  can be either  $O_z^{\Gamma_L}$  or  $O_{\pm}^{\Gamma_L}$ . Hence the contributions of  $\Lambda\Gamma_L$  to the variance is equal to zero for each polarization. Regarding  $\Lambda\Gamma_S$ , we consider the operator  $U$  defined in the space  $[I] \oplus [F]$  by

$$U|A, M_{l_a}, M_{s_a}\rangle = |A, -M_{l_a}, -M_{s_a}\rangle$$

and remark that (1)  $U$  commutes with  $\Lambda$ ; (2)  $U$  anticommutes with  $\Gamma_S$ ; (3)  $U$  commutes with  $O_z^{\Lambda} = P_{[I]}zP_{[F]}zP_{[I]}\Lambda P_{[A]}$ ; and, (4) denoting  $O_{\pm}^{\Lambda} = P_{[I]}(x \pm iy)P_{[F]}(x \mp iy)P_{[I]}\Lambda P_{[A]}$ , we have  $UO_{\pm}^{\Lambda} = O_{\mp}^{\Lambda}U$ . The same argument used in (A2) yields

$$\text{Tr}(O_+^{\Lambda}\Gamma_S) = \text{Tr}(O_+^{\Lambda}U^2\Gamma_S) = -\text{Tr}(O_-^{\Lambda}\Gamma_S)$$

and  $\text{Tr}(O_z^{\Lambda}\Gamma_S) = -\text{Tr}(O_z^{\Lambda}\Gamma_S)$  so that  $\text{Tr}(O_z^{\Lambda}\Gamma_S) = 0$ . The overall contribution of the crossed terms to the variance is then

$$[\text{Tr}(O_-^{\Lambda}\Gamma_S) + \text{Tr}(O_z^{\Lambda}\Gamma_S) + \text{Tr}(O_+^{\Lambda}\Gamma_S)]/3 = 0.$$

We conclude that the crossed terms between  $\Lambda$  and  $\Gamma$  do not contribute to the overall variance. Furthermore, the calculation presented in the main text shows that the increase of variance related to a given polarization,  $\text{Tr}(O_+^{\Lambda}\Gamma_S)$ , for example, also reduces to zero in the case of intermediate coupling.

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