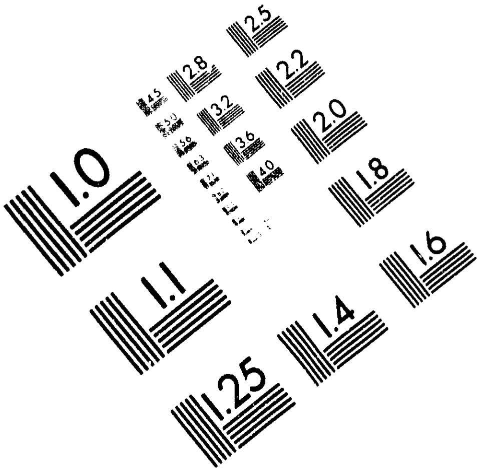
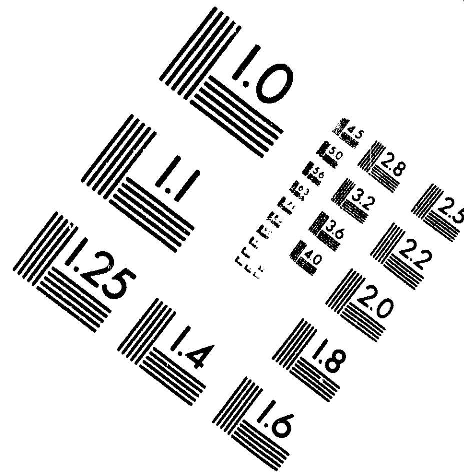
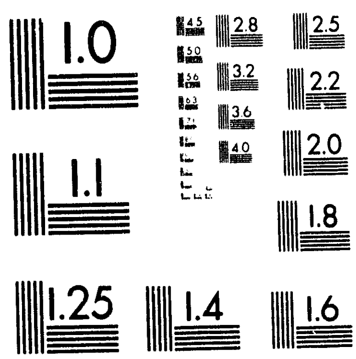
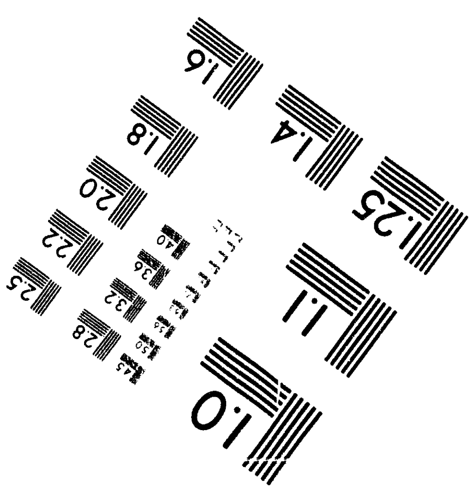


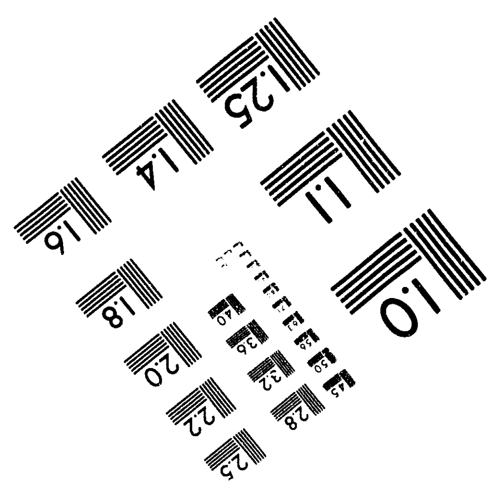


AIIM

Association for Information and Image Management
1100 Wayne Avenue, Suite 1100
Silver Spring, Maryland 20910
301/587-8202







MANUFACTURED TO AIIM STANDARDS
BY APPLIED IMAGE, INC.

2/

Conf-9211211--3

UCRL- JC-113642
PREPRINT

Configuration Interaction in LTE Spectra of Heavy Elements

A. Bar-Shalom and J. Oreg
Nuclear Research Center Negev, Beer Sheva, Israel

W. Goldstein
Lawrence Livermore National Laboratory
Livermore, CA.

This Paper Prepared for Submittal for the 5th International Workshop on Radiative Properties of Dense Matter

Santa Barbara, CA.
November 2-6, 1992

November 1992

Lawrence Livermore National Laboratory

DISCLAIMER

Configuration Interaction in LTE Spectra of Heavy Elements

A. Bar-Shalom and J. Oreg
Nuclear Research Center Negev, P. O. Box , Beer Sheva Israel

and

W. H.Goldstein
L-Division, Lawrence Livermore National Laboratory, Livermore, CA 94550

Abstract

We present a method for including the effects of configuration interaction (CI) between relativistic subconfigurations of an electron configuration in the calculation of emission and absorption spectra of plasmas in local thermodynamic equilibrium (LTE). Analytical expressions for the correction to the intensities, owing to CI, of an unresolved transition array (UTA) and of a supertransition array (STA) are obtained when the correction is small compared to the spin-orbit splitting, bypassing the need to diagonalize energy matrices. These expressions serve as working formulas in the STA model and, in addition, reveal *a priori* the conditions under which CI effects are significant. Examples of the effect are presented.

I. Introduction

The supertransition array (STA) model provides a method for simulating the spectra of of LTE plasmas, under the assumption that j-j coupling is a good approximation. The model was formulated in terms of transitions between j-j coupled electron sub-configurations, and configuration interaction (CI) was neglected. To include CI the energy matrices for levels involved in transitions must be diagonalized. This approach is impractical for the case of LTE spectra of complex atoms because immense numbers of levels contribute. In this work we demonstrate a method to bypass the need for matrix diagonalizations and include the dominant effects of CI within the STA model.[1,2,3] This dominant effect is the interaction between relativistic sub-configurations of the same LS configuration.

The CI effect on radiative transition arrays was first investigated by Bauche *et al.*[4] As indicated in Ref. 4, the effects of CI can be separated into a small, second order, energy shift, and a possibly large change in intesity. In this work we obtain analytic expressions for the latter correction in the unresolved transition array (UTA) and STA models. These expressions serve both to supply working formulas for STA calculations and give practical rules for determining *a priori* when CI is important.

We first show that although the number of "relativistic," or j-j, UTAs (called SOSAs by Bauche *et al.*[5]) contained within a single "non-relativistic," or LS, UTA may be very large, in general each non-relativistic UTA splits into only three sub-arrays, which we call J-Transition Arrays (JTAs). Similarly a "non-relativistic" STA splits to only three "extended" JTAs. The effect of CI is mainly to redistribute intensity among the three JTAs.

Section II containes a short theoretical background. In section III we define the JTAs and present the analytic expressions for their moments (intensities and average energies). The average energy of a "non-relativistic" UTA is then expressed in terms of the moments of the three JTAs. Section IV presents the expression for the CI-induced correction in the average energy of a "non-relativistic" UTA. The effect of CI on the JTA intensities is analyzed in section V, where we present the analytic expressions for the corrected JTA intensities, and demonstrate the effect in specific simple examples. In section VI we extend the treatment to the STA model. Section VII presents calculations of LTE spectra showing the effect of CI under various conditions. All detailed derivations relegated to the appendices.

II. Theoretical Background

The STA model has been presented in several previous works.[1,2,3] The reader is referred to these references for further details. In this section we mention only briefly the most relevant points. A superconfiguration is a collection of configurations constructed by distributing the electrons occupying a super-shell amongst its constituent electron shells or sub-shells in all possible ways. UTAs and STAs are the sets of transitions between two configurations and two superconfigurations, respectively. The STA model is fully relativistic and, as previously mentioned, is based on configurations that are manifolds of pure j-j coupled basis states.

In the development that follows, it will be neccessary to compare transition array moments expressed in terms of j-j coupled states to those expressed in terms of the physical states of an LS coupled configuration. Note that the latter are generally linear combinations of the former. In preparation, we present here several definitions, and a simple rule involving partial averages.

The average energy of a transition array is defined as

$$\overline{E} \equiv \frac{\sum_{i,j} w_{ij} E_{ij}}{\sum_{i,j} w_{ij}} \tag{1}$$

where E_{ij} the energy difference between states i and j and the weight w_{ij} is transition line intensity,

$$w_{ij} = N_i f_{ij} \tag{2}$$

in terms of the initial population N_i and the transition probability f_{ij}. In the UTA model, the population distribution within a configuration is assumed to be statistical and the weights are simply $w_{ij} = g_i f_{ij}$ where g_i is the statistical weight of i.

We denote by $E_c^{j_\alpha j_\beta}$ the average energy of the $j_\alpha \Rightarrow j_\beta$ UTA between two j-j configurations, c and c', where $j_\alpha \equiv (n_\alpha l_\alpha j_\alpha)$, and

$$c = (j_1)^{q_{j_1}}(j_2)^{q_{j_2}}\ldots(j_\alpha)^{q_{j_\alpha}}\ldots(j_\beta)^{q_{j_\beta}}\ldots\ ,\ c' = (j_1)^{q_{j_1}}(j_2)^{q_{j_2}}\ldots(j_\alpha)^{q_{j_\alpha}-1}\ldots(j_\beta)^{q_{j_\beta}+1} \tag{3}$$

Similarly, the average energy of a "non-relativistic" UTA between the two configurations

$$A = (n_1 l_1)^{q_1}(n_2 l_2)^{q_2}\ldots(n_\alpha l_\alpha)^{q_\alpha}\ldots(n_\beta l_\beta)^{q_\beta}\ ,\ A' = (n_1 l_1)^{q_1}(n_2 l_2)^{q_2}\ldots(n_\alpha l_\alpha)^{q_\alpha - 1}\ldots(n_\beta l_\beta)^{q_\beta + 1} \tag{3'}$$

characterized by the single orbital transition $n_\alpha l_\alpha \Rightarrow n_\beta l_\beta$ is

$$E_A^{\alpha\beta} \equiv \frac{\sum_{k\in A\ l\in A'} w_{kl} E_{kl}}{\sum_{k\in A\ l\in A'} w_{kl}} \tag{4}$$

where k and l are physical states contained in A and A' respectively, and include therefore the CI between j-j sub-configurations.

The results of Bauche *et al.* (5,6) for these average energies can be written in a compact form as

$$E_c^{j_\alpha j_\beta} = D_0^{j_\alpha j_\beta} + \sum_{j_a} (q_{j_a} - \delta_{j_a j_\alpha}) \mathcal{D}_{j_a}^{j_\alpha j_\beta} \ldots \tag{5}$$

$$E_A^{\alpha\beta} = D_0^{\alpha\beta} + \sum_a (q_a - \delta_{a\alpha}) \mathcal{D}_a^{\alpha\beta} \tag{6}$$

where the ordinary D's and italic $\mathcal{D}$"s are independent of the occupation numbers and given explicitly in Appendix A in terms of radial integrals. In Eq. (6), and hereafter, a non-relativistic orbital $n_a l_a$ will be denoted simply by a.

The result (6) was given by Bauche *et al.*[6] only in the non-relativistic limit. It is shown in Appendix A, though, that Eq. (6) holds true to a very good approximation also in a fully relativistic treatment where the "non-relativistic" radial integrals in (6) are taken as specific averages of the relativistic ones.

We will use quite frequently the following simple rule. Let G be a group of numbers E_i and g non overlapping subgroups comprising G.. The average of the E_i weighted by w_i in G, defined as

$$E_G = \sum_{i \in G} w_i E_i / w_G \quad , \quad w_G = \sum_{i \in G} w_i \tag{7}$$

can be written in terms of the partial averages

$$E_g = \sum_{i \in g} w_i E_i / w_g \quad , \quad w_g = \sum_{i \in g} w_i \tag{8}$$

as

$$E_G = \sum_{g \in G} w_g E_g / w_G \quad , \quad w_G = \sum_{g \in G} w_g \tag{9}$$

III. J-Transition Arrays

Consider the "non-relativistic" UTA, A ⇒ A' defined by Eq. (3'). Each shell $(nl)^q$ containing q electrons is in fact a union of all subshells (nlj),

$$(nl)^q = \sum_{\{q_- + q_+ = q\}} [(nl_+)^{q_+} + (nl_-)^{q_-}] \tag{10}$$

where $nl_\pm \equiv nlj$, ($j = l \pm 1/2$). Of course, the $l \pm 1/2$ subshells become degenerate in the non-relativistic limit.

Depending on the number of partitions of q, the number of relativistic UTAs $c \Rightarrow c'$ (*Cf.* Eq. (3)) in contained in $A \Rightarrow A'$ may be very large. However, the mean energies of these UTAs naturally cluster into three dinstinct arrays characterized by the three suborbital transitions (the principal number n is omitted hereafter when convenient) $j_\alpha \Rightarrow j_\beta$, with

$$l_{\alpha_-} \Rightarrow l_{\beta_-} \;, l_{\alpha_+} \Rightarrow l_{\beta_+} \quad \text{and} \quad \begin{cases} l_{\alpha_+} \Rightarrow l_{\beta_-} \ \text{for} \ 0 < l_\alpha < l_\beta \\ l_{\alpha_-} \Rightarrow l_{\beta_+} \ \text{for} \ 0 < l_\beta < l_\alpha \end{cases} \tag{11}$$

The fourth possibility

$$\begin{cases} l_{\alpha_+} \Rightarrow l_{\beta_-} & \text{for} \quad 0 < l_\beta < l_\alpha \\ l_{\alpha_-} \Rightarrow l_{\beta_+} & \quad\; 0 < l_\alpha < l_\beta \end{cases} \tag{12}$$

is eliminated by the selection rule

$$|j_\alpha - j_\beta| < 1 \quad , \quad |l_\alpha - l_\beta| = 1 \tag{13}$$

When an active orbitals has $l=0$ these selection rule yields only two arrays. Each array $j_\alpha \Rightarrow j_\beta$ – which will be called a J-Transition Array (JTA) – is actally an STA that includes many relativistic UTAs with nearly the same mean energy.

As an example consider the "non-relativistic" UTA

$$A = \prod_{a \neq 3d,4f} (n_a l_a)^{q_a}\, 3d^3 \;\Rightarrow\; A' = \prod_{a \neq 3d,4f} (n_a l_a)^{q_a}\, 3d^2 4f \tag{14}$$

for the orbital transition $3d \Rightarrow 4f$. This transition array comprises relativistic UTAs $c \Rightarrow c'$, where

$$c \in A : \prod_{a \neq 3d,4f} \sum_{\{q_{a_+} + q_{a_-} = q_a\}} (n_{a_+} l_{a_+})^{q_{a_+}} (n_{a_-} l_{a_-})^{q_{a_-}}$$
$$[(3d_+)^3 + (3d_+)^2(3d_-) + (3d_+)(3d_-)^2 + (3d_-)^3]$$

$$c' \in A' : \prod_{a \neq 3d,4f} \sum_{\{q_{a_+} + q_{a_-} = q_a\}} (n_{a_+} l_{a_+})^{q_{a_+}} (n_{a_-} l_{a_-})^{q_{a_-}}$$

$$[(3d_+)^2 (4f_-) + (3d_-)^2 (4f_-) + (3d_+)\ (3d_-)(4f_-)$$
$$+ (3d_+^2)\ (4f_+) + (3d_-^2)\ (4f_+) + (3d_+)\ (3d_-)(4f_+)]$$

and the 3 JTAs comprise all transitions from c to c' with $3d_- \Rightarrow 4f_-$, $3d_+ \Rightarrow 4f_-$ and $3d_+ \Rightarrow 4f_+$.

In Appendix B it is shown that the normalized JTA intensity is simply

$$\bar{W}^{j_\alpha j_\beta} = \frac{1}{2} g_{j_\alpha} g_{j_\beta} \begin{Bmatrix} j_\alpha & l_\alpha & \frac{1}{2} \\ l_\beta & j_\beta & 1 \end{Bmatrix}^2 \tag{15}$$

and its average energy is

$$E_A^{j_\alpha j_\beta} = D_0^{j_\alpha j_\beta} + \sum_a (q_a - \delta_{a\alpha})\, \bar{D}_a^{j_\alpha j_\beta} \quad , \qquad q_\alpha > 0 \quad , \quad q_\beta < g_\beta \tag{16}$$

where the barred D's are defined in Appendix B. The remarkable feature of Eq. (16) is that, although it holds for transitions between relativistic sub-configurations, it is expressed in terms of the orbital occupation numbers of the "non-relativistic" A $\Rightarrow$ A' UTA.

IV. The CI Shift in the Average Transition Energy of a "Non-Relativistic" UTA

The average transition energy of the A $\Rightarrow$ A' UTA, without CI effects, can be written

$$E_A^{\alpha\beta} = \frac{\sum_{c \in A\ c' \in A'} \sum_{i \in c\ j' \in c'} g_i f_{ij} E_{ij}}{\sum_{c \in A\ c' \in A} \sum_{i \in c\ j' \in c'} g_i f_{ij}} \tag{17}$$

It follows from Eq. (9) that

$$E_A^{\alpha\beta} = \sum_{j_\alpha j_\beta} \bar{W}^{j_\alpha j_\beta} E_A^{j_\alpha j_\beta} \tag{18}$$

The CI-induced shift in the average energy of the A $\Rightarrow$ A' UTA follows from a comparison of Eqs. (4) and (18), or, equivalently, (6) and (16):

$$\delta E_A^{\alpha\beta} \equiv E_A^{\alpha\beta} - E_A^{\alpha\beta} = [D_0^{\alpha\beta} - \sum_{j_\alpha j_\beta} \bar{W}^{j_\alpha j_\beta} D_0^{j_\alpha j_\beta}] + \sum_a (q_a - \delta_{a\alpha}) [D_a^{\alpha\beta} - \sum_{j_\alpha j_\beta} \bar{W}^{j_\alpha j_\beta} \bar{D}_a^{j_\alpha j_\beta}] \tag{19}$$

By substituting explicit forms for the expressions appearing in (19) and rearranging terms, it is possible to show that

$$\delta E_A^{\alpha\beta} = \left\{ \frac{q_\alpha - 1 + \delta_{q_\alpha, 0}}{4l_\alpha + 1} - \frac{q_\beta - \delta_{q_\beta, (4l_\beta + 2)}}{4l_\beta + 1} \right\} \Gamma^{\alpha\beta} \tag{20}$$

where $\Gamma^{\alpha\beta}$ is independent of the occupation numbers.Since Eq. (20) is one of our main results we write here the detailed form of $\Gamma^{\alpha\beta}$ in terms of the relativistic Slater inıegrals:

$$\Gamma^{\alpha\beta} = \Phi^0 \sum_{j_\alpha j_\beta} (-1)^{j_\alpha + j_\beta} F^0(j_\alpha, j_\beta) + \sum_{j_\alpha, j_\beta} g_{j_\alpha} g_{j_\beta} \left\{ \sum_{\substack{k \neq 0 \\ \text{even}}} \Phi^k(j_\alpha, j_\beta)\, F^k(j_\alpha, j_\beta) + \gamma(j_\alpha, j_\beta)\, G^1(j_\alpha, j_\beta) \right\} \tag{21}$$

where $F^k(j_\alpha, j_\beta)$ and $G^k(j_\alpha, j_\beta)$ are the direct and exchange Slater integrals,

$$\Phi^0 \equiv (-1)^{j_\alpha + j_\beta} \left[\frac{g_{j_\alpha} g_{j_\beta}}{g_\alpha g_\beta} - \bar{W}^{j_\alpha j_\beta} \right] = \frac{2[l_\alpha(l_\alpha + 1) + l_\beta(l_\beta + 1) - 2}{g_\alpha g_\beta}$$

$$\Phi^{k}(j_\alpha,j_\beta)=\begin{pmatrix} l_\alpha & k & l_\alpha \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_\beta & k & l_\beta \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times\frac{1}{4}\left[\frac{1}{2}g_{j_\alpha}g_{j_\beta}\begin{Bmatrix} j_\alpha & 1 & j_\beta \\ l_\beta & \frac{1}{2} & l_\alpha \end{Bmatrix}^2 g_\alpha g_\beta\begin{Bmatrix} j_\alpha & k & j_\alpha \\ l_\alpha & \frac{1}{2} & l_\alpha \end{Bmatrix}\begin{Bmatrix} j_\beta & k & j_\beta \\ l_\beta & \frac{1}{2} & l_\beta \end{Bmatrix}\begin{Bmatrix} j_\alpha & k & j_\alpha \\ j_\beta & 1 & j_\beta \end{Bmatrix}+\begin{Bmatrix} l_\alpha & k & l_\alpha \\ l_\beta & 1 & l_\beta \end{Bmatrix}\right],\ (k\neq k')$$

(22)

and

$$\gamma(j_\alpha,j_\beta)=\frac{g_\alpha g_\beta}{12}\begin{pmatrix} l_\alpha & 1 & l_\beta \\ 0 & 0 & 0 \end{pmatrix}^2\begin{Bmatrix} j_\alpha & 1 & j_\beta \\ l_\beta & \frac{1}{2} & l_\alpha \end{Bmatrix}^2\left[1-\frac{1}{2}g_{j_\alpha}g_{j_\beta}\begin{Bmatrix} j_\alpha & 1 & j_\beta \\ l_\beta & \frac{1}{2} & l_\alpha \end{Bmatrix}^2\right] \tag{23}$$

The following features of Eq. (20) should be noted: the selection rule (13) is inherent in the n-j symbols; only the active orbitals appear; the exchange part includes only $G^1(j_\alpha,j_\beta)$; $\Gamma^{\alpha\beta}$ depends on the overlap between the active orbitals mainly through the dominant $G^1(j_\alpha,j_\beta)$ integral; and the sum in Eq. (21) is over the 4 possibilities of $j_a\, j_b$. The four contributions of $F^0(j_\alpha,j_\beta)$ cancel each other owing to the alternating signs; in the linear approximation of Bauche *et al.*(7) the cancellation is exact, while in general the total contribution is negligible.

The analytic expression (20) yields two simple rules for identifying *a priori* the cases where CI is significant. (1) The CI effect increases as the occupation number of the active shell α increases and that of β decreases; the strongest effect occurs when the shell α is full and β is empty; and (2) the effect is increases with increasing overlap between the active orbitals. Thus 1s-2p , 2p-3d, 3d-4f, transitions will have the strongest effect while for the 3d-4p transition the effect is expected to be small. These rules are demonstrated below in examples.

V. The Effect of CI on the JTA Intensities

The normalized JTA intensities in pure j-j coupling, Eq. (15), is summarized for the strongest transitions in Table 1. Evidently only two JTAs have significant stength for each type of transition. For the s -p transition only the ++ and +- combinations exist, while for others the +- transitions are very weak.

Configuration interaction shifts level energies and redistributes oscillator strength. If the interaction is very strong compared to the spin-orbit interaction, the three JTAs will completely intermix, forming a single structure. In this case the intensity redistribution will have no effect on the transition array. We are therefore primarily interested in cases where the CI is strong enough to cause an apparent effect, but not strong enough to actually merge the distinct JTA structures. In these cases individual transition lines are shifted to $E_{ij} \Rightarrow E_{ij} = E_{ij} + \Delta E_{ij}$, and their intensities are changed by $N_i f_{ij} \Rightarrow S_{ij}$, but the JTA structure still exists and each individual line can still be attributed to one of the three JTAs.

	++	--	+-
s-p	2/3	0	1/3
p-d	9/15	5/15	1/15
d-f	20/35	14/35	1/35
f-g	35/63	27/63	1/63

Table 1: Pure j-j JTA intensities

Using again Eq. (9) we can write the "non-relativistic" UTA average energy (*cf.* Eq.(20)) in terms of the CI-corrected JTA energies and intensities as

$$E_A^{\alpha\beta} = \frac{\sum_{i \in A\, j \in A'} S_{ij} E_{ij}}{\sum_{i \in A\, j \in A'} S_{ij}} = \frac{\sum_{j_\alpha j_\beta} S_A^{j_\alpha j_\beta} E_A^{j_\alpha j_\beta}}{\sum_{j_\alpha j_\beta} S_A^{j_\alpha j_\beta}} \tag{24}$$

where the CI-corrected JTA intensities are

$$S_A^{j_\alpha j_\beta} = \sum_{\substack{i \in A\, j \in A' \\ j_\alpha \Rightarrow j_\beta}} S_{ij} \tag{25}$$

and the their shifted average energies are

$$E_A^{j_\alpha j_\beta} = \sum_{\substack{i \in A\, j \in A' \\ j_\alpha \Rightarrow j_\beta}} S_{ij} E_{ij} / S_A^{j_\alpha j_\beta} \quad . \tag{26}$$

The sums in (25) and (26) are over all transitions contained in the $j_\alpha \Rightarrow j_\beta$ JTA.

We will consider the corrected JTA intensities $S_A^{j_\alpha j_\beta}$ as unknowns to be solved for under the following assumptions. Since each JTA is distinct from others, and unresolved within itself, and since the CI effect on level energies is small (second order), we can approximate

$$E_A^{j_\alpha j_\beta} \approx E_A^{j_\alpha j_\beta} \tag{27}$$

yielding

$$E_A^{\alpha\beta} \approx \sum_{j_\alpha j_\beta} \overline{S}_A^{j_\alpha j_\beta} E_A^{j_\alpha j_\beta} \tag{28}$$

where the normalized intensities are

$$\overline{S}_A^{j_\alpha j_\beta} = S_A^{j_\alpha j_\beta} \Big/ \sum_{j_\alpha j_\beta} S_A^{j_\alpha j_\beta} \quad . \tag{29}$$

From (28) and (18) we can now write the following equation for the intensities

$$\delta E_A^{\alpha\beta} = \sum_{j_\alpha j_\beta} (\overline{S}_A^{j_\alpha j_\beta} - \overline{W}^{j_\alpha j_\beta}) E_A^{j_\alpha j_\beta} \tag{30}$$

Further, as shown in Table 1, the intensity of the + - transition is very small. We shall see below that the CI effect tends to eliminate it almost completely. We therefore ignore it and assume

$$\overline{S}_A^{\alpha_+\beta_+} + \overline{S}_A^{\alpha_-\beta_-} = 1 \quad .$$

Explicitly we have

$$\overline{S}_A^{\alpha_+\beta_+} E_A^{\alpha_+\beta_+} + (1 - \overline{S}_A^{\alpha_+\beta_+}) E_A^{\alpha_-\beta_-} = E_A^{\alpha\beta} + \delta E_A^{\alpha\beta} \quad . \tag{32}$$

leading to the following analytic expressions for the CI-corrected intensities:

$$\bar{S}_A^{\alpha_-\beta_-} = \varphi_A^{\alpha_-\beta_-} + \frac{\delta E_A^{\alpha\beta}}{E_A^{\alpha_-\beta_-} - E_A^{\alpha_+\beta_+}}, \quad \varphi_A^{\alpha_-\beta_-} = \frac{E_A^{\alpha\beta} - E_A^{\alpha_+\beta_+}}{E_A^{\alpha_-\beta_-} - E_A^{\alpha_+\beta_+}} \approx \bar{W}^{\alpha_-\beta_-} \tag{33}$$

$$\bar{S}_A^{\alpha_+\beta_+} = \varphi_A^{\alpha_+\beta_+} - \frac{\delta E_A^{\alpha\beta}}{E_A^{\alpha_-\beta_-} - E_A^{\alpha_+\beta_+}}, \quad \varphi_A^{\alpha_+\beta_+} = \frac{E_A^{\alpha_-\beta_-} - E_A^{\alpha\beta}}{E_A^{\alpha_-\beta_-} - E_A^{\alpha_+\beta_+}} \approx \bar{W}^{\alpha_+\beta_+} \ . \tag{34}$$

It should be pointed out here that we have obtained the CI-corrected JTA intensities without diagonalizating the energy.

Before considering the effect o STA intensities of CI, we present simple examples in closed shell systems where direct diagonalization is compared with the pure j-j intensities of Table 1. (The use of closed shell examples simplifies the line spectrum sufficiently to clearly demonstrate the CI effect; he scaling of the effect with the occupation numbers of the active shells is given exactly by Eq. (20).) The upper drawing of Fig.1 represents the spectrum of the 3d-4f transition in nickelike Tm. In this case the active electron is promoted from a closed shell to an empty one. In addition, the 3d and 4f orbitals strongly overlap. As expected from the rules obtained above, this case exhibits a strong CI effect. The heavy and thin traces in the figure describe the transitions with and without CI, respectively. Note that the CI shifts are indeed small, but the JTA intensities invert. Another interesting point is that the weak +- transition disappears almost completely. This effect is observed in all other examples, as well, and was used to simplify the equations for the corrected intensities, (33) and (34). The second and third drawings in Fig 1. present the results for the 2p-3d transition in neonlike and argonlike Fe, respectively. All the arguments used in the previous case hold true also here, and we obtain again a strong effect. The lower drawing of Fig. 1 is the 3d-4p transition in nicklelike Tm. Since, in this case, the active orbitals do not significantly overlap, the effect is small and the JTA intensities are similar to their pure j-j values.

VI. The effect of CI on the STA spectra

The STA model is fully relativistic, and describes transitions in terms of j-j configurations. The three STAs corresponding to the three sub-orbital transitions $j_\alpha \Rightarrow j_\beta{}'$, $\alpha \Rightarrow \beta$, of Eq.(11), we define as "extended" JTAs. Taken together, these three STAs form an extended, "non-relativistic" STA, corresponding to the orbital-to-orbital transition $\alpha \Rightarrow \beta$.

Despite the vast number of overlapping UTAs in such an extended STA, in many cases the JTA structure remains apparent, and the effect of CI again redistributes the intensities among these extended JTAs. We will develop analytic expressions for the corrected STA intensities similar to (33) and (34) following the same steps.

Using the mean average rule, (9), we write the average transition energy of an extended STA without CI in terms of those of the three STAs it includes:

$$E_{STA}^{\alpha\beta} = \sum_{j_\alpha j_\beta} \overline{W}_{STA}^{j_\alpha j_\beta} E_{STA}^{j_\alpha j_\beta} \tag{35}$$

where $\overline{W}_{STA}^{j_\alpha j_\beta}$ is the normalized intensity of the $j_\alpha \Rightarrow j_\beta$ STA, and is given in terms of the average transition probability $f_A^{j_\alpha j_\beta}$ of the JTA, obtained analytically in Appendix B,

$$W_{STA}^{j_\alpha j_\beta} \equiv \sum_{A\in SC} N_A f_A^{j_\alpha j_\beta}, \qquad \overline{W}_{STA}^{j_\alpha j_\beta} \equiv W_{STA}^{j_\alpha j_\beta} \Big/ \sum_{j_\alpha j_\beta} W_{STA}^{j_\alpha j_\beta}, \tag{36}$$

The average energy of the JTA is

$$E_{STA}^{j_\alpha j_\beta} = \frac{\sum_{A\in SC} N_A f_A^{j_\alpha j_\beta} E_A^{j_\alpha j_\beta}}{\sum_{A\in SC} N_A f_A^{j_\alpha j_\beta}} \tag{37}$$

The populations N_A of the configurations A are not removed by the normalization as in the UTA case since the energy difference between configurations within a super configuration may be large compared with the corresponding Boltzmann factors.[1]

Equations (35) and (36) assume statistical populations within the "non-relativistic" configurations A. Making this assumption only within relativistic configurations, as is done in the STA model, we have instead of (36) and (37)

$$W_{STA}^{j_\alpha j_\beta} \equiv \sum_{A\in SC} \sum_{c\in A} N_c f_c^{j_\alpha j_\beta} \tag{38}$$

$$E_{STA}^{j_\alpha j_\beta} = \frac{\sum_{A\in SC} \sum_{c\in A} N_c f_c^{j_\alpha j_\beta} E_c^{j_\alpha j_\beta}}{\sum_{A\in SC} \sum_{c\in A} N_c f_c^{j_\alpha j_\beta}} \tag{39}$$

Since the extended JTAs are simply relativistic STAs, explicit formulas for their intensities and average energy, (38) and (39), have alreadyt been presented.[1-3]

As for UTAs we can write the average energy of the extended STA, *including CI*, in terms of the CI-corrected intensities and energies. Using the extended JTA moments,

$$S_{STA}^{j_\alpha j_\beta} = \sum_{\substack{i,j\in STA \\ (j_\alpha \Rightarrow j_\beta)}} S_{ij} \tag{40}$$

for the corrected intensity, and

$$E_{STA}^{j_\alpha j_\beta} = \sum_{\substack{i,j\in STA \\ (j_\alpha \Rightarrow j_\beta)}} S_{ij} E_{ij} / S_{STA}^{j_\alpha j_\beta} \tag{41}$$

for the average energy, the mean average rule yields

$$\begin{cases} E_{STA}^{\alpha\beta} = \dfrac{\sum_{A\in SC} \sum_{i\in A\, j\in A'} S_{ij} E_{ij}}{\sum_{A\in SC} \sum_{i\in A\, j\in A'} S_{ij}} = \sum_{j_\alpha j_\beta} \overline{S}_{STA}^{j_\alpha j_\beta} E_{STA}^{j_\alpha j_\beta} \\ \overline{S}_{STA}^{j_\alpha j_\beta} = \sum_{j_\alpha j_\beta} S_{STA}^{j_\alpha j_\beta} \end{cases} \tag{42}$$

Assuming again that the average JTA energy is little affected by CI we can write

$$E_{STA}^{j_\alpha j_\beta} \approx E_{STA}^{j_\alpha j_\beta} \tag{43}$$

and the CI shift in the average energy of the extended STA will be

$$\delta E^{\alpha\beta}_{STA} = \sum_{j_\alpha j_\beta} (\overline{S}^{j_\alpha j_\beta}_{STA} - \overline{W}^{j_\alpha j_\beta}_{STA}) E^{j_\alpha j_\beta}_{STA} \tag{44}$$

Now, using the (very good) statistical approximation for all levels $i \in C \in A$,

$$\frac{N_A}{g_A} = \frac{N_c}{g_c} = \frac{N_i}{g_i} = N_0 , \tag{45}$$

where the N's and g's are the corresponding populations and statistical weights, respectively, the shift, Eq. (44), is simply the sum of the shifts, (20), of the included UTAs. Therefore, from (20), we obtain the expression

$$\delta E^{\alpha\beta}_{STA} \equiv \frac{\sum_{A \in SC} N_A f_A \delta E^{\alpha\beta}_A}{\sum_{A \in SC} N_A f_A}$$

$$= \left\{ \frac{< q_\alpha - 1 + \delta_{q_\alpha, 0} >_{STA}}{4l_\alpha + 1} - \frac{< q_\beta - \delta_{q_\beta, (4l_\beta + 2)} >_{STA}}{4l_\beta + 1} \right\} \Gamma^{\alpha\beta} \tag{46}$$

where

$$f_A \equiv \sum_{j_\alpha j_\beta} f_A^{j_\alpha j_\beta} \tag{47}$$

with the occupation number averages given by

$$< q_a >_{STA} \equiv \frac{\sum_{A \in STA} N_A f_A q_a}{\sum_{A \in STA} N_A f_A} \tag{48}$$

These occupation number averages, in both "non-relativistic" and relativistic representations, are easily obtained within the STA model as, respectively,

$$< q^\alpha_a >_{STA} = \frac{g^\alpha_a X_a U_{Q-2}(g^{\alpha\beta a})}{U_{Q-1}(g^{\alpha\beta})} , \qquad X_s = e^{-\frac{\varepsilon_s - \mu}{kT}}$$

and

$$< q_a^\alpha >_{STA} = \frac{\sum_{j_\alpha j_\beta} \begin{Bmatrix} j_\alpha & 1 & j_\beta \\ l_\beta & 1/2 & l_\alpha \end{Bmatrix}^2 g_{j_\alpha} g_{j_\beta} \sum_{j_a \in a} g_{j_a}^{j_\alpha} X_{j_a} U_{Q-2}(g^{j_\alpha j_\beta j_a})}{\sum_{j_\alpha j_\beta} \begin{Bmatrix} j_\alpha & 1 & j_\beta \\ l_\beta & 1/2 & l_\alpha \end{Bmatrix}^2 g_{j_\alpha} g_{j_\beta} X_{j_\alpha} U_{Q-1}(g^{j_\alpha j_\beta})}, \quad X_{j_s} = e^{-\frac{\varepsilon_{j_s} - \mu}{kT}}$$

where the quantities UQ-1, UQ-2 are reduced partition functions as defined in Ref. 1.

Knowing the CI shift (41) we can now use (40) to solve for the corrected JTA intensities. Following the same steps that led to Eqs. (33) and (34) in the UTA case, we obtain for the corrected STA intensities

$$\bar{S}_{STA}^{\alpha_-\beta_-} = \varphi_{STA}^{\alpha_-\beta_-} + \frac{\delta E_{STA}^{\alpha\beta}}{E_{STA}^{\alpha_-\beta_-} - E_{STA}^{\alpha_+\beta_+}}, \quad \varphi_{STA}^{\alpha_-\beta_-} = \frac{E_{STA}^{\alpha\beta} - E_{STA}^{\alpha_+\beta_+}}{E_{STA}^{\alpha_-\beta_-} - E_{STA}^{\alpha_+\beta_+}} \approx \bar{W}_{STA}^{\alpha_-\beta_-} \tag{49}$$

$$\bar{S}_{STA}^{\alpha_+\beta_+} = \varphi_{STA}^{\alpha_+\beta_+} - \frac{\delta E_{STA}^{\alpha\beta}}{E_{STA}^{\alpha_-\beta_-} - E_{STA}^{\alpha_+\beta_+}}, \quad \varphi_{STA}^{\alpha_+\beta_+} = \frac{E_{STA}^{\alpha_-\beta_-} - E_{STA}^{\alpha\beta}}{E_{STA}^{\alpha_-\beta_-} - E_{STA}^{\alpha_+\beta_+}} \approx \bar{W}_{STA}^{\alpha_+\beta_+} \tag{50}$$

where δE is given by (42) and the E's are STA average energies as given by the STA theory.[1-3]

VII. Examples of STA spectra demonstrating the CI effect

We conclude with several examples demonstrating the effect of CI on STA spectra for four cases. In Fig.2 we present the 3d-4f transition of Er in LTE at temperature T= 60 eV and density ρ=0.04 gm/cc. Under these conditions the average 3d occupation number is close to 10 while the 4f shell is on the average half empty, leading to a strong CI effect. The intensities of the ++ and -- STAs are indeed exchanged. In Fig.3 we present a Gd spectrum at 60 eV and 0.04 gm/cc. Here, the overlap of the JTAs is much larger since Z is smaller. Still we note a change in the spectrum owing to CI. Finally, for Xe at 60 eV and 0.04 gm/cc we see in Fig.4 that the JTAs are almost completely overlapping and CI merely shifts the entire array with no effect on the internal structure.

*Work performed under the auspcies of the U.S.Dept. of Energy by the Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

VIII. References

1. A. Bar-Shalom, J. Oreg, W. H. Goldstein, D. Shvarts and A. Zigler, Phys. Rev. A40, 3183(1989).
2. "Calculation of Emission and Absorption Spectra of LTE Plasma by the STA method",A. Bar-Shalom, J. Oreg and W. H. Goldstein, in 'Radiative Properties of Hot Dense Matter' ed., W. H. Goldstein, C. Hooper, J. Gautier, J. Seely and R. Lee, World Scientific (1990)
3. "Recent Development in the Super Transition Array Model for Spectral Simulation of LTE Plasmas", A. Bar Shalom, J. Oreg and W. H. Goldstein, in "Atomic Processes in Plasmas",ed. E. S. Marmar and J. L. Terry, AIP (1991)
4. C. Bauche-Arnolt, J. Bauche and M. Klapisch, J. Phys. B24, 1 (1991)
5. C. Bauche-Arnolt, J. Bauche and M. Klapisch, Phys. Rev. A25, 2641 (1982)
6. C. Bauche-Arnolt, J. Bauche and M. Klapisch, Phys. Rev. A20, 2424 (1979)
7. J. Bauche, C. Bauche-Arnolt, E.Luc-Koenig and M. Klapisch, J. Phys. B15, 2325 (1982)
8. I.I.Sobel'man, "Introduction to the Theory of Atomic Spectra" Pergamon Press. Oxford (1972)

Captions

Fig. 1 The CI effect in closed shell systems: comparison of direct diagonalization and with pure j-j results

Fig. 2 The 3d-4f transition of Er LTE spectra

Fig. 3 The Gd spectrum

Fig. 4 The Xe spectrum

Appendix A. Average UTA energies

The results of Bauche *et al.*[5] for the average energies of the UTA between the relativistic configurations C and C' of Eq. (3) connected by the orbital transition $j_\alpha \Rightarrow j_\beta$ can be written in a compact form as follows:

$$E_C^{j_\alpha j_\beta} \equiv \sum_{i \in C\, j \in C'} w_{ij} E_{ij} \Big/ \sum_{i \in C\, j \in C'} w_{ij} = D_0^{j_\alpha j_\beta} + \sum_{j_a} \left(q_{j_a} - \delta_{j_a j_\alpha}\right) \mathcal{D}_{j_a}^{j_\alpha j_\beta} \qquad \text{A.1}$$

where

$$D_0^{j_\alpha j_\beta} = \langle j_\beta \rangle - \langle j_\alpha \rangle \qquad \text{A.2}$$

$$\langle j_a \rangle \equiv \langle j_a | h_D | j_a \rangle \qquad \text{A.3}$$

with the Dirac single particle Hamiltonian h_D,

$$\mathcal{D}_{j_a}^{j_\alpha j_\beta} \equiv D_{j_a}^{j_\alpha j_\beta} + A^{j_\alpha j_\beta} \left\{ \frac{\delta_{j_a j_\alpha}}{2j_\alpha} - \frac{\delta_{j_a j_\beta}}{2j_\beta} \right\} \qquad \text{A.4}$$

$$D_{j_a}^{j_\alpha j_\beta} \equiv \langle j_a, j_\beta \rangle - \langle j_a, j_\alpha \rangle \qquad \text{A.5}$$

$$\langle j_r, j_s \rangle = F^0(j_r, j_s) - \frac{g_{j_s}}{\left(g_{j_s} - \delta_{j_r j_s}\right)} \sum_k \begin{pmatrix} j_r & k & j_s \\ 1/2 & 0 & -1/2 \end{pmatrix}^2 G^k(j_r, j_s) \qquad \text{A.6}$$

$$A^{j_\alpha j_\beta} \equiv F^{j_\alpha j_\beta} + \sum_k \frac{g_{j_\alpha} g_{j_\beta} \delta_{k,1} - 3}{3} \begin{pmatrix} j_\alpha & k & j_\beta \\ 1/2 & 0 & -1/2 \end{pmatrix}^2 G^k(j_\alpha, j_\beta) \qquad \text{A.7}$$

$$F^{j_\alpha j_\beta} \equiv - \sum_{\substack{k \neq 0 \\ \text{even}}} g_{j_\alpha} g_{j_\beta} \begin{Bmatrix} k & j_\alpha & j_\alpha \\ 1 & j_\beta & j_\beta \end{Bmatrix} \begin{pmatrix} j_\alpha & k & j_\alpha \\ 1/2 & 0 & -1/2 \end{pmatrix} \begin{pmatrix} j_\beta & k & j_\beta \\ 1/2 & 0 & -1/2 \end{pmatrix} F^k(j_\alpha, j_\beta) \qquad \text{A.8}$$

where F^k and G^k are the Slater integrals and $g_{j_s} \equiv 2j_s + 1$.

We turn now to Eq. (6) and show that this equation holds true also in the fully relativistic treatment using averaged radial integrals. The results of ref. (6) for the non relativistic average energy of the UTA between the two configurations A and A' of Eq. (3') connected by the orbital transition $n_\alpha l_\beta \Rightarrow n_\beta l_\beta$ $(\alpha \Rightarrow \beta)$ can be written in a compact form as:

$$E_A^{\alpha\beta} = D_0^{\alpha\beta} + \sum_a (q_a - \delta_{a\alpha})\, \mathcal{D}_a^{\alpha\beta} \qquad \text{A.9}$$

where

$$D_0^{\alpha\beta} \equiv \langle\beta\rangle - \langle\alpha\rangle \qquad \text{A.10}$$

$$\langle a\rangle \equiv \langle a|h\ |a\rangle \qquad \text{A.11}$$

with the Schrodinger single particle Hamiltonian h

$$\mathcal{D}_a^{\alpha\beta} \equiv D_a^{\alpha\beta} + A^{\alpha\beta}\{\frac{\delta_{a\alpha}}{4l_\alpha+1} - \frac{\delta_{a\beta}}{4l_\beta+1}\} \qquad \text{A.12}$$

$$D_a^{\alpha\beta} \equiv \langle a,\beta\rangle - \langle a,\alpha\rangle \qquad \text{A.13}$$

$$\langle a,b\rangle \equiv F^0(l_a, l_b) - \frac{1}{2}\frac{g_a}{g_a - \delta_{ab}}\sum_k \begin{pmatrix} l & k & l_b \\ 0 & 0 & 0 \end{pmatrix}^2 G^k(l_a, l_b) \qquad \text{A.14}$$

$$A^{\alpha\beta} \equiv F^{\alpha\beta} + \frac{g_\alpha g_\beta}{4}\sum_k \begin{pmatrix} l & k & l_\beta \\ 0 & 0 & 0 \end{pmatrix}^2 \{\frac{2}{3}\delta_{k,1} - \frac{2}{g_\alpha g_\beta}\} G^k(l_\alpha, l_\beta) \qquad \text{A.15}$$

$$F^{\alpha\beta} \equiv \frac{g_\alpha g_\beta}{4}\sum_{\substack{k\neq 0\\ \text{even}}} \begin{pmatrix} l_\alpha & k & l_\alpha \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_\beta & k & l_\beta \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} l_\alpha & k & l_\alpha \\ l_\beta & 1 & l_\beta \end{Bmatrix} F^k(l_\alpha, l_\beta) \qquad \text{A.16}$$

where F^k and G^k are here the non-relativistic Slater integrals.

In a fully relativistic treatment, the non-relativistic expression A.9 can be related to the relativistic analog A.1, by comparing the corresponding configuration average energies, which, unlike transition energies, are independent of CI. In this way, we obtain

$$\langle a \rangle \equiv \frac{\sum_{j_a} g_{j_a} \langle j_a \rangle}{g_a} \qquad \text{A.17}$$

which relates $D_0^{j_\alpha j_\beta}$ to $D_0^{\alpha\beta}$, and, for the two-body contributions,

$$\langle a, b \rangle \equiv \frac{\sum_{j_a} g_{j_a} \left(g_{j_b} - \delta_{j_a j_b} \right) \langle j_a , j_b \rangle}{g_a \left(g_b - \delta_{ab} \right)} \qquad \text{A.18}$$

Using A.6 and A.14, this leads to

$$G^k(l_a, l_b) = \sum_{j_a \in a \; j_b \in b} \frac{1}{2} g_{j_a} g_{j_b} \begin{Bmatrix} j_a & j_b & k \\ l_b & l_a & \frac{1}{2} \end{Bmatrix}^2 G^k(j_a, j_b) \qquad \text{A.19}$$

Radial integrals of the type F^k ($k \neq 0$) do not appear in the expressions for the configuration average energies. However, since they depend only weakly on j we can safely use the linear approximation of Bauche *et al.*[7] to obtain

$$F^k(l_a, l_b) = \frac{\sum_{j_a \in a \; j_b \in b} g_{j_a} g_{j_b} F^k(j_a, j_b)}{\sum_{j_a \in a \; j_b \in b} g_{j_a} g_{j_b}} \qquad \text{A.20}$$

These averages, unlike transition average energies, are independent of CI. Since the single electron parts D_0 in Eq. (A.9) is a difference of configuration average energies, it represents the exact relativistic single particle contibution when expressed in terms of the relativistic quantities as in A.17. For the two-body parts of (A.9) we take again the averages (A.18) or, equivalently, (A.19) and (A.20), since usually the relativistic slater integrals depend only weakly on j (though they can differ greatly from their non-relativistic analogs) and in that case the result is exact.

Appendix B. The intensity and average energy of a JTA

The total intensity of the relativistic UTA between the configurations C and C' of Eq. (3), connected by the orbital transition $j_\alpha \Rightarrow j_\beta$ is given by

$$W_c^{j_\alpha j_\beta} \equiv \sum_{i\in c\, j\in c'} N_i f_{ij} = N_c f_c^{j_\alpha j_\beta} \qquad \text{B.1}$$

where N_i is the population of level i (assumed statistical, $N_i = N_0 g_i$, within a configuration),

$$N_c = \sum_{i\in c} N_i \qquad \text{B.2}$$

is the population of the configuration C, and the average transition probability is

$$f_c^{j_\alpha j_\beta} \equiv \frac{1}{g_c} \sum_{i\in c\, j\in c'} g_i f_{ij} \qquad \text{B.3}$$

with the statistical weight

$$g_c \equiv \sum_{i\in c} g_i = \prod_a \begin{pmatrix} g_{j_a} \\ q_{j_a} \end{pmatrix} \qquad \text{B.4}$$

The analytical result for the average transition probability is [8]

$$f_c^{j_\alpha j_\beta} = \varphi^{j_\alpha j_\beta} Q_c^{j_\alpha j_\beta} \qquad \text{B.5}$$

where

$$\varphi^{j_\alpha j_\beta} = \kappa_{\alpha\beta} g_\alpha g_\beta \begin{Bmatrix} j_\alpha & 1 & j_\beta \\ l_\beta & 1/2 & l_\alpha \end{Bmatrix}^2 \qquad \text{B.6}$$

with

$$\kappa_{\alpha\beta} = \kappa' E^{\alpha\beta} (M'^{(1)}_{\alpha\beta})^2 \begin{pmatrix} l_\alpha & 1 & l_\beta \\ 0 & 0 & 0 \end{pmatrix}^2 ,$$

where k' is a constant defined by the chosen units, $E^{j_\alpha j_\beta} \approx E^{\alpha\beta}$ is an average transition energy, $M'^{(1)}_{j_\alpha j_\beta} \approx M'^{(1)}_{\alpha\beta}$ is an average radial transition integral, and $Q_c^{j_\alpha j_\beta}$ is given in terms of the occupation numbers of the active orbitals in C:

$$Q_c^{j_\alpha j_\beta} \equiv q_{j_\alpha}(g_{j_\beta} - q_{j_\beta}) \qquad \text{B.7}$$

Assuming statistical level populations within the configuration A,

$$\frac{N_A}{g_A} = \frac{N_c}{g_c} = \frac{N_i}{g_i} = N_0 , \qquad \text{B.8}$$

we obtain for the total $j_\alpha \Rightarrow j_\beta$ JTA intensity

$$W_A^{j_\alpha j_\beta} \equiv \sum_{i \in A\ j \in A'} N_i f_{ij}^{j_\alpha j_\beta} = \frac{N_A}{g_A} \sum_{c \in A} g_c f_c^{j_\alpha j_\beta} = N_A f_A^{j_\alpha j_\beta} \qquad \text{B.9}$$

where

$$f_A^{j_\alpha j_\beta} \equiv \frac{1}{g_A} \sum_{c \in A} g_c f_c^{j_\alpha j_\beta} = \varphi^{j_\alpha j_\beta} Q_A^{j_\alpha j_\beta} \qquad \text{B.10}$$

and, using standard binomial relations,

$$Q_A^{j_\alpha j_\beta} \equiv \frac{1}{g_A} \sum_{c \in A} g_c Q_c^{j_\alpha j_\beta} = g_{j_\alpha} g_{j_\beta} \frac{q_\alpha (g_\beta - q_\beta)}{g_\alpha g_\beta}$$ B.11

Using the identity

$$\sum_{j_\alpha j_\beta} g_{j_\alpha} g_{j_\beta} \begin{Bmatrix} j_\alpha & 1 & j_\beta \\ l_\beta & \frac{1}{2} & l_\alpha \end{Bmatrix}^2 = 2$$ B.12

we obtain for the total UTA intensity

$$\sum_{j_\alpha j_\beta} f_A^{j_\alpha j_\beta} = 2\kappa_{\alpha\beta} q_\alpha (g_\beta - q_\beta)$$ B.13

The normalized JTA intensity is therefore obtained from the relations between n-j symbols yielding

$$\overline{W}^{j_\alpha j_\beta} \equiv \frac{f_A^{j_\alpha j_\beta}}{\sum_{j_\alpha j_\beta} f_A^{j_\alpha j_\beta}} = \frac{1}{2} g_{j_\alpha} g_{j_\beta} \begin{pmatrix} j_\alpha & 1 & j_\beta \\ 1/2 & 0 & -1/2 \end{pmatrix}^2$$ B.14

The following relations are easily verified

$$\sum_{j_\alpha} \overline{W}^{j_\alpha j_\beta} = \frac{g_{j_\beta}}{g_\beta} \quad , \quad \sum_{j_\beta} \overline{W}^{j_\alpha j_\beta} = \frac{g_{j_\alpha}}{g_\alpha}$$ B.15

From Eq. (9) we obtain for the JTA's average energy

$$E_A^{j_\alpha j_\beta} = \frac{\sum_{c\in A} g_c f_c^{j_\alpha j_\beta} E_c^{j_\alpha j_\beta}}{\sum_{c\in A} g_c f_c^{j_\alpha j_\beta}} \tag{B.16}$$

$$= D_0^{j_\alpha j_\beta} + \frac{\sum_{c\in A} \sum_{j_a} (q_{j_a} - \delta_{j_a j_\alpha}) g_c Q_c^{j_\alpha j_\beta} D_{j_a}^{j_\alpha j_\beta}}{g_A Q_A^{j_\alpha j_\beta}} \tag{B.17}$$

Again using binomial relations, we obtain

$$E_A^{j_\alpha j_\beta} = D_0^{j_\alpha j_\beta} + \sum_a (q_a - \delta_{a\alpha}) \bar{D}_a^{j_\alpha j_\beta} \tag{B.18}$$

where the barred D's are averages of the form

$$\bar{D}_a^{j_\alpha j_\beta} \equiv \frac{1}{g_a^{\alpha\beta}} \sum_{j_a} g_{j_a}^{j_\alpha j_\beta} D_{j_a}^{j_\alpha j_\beta} \tag{B.19}$$

It should be emphasized that although Eq. B.16 contains only j-j occupation numbers, the result B.18 is given in terms of the "non-relativistic" occupation numbers.

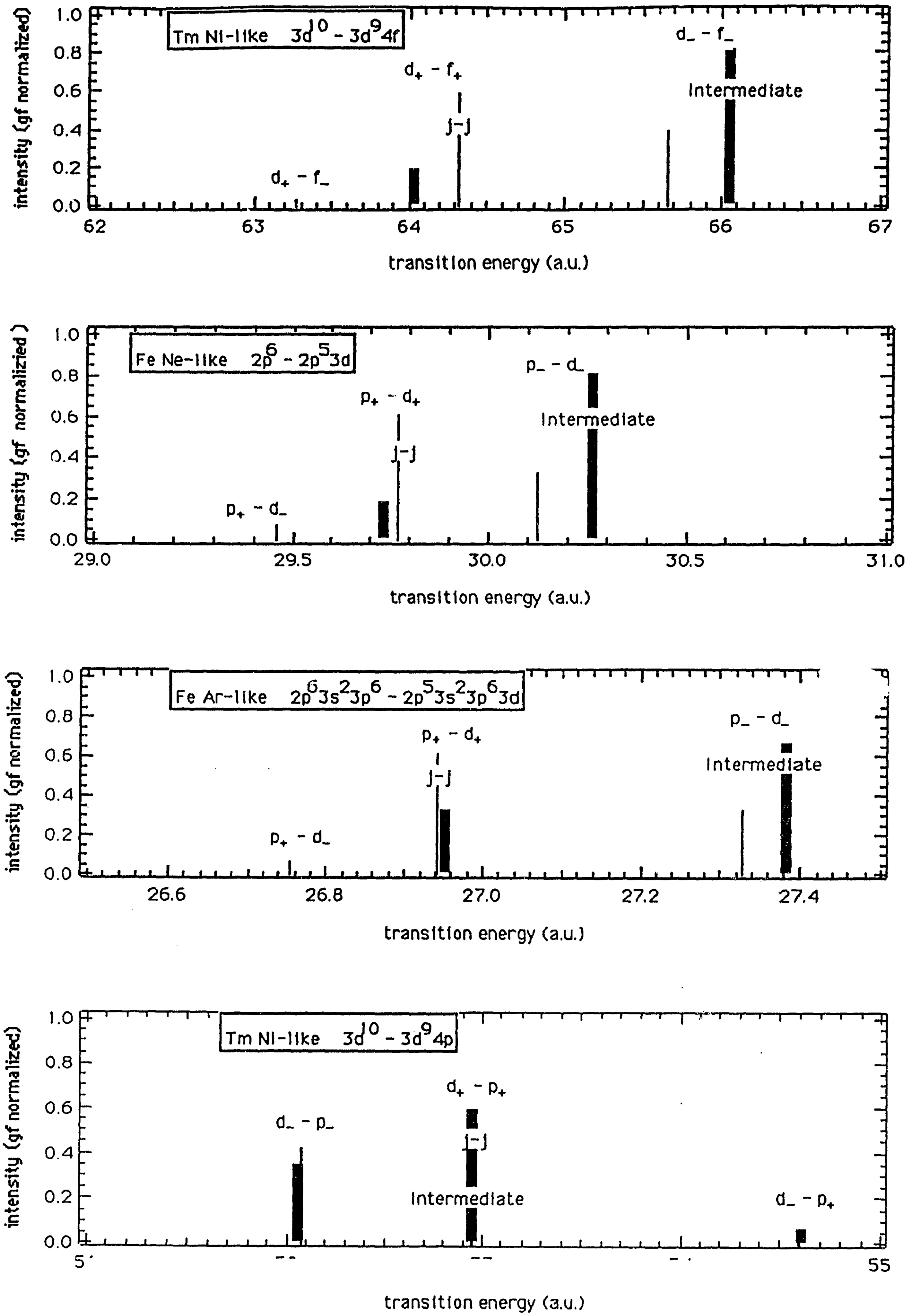


Fig. 1: configuration interaction effect -comparison with pure j-j results

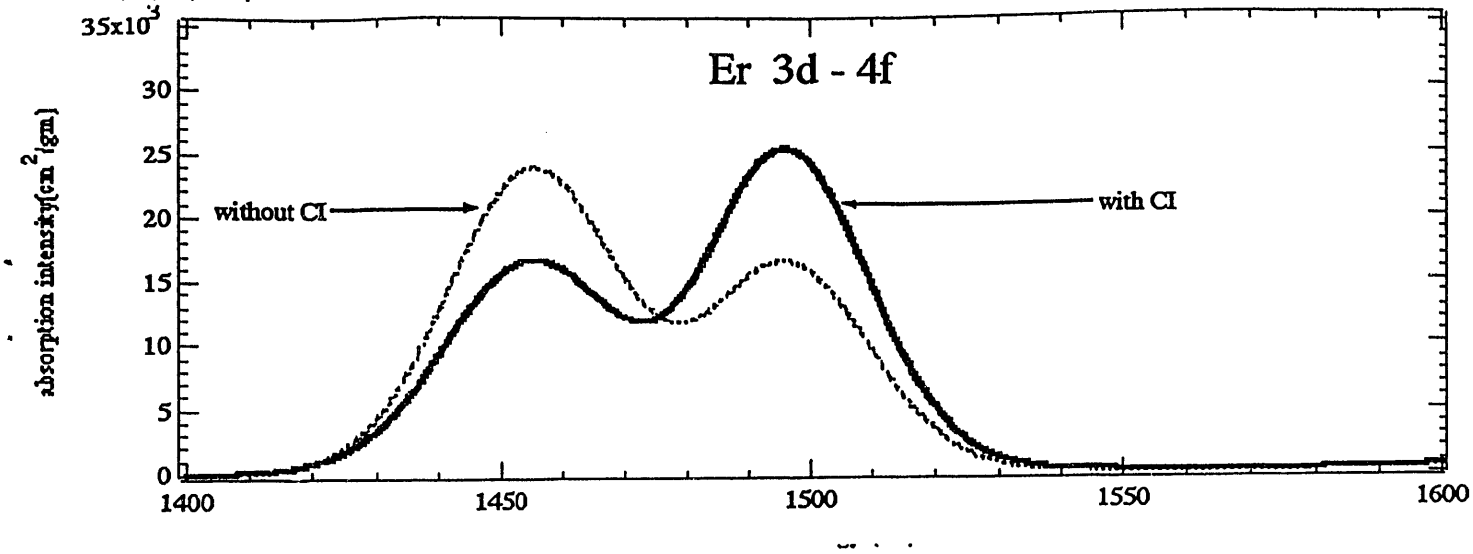


Fig 2: the of 3d-4f transition spectrum of Er at T=60eV and ρ=0.04gm/cc

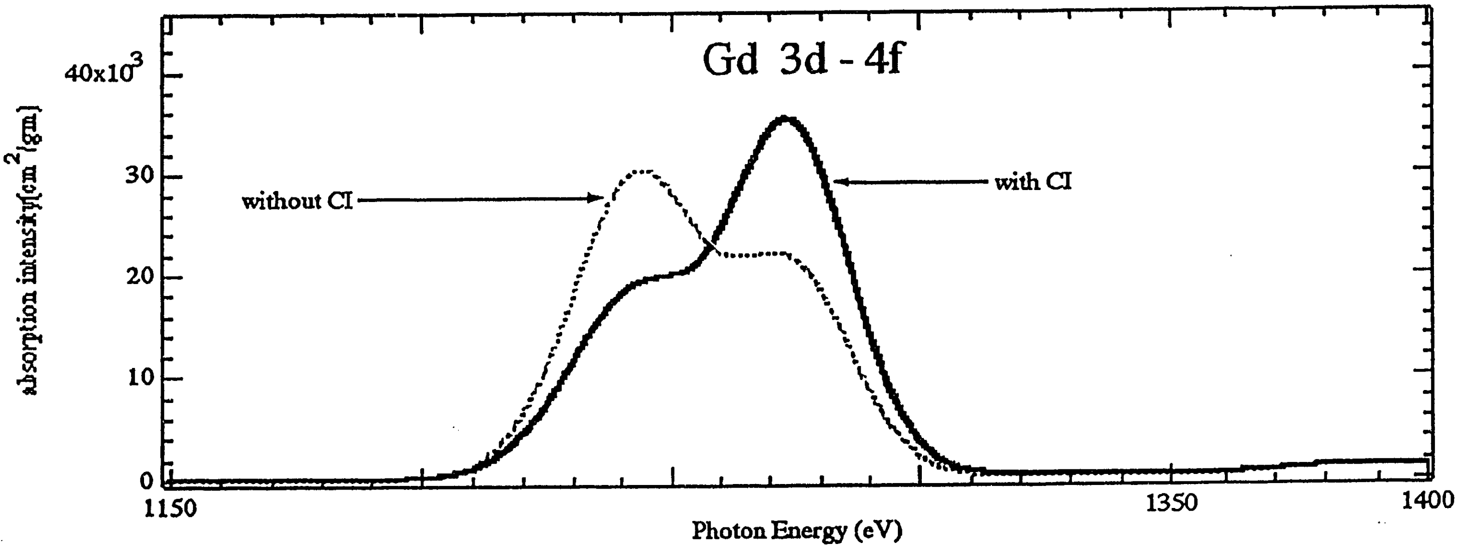


Fig 3: the of 3d-4f transition spectrum of Gd at T=60eV and ρ=0.04gm/cc

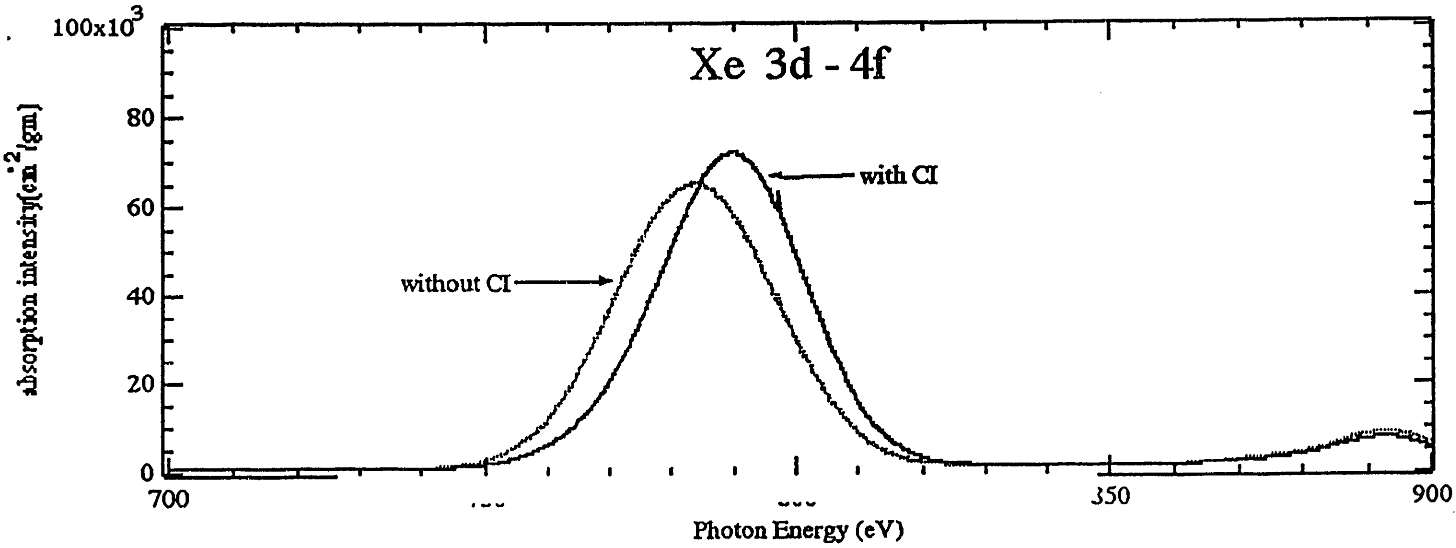


Fig 4: the of 3d-4f transition spectrum of Xe at T=60eV and ρ=0.04gm/cc

DATE

FILMED

9/14/93

END