Effect of configuration interaction on shift widths and intensity redistribution of transition arrays

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Opacity calculations are generally restricted to single configurations approximation with no configuration interaction (CI). The theory for the inclusion of the CI effect on intensity distribution on transition arrays has recently been developed and added to the supertransition array model. However, in an experiment performed recently at NRL, presented in this work, it became apparent that the global shift and width of transition arrays, due to the CI effect, are significant and must be included in the calculations. This feature was also noticed in an LLNL experiment published recently on iron plasma. In these cases the dominant arrays originate from $\Delta n=0$ transitions where this effect is particularly significant. In this work we extend the theory, bypassing the impractical need for matrix diagonalizations, and derive analytic expressions for the CI-corrected array moments including CI shifts, widths, and the adjusted intensity distribution. Examples are presented comparing the theoretical results with detailed calculations and with the experiments. [S1063-651X(99)04303-2]

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I. INTRODUCTION

The supertransition array (STA) [1–7] and SCROLL [8, 9] models for the interpretation of local thermodynamic equilibrium (LTE) and non-LTE plasma spectra, respectively, are both based on a relativistic j-j scheme with no configuration interaction (CI). These models constructs the entire spectrum by a set of Gaussians each describing a supertransition array and reveals the spectral details by splitting STAs in steps until convergence. The result is the detailed configuration accounting (DCA) spectrum where the fundamental array is a unresolved transition array [10] (UTA) between a pair of ordinary relativistic configurations.

The effect of CI on unresolved transition arrays was first investigated by Bauche *et al.* [10] indicating small second order energy shifts, and a possibly large changes in the intensity distribution. In a previous work [4], the dominant effect on supertransition arrays (STAs), i.e., the redistribution of the intensities of STAs, was added to the models indirectly by-passing the impractical need for matrix diagonalizations. However, the CI energy level shifts, manifested as a global shift and in an increase of the variance of STAs were neglected. These effects become important when the electrostatic interaction is strong enough, in particular for $\Delta n=0$ transitions. In this case CI mixing is large due to the overlap of the two active orbitals $\mathbf{j}_\alpha=n_\alpha l_\alpha j_\alpha$ and $\mathbf{j}_\beta=n_\beta l_\beta j_\beta$, giving rise to a large Slater integral $G^1(\mathbf{j}_\alpha,\mathbf{j}_\beta)$. The effect of CI shifts and widths is striking in two recent experiments where $\Delta n=0$ transitions are the most dominant. The first experiment was performed at Lawrence Livermore National Laboratory (LLNL) using iron target at low temperature and density [11]. The second experiment, presented in this work, was performed at the Naval Research Laboratory (NRL) on tungsten-doped plastic targets. The main purpose of this work, however, is to extend the CI theory [4] and derive analytic expressions for the CI-corrected UTA and STA moments, including CI shifts, widths and adjusted intensity distribution. As in our previous work [4], we account for the CI dominant contribution, i.e., CI among nlj configurations belonging to the same parent nl configuration.

Coupled equations for the CI shifted average energies and intensities of STAs and their solutions are derived. In addition analytic expressions for the CI-corrected variances of STAs are obtained. Examples are presented comparing the theoretical results with detailed calculations and with the experiments.

In the next section we define the relevant quantities. In Sec. III we present the analytic expressions for the CI-corrected widths, shifts, and intensities of UTAs and STAs. The detailed derivation of these expressions is given in the appendixes. In Sec. IV we test the model assumptions and demonstrate the importance of these order effects with a few theoretical examples. Section V focuses on comparison with the experiments. In particular we present and discuss here the NRL tungsten experiment. Summary and discussion are given in Sec. VI.

II. DEFINITIONS AND NOTATIONS

A. The nlj and nl UTAs

In the development that follows it will be necessary to compare quantities related to ''relativistic'' nlj configurations, constructed from $\mathbf{j}_s\equiv n_s l_s j_s$ orbitals, with the corresponding ''nonrelativistic'' nl configurations, constructed

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from $\ell_s \equiv n_s l_s$ orbitals, where the index s distinguishes different shells. For simplicity we use the short notation $s \equiv \ell_s \equiv n_s l_s$ and $s_\pm \equiv \mathbf{j}_s \equiv n_s l_s j_s$ for $j_s = l_s \pm \frac{1}{2}$, respectively.

We denote nl and nlj configurations by $A = \Pi_s \ell_s^{q_s}$, and $c = \Pi_{\mathbf{j}_s} \mathbf{j}_s^{q_{\mathbf{j}_s}}$, respectively, where the q's are the corresponding shell occupation numbers. A nl UTA -$A^{\alpha\beta}$ is a transition array between two nonrelativistic configurations, $A \rightarrow A' = \Pi_s \ell_s^{q'_s}$ connected by the orbital transition $\alpha \rightarrow \beta$, i.e., $q'_s = q_s - \delta_{s\alpha} + \delta_{s\beta}$. Similarly, a nlj UTA (termed SOSA [10b]) is a transition array between two relativistic nlj configurations $c \rightarrow c'$ connected by the orbital transition $\mathbf{j}_\alpha \rightarrow \mathbf{j}_\beta$ and is denoted by $c^{j_\alpha j_\beta}$.

The nth moment of a nl UTA is defined by [10]

$$\mu^{(n)} \equiv \sum_{i \in A,\ i' \in A'} \overline{S_{ii'}} \varepsilon_{ii'}^n , \tag{1}$$

where $\varepsilon_{ii'}$ is the transition energy and $\overline{S_{ii'}} = |d_{ii'}|^2$ is the corresponding normalized intensity, given in terms of the transition matrix elements $d_{ii'}$ (normalized). The states i and i' diagonalize the Hamiltonian within A and A', respectively, i.e., $\varepsilon_{ii'} = H_{i'i'} - H_{ii}$.

It was shown [10] that $\mu^{(n)}$ is a matrix trace and is invariant in any coupling scheme. For example,

$$\mu^{(1)} = \sum_{k \in A} (d_{AA'} H_{A'A'} d_{A'A})_{kk} - \sum_{k' \in A'} (d_{A'A} H_{AA} d_{AA'})_{k'k'}$$
$$\equiv \sum_{k \in A,\ k'l' \in A'} d_{kk'} H_{k'l'} d_{l'k} - \sum_{k' \in A',\ k,l \in A} d_{k'k} H_{kl} d_{lk'} \tag{2}$$

reduces to Eq. (1) when using the diagonalized states of the Hamiltonian within A and A' separately.

In the j-j scheme k,k' are j-j diagonalized states of the configurations $c \in A$ and $c' \in A'$, respectively, but not of A and A'. In this case nondiagonal matrix elements connecting states of every $c \in A$ (i.e., CI) and separately for every $c' \in A'$ must be included in Eq. (2).

Ignoring CI the transition energies are $E_{kk'} = H_{k'k'} - H_{kk}$ and

$$\mu_{\text{no CI}}^{(n)} \equiv \sum_{c \in A,\ c' \in A'} \sum_{k \in c,\ k' \in c'} \overline{w_{kk'}} (E_{kk'})^n, \tag{3}$$

where $\overline{w_{kk'}}$ is the normalized intensity without CI. Hereafter we use the notations ε and E for transition energies (and S and w for intensities) with and without CI, respectively.

B. *J*-transition arrays (JTAs)

Consider the nl UTA - $A \rightarrow A' \equiv A^{\alpha\beta}$. Each nl shell in both A and A' containing q electrons is in fact a union of all nlj subshells written as

$$nl^q = \cup_{\{q_- + q_+ = q\}} (nl_-^{q_-}\ \ nl_+^{q_+}). \tag{4}$$

Of course, the subshells become degenerate in the nonrelativistic limit. Ignoring CI, the nl UTA $A^{\alpha\beta}$ can be constructed from all the included nlj UTAs. Depending on the number of partitions $\{q_- + q_+ = q\}$ for all $nl \in A$, the number of nlj UTAs $c \rightarrow c'$, contained in $A \rightarrow A'$ may be very large. However, the mean energies of these nlj UTAs naturally cluster into three distinct arrays characterized by the three suborbital transitions $\mathbf{j}_\alpha \rightarrow \mathbf{j}_\beta$

$$\alpha_- \rightarrow \beta_-, \quad \alpha_+ \rightarrow \beta_+, \quad \text{and} \quad \begin{cases} \alpha_+ \rightarrow \beta_- & \text{for} \quad l_\beta < l\alpha, \\ \alpha_- \rightarrow \beta_+ & \text{for} \quad l_\alpha < l_\beta. \end{cases} \tag{5}$$

The fourth possibility is eliminated by selection rules. For an active orbital with $l=0$ the selection rules yield of course only two arrays. Each of these arrays, called *J*-transition arrays (JTAs), is denoted by $A^{j_\alpha j_\beta} \equiv \cup_{c \in A} c^{j_\alpha j_\beta}$ and includes many nlj UTAs with nearly the same mean energy.

When CI among all $c \in A$ and $c' \in A'$ is gradually switched on, each transition line can still be attributed to one of the three JTAs and the JTA three-array structure remains. Only the JTA moments are changed. When the electrostatic interaction is very strong compared to the spin-orbit interaction, the three JTAs completely intermix, forming a single structure. However, as we shall see, a significant effect on the spectral shift and width of the entire $A \rightarrow A'$ array may still be observed. The same features hold for extended JTAs defined for STAs below. In this work we evaluate CI effect on the moments of JTAs (for UTAs) and of *extended* JTAs (for STAs).

C. *J*-transition arrays of STAs

For convenience we give here briefly the definitions of the required concepts of the STA model.

1. Supershells and superconfigurations

A supershell is a union of adjacent ordinary shells. A superconfiguration is defined on a given supershell structure by assigning an occupation number to each supershell. These occupation numbers are distributed among the ordinary shells of the corresponding supershell in all possible ways, giving rise to many ordinary configurations.

2. Supertransition arrays

A supertransition array is the bulk of all the transition lines, between two superconfigurations connected by a single electron jump. These definitions apply to both nlj shells and nl shells. We denote a general nlj superconfiguration by Ξ and a nlj STA by either $\Xi \rightarrow \Xi'$ where Ξ and Ξ' are the initial and final nlj superconfigurations, or by $\Xi^{j_\alpha j_\beta}$ where $\mathbf{j}_\alpha \rightarrow \mathbf{j}_\beta$ is the specific electron jump. In this case Ξ' contains all the nlj configuration c' obtained from all $c \in \Xi$ by this electron jump. A nlj STA is thus a collection of nlj UTAs: $\Xi^{j_\alpha j_\beta} \equiv \cup_{c \in \Xi} c^{j_\alpha j_\beta}$. Its moments are routinely calculated in both the STA and SCROLL models using partition function algebra [1,7]. Similarly a nl STA denoted by $\Omega^{\alpha\beta}$ is the transition array between two nl superconfigurations $\Omega \rightarrow \Omega'$ connected by the nl orbital jump $\alpha \rightarrow \beta$.

3. Extended JTAs

As for $A^{\alpha\beta}$ above, a nl STA $\Omega^{\alpha\beta}$ (or $\Omega \rightarrow \Omega'$) consists of three "extended" JTAs $\Omega^{j_\alpha j_\beta}$ for the three nlj-orbital transitions of Eq. (5). Ω represents a nl superconfiguration constructed from nl supershells. When CI is ignored a nl supershell can be viewed as a nlj supershell where, for each nl, both nl_- and nl_+ are included. The distribution of the occupation number Q, of a nl supershell, among all its inner shells, in all possible ways, automatically includes all the partitions of Eq. (4) for each of the included nl shells. The ''extended'' JTAs $\Omega^{j_\alpha j_\beta}$ can therefore be viewed as a special cases of a nlj STA. The only difference between $\Omega^{j_\alpha j_\beta}$ and ordinary nlj STA $\Xi^{j_\alpha j_\beta}$ is that in $\Omega^{j_\alpha j_\beta}$ both $nl_- nl_+$ must be included in the same nlj supershell. The JTA $A^{j_\alpha j_\beta} \equiv \cup_{c\in A} c^{j_\alpha j_\beta}$ defined above is actually an example of such nlj STA, where each nl shell is considered as a nlj supershell $(nl_- nl_+)$. In the next section we will first discuss in detail JTAs of the nl UTA $A \rightarrow A'$. The results for extended JTAs will follow.

III. THE CI CORRECTION TO THE JTA SPECTRUM

A. UTA moments

1. The variance of the nl UTA $A^{\alpha\beta}$

The variance of $A^{\alpha\beta}$ is defined by

$$[\Delta^2(A^{\alpha\beta})]_{\rm CI} = \sum_{i\in A,\ i'\in A'} \overline{S}_{ii'}\varepsilon_{ii'}^2 - (\varepsilon_A^{\alpha\beta})^2, \tag{6}$$

where

$$\overline{S}_{ii'} \equiv S_{ii'}/S_A^{\alpha\beta}, \quad S_A^{\alpha\beta} = \sum_{i\in A,\ i'\in A'} S_{ii'}, \tag{7}$$

and

$$\varepsilon_A^{\alpha\beta} = \sum_{i\in A,\ i'\in A'} \overline{S}_{ii'}\varepsilon_{ii'}. \tag{8}$$

The index CI in Eq. (6) indicates that when working in j-j basis, CI among all $c\in A$ and $c'\in A'$ is included.

It is shown in Appendix A that assuming a single set of radial orbitals (generated from the same potential) for all the states of

$$\left[A = \left(\prod_{s\notin\alpha,\beta} \ell_s^{q_s}\right)\ell_\alpha^{q_\alpha}\ell_\beta^{q_\beta} \rightarrow A' = \left(\prod_{s\notin\alpha,\beta} \ell_s^{q_s}\right)\ell_\alpha^{q_\alpha-1}\ell_\beta^{q_\beta+1}\right], \tag{9}$$

the results of Bauche *et al.* [10a] can be written as

$$[\Delta^2(A^{\alpha\beta})]_{\rm CI} = \Delta_{\rm SO}^2(A^{\alpha\beta}) + \Delta_{\rm ES}^2(A^{\alpha\beta}), \tag{10}$$

where

$$\Delta_{\rm SO}^2(A^{\alpha\beta}) = \frac{1}{4}\{l_\alpha(l_\alpha+1)\zeta_\alpha^2 + l_\beta(l_\beta+1)\zeta_\beta^2 - [l_\alpha(l_\alpha+1) + l_\beta(l_\beta+1) - 2]\zeta_\alpha\zeta_\beta\} \tag{11}$$

is the spin orbit contribution, and the electrostatic contribution is

$$\Delta_{\rm ES}^2(A^{\alpha\beta}) = \sum_s (q_s - \delta_{s\alpha})(g_s - q_s - \delta_{s\beta})\sigma^2(s), \tag{12}$$

$$\sigma^2(s) = \frac{\Delta^2(\ell_s\ell_\alpha \rightarrow \ell_s\ell_\beta)}{(g_s - 1 - \delta_{s\alpha} - \delta_{s\beta})}, \tag{13}$$

where $g_s = 4l_s + 2$ and $\Delta^2(\ell_s\ell_\alpha \rightarrow \ell_s\ell_\beta)$ are combinations of radial Slater integrals given explicitly in Ref. [10a].

2. The variance of nlj UTA

For the nlj UTA $c^{j_\alpha j_\beta}$ the variance is defined by

$$\Delta^2(c^{j_\alpha j_\beta}) = \sum_{k\in c,\ k'\in c'} \overline{w}_{kk'}E_{kk'}^2 - (E_c^{j_\alpha j_\beta})^2, \tag{14}$$

$$\overline{w}_{k,k'} \equiv \frac{w_{k,k'}}{w_c^{j_\alpha j_\beta}}, \tag{15}$$

$$w_c^{j_\alpha j_\beta} = \sum_{k\in c,\ k'\in c'} w_{kk'}, \tag{16}$$

$$E_c^{j_\alpha j_\beta} = \sum_{k\in c,\ k'\in c'} \overline{w}_{kk'}E_{kk'}, \tag{17}$$

and the corresponding results of Bauche *et al.* [10b] for

$$\left[c = \left(\prod_s \mathbf{j}_s^{q_s}\right)\mathbf{j}_\alpha^{q_\alpha}\mathbf{j}_\beta^{q_\beta} \rightarrow c' = \left(\prod_s \mathbf{j}_s^{q_s}\right)\mathbf{j}_\alpha^{q_\alpha-1}\mathbf{j}_\beta^{q_\beta+1}\right] \tag{18}$$

can be written as

$$\Delta^2(c^{j_\alpha j_\beta}) = \sum_s (q_{\mathbf{j}_s} - \delta_{\mathbf{j}_s\mathbf{j}_\alpha})(g_{j_s} - q_{\mathbf{j}_s} - \delta_{\mathbf{j}_s\mathbf{j}_\beta})\sigma^2(\mathbf{j}_s) \tag{19}$$

where $g_{j_s} = 2j_s + 1$ and

$$\sigma^2(\mathbf{j}_s) = \frac{\Delta^2(\mathbf{j}_s\mathbf{j}_\alpha \rightarrow \mathbf{j}_s\mathbf{j}_\beta)}{(g_{j_s} - 1 - \delta_{\mathbf{j}_s\mathbf{j}_\alpha} - \delta_{\mathbf{j}_s\mathbf{j}_\beta})}. \tag{20}$$

$\Delta^2(\mathbf{j}_s\mathbf{j}_\alpha \rightarrow \mathbf{j}_s\mathbf{j}_\beta)$ are combination of relativistic radial Slater integrals [10(b), 5].

B. The CI effect on JTA widths

1. Expressing an average in terms of partial averages

We will use the following averaging rule. Let B be a set of elements x_i and let b be a subset of B. The weighted averages and variances of B and b, with the weight f_i for x_i, are

$$X_B \equiv \frac{1}{f_B}\sum_{i\in B} f_i x_i, \quad f_B \equiv \sum_{i\in B} f_i, \tag{21}$$

$$X_b \equiv \frac{1}{f_b}\sum_{i\in b} f_i x_i, \quad f_b \equiv \sum_{i\in b} f_i, \tag{22}$$

$$\Delta_B^2 \equiv \frac{1}{f_B}\sum_{i\in B} f_i(x_i - X_B)^2, \tag{23}$$

$$\Delta_b^2 \equiv \frac{1}{f_b} \sum_{i \in b} f_i (x_i - X_b)^2. \tag{24}$$

It is straightforward to show [5] that if the subsets $b \subset B$ do not overlap and cover B, then

$$\Delta_B^2 = \Delta_{1B}^2 + \Delta_{2B}^2, \tag{25}$$

where Δ_{1B}^2 is the contribution of the centers of the various subsets b to the variance of B, i.e.,

$$\Delta_{1B}^2 = \Delta_{\bar{B}}^2 \equiv \frac{1}{f_B} \sum_{b \in B} f_b (X_b - X_B)^2 \tag{26}$$

and Δ_{2B}^2 is the contribution of the variances Δ_b^2 to the variance of B:

$$\Delta_{2B}^2 \equiv \frac{1}{f_B} \sum_{b \in B} f_b \Delta_b^2. \tag{27}$$

2. The JTA *moments with no* CI

Ignoring CI and assuming that the states of all $c \in A$ and $c' \in A'$ are obtained from a single set of radial orbitals we can write the moments of $A^{\alpha\beta}$ in terms of those of the various JTAs $A^{j_\alpha j_\beta}$ and subarrays $c^{j_\alpha j_\beta}$.

Intensity:

$$w_A^{\alpha\beta} = \sum_{\mathbf{j}_\alpha \mathbf{j}_\beta} w_A^{j_\alpha j_\beta}, \tag{28}$$

$$w_A^{j_\alpha j_\beta} = \sum_{c \in A} w_c^{j_\alpha j_\beta}. \tag{29}$$

Average energy:

$$E_A^{\alpha\beta} = \sum_{\mathbf{j}_\alpha \mathbf{j}_\beta} \overline{w_A^{j_\alpha j_\beta}} \; E_A^{j_\alpha j_\beta}, \tag{30}$$

where

$$\overline{w_A^{j_\alpha j_\beta}} \equiv \frac{w_A^{j_\alpha j_\beta}}{w_A^{\alpha\beta}}, \tag{31}$$

$$E_A^{j_\alpha j_\beta} = \sum_{c \in A} \overline{w_c^{j_\alpha j_\beta}} E_c^{j_\alpha j_\beta}, \tag{32}$$

and

$$\overline{w_c^{j_\alpha j_\beta}} = \frac{w_c^{j_\alpha j_\beta}}{w_A^{j_\alpha j_\beta}}. \tag{33}$$

Variance: using the averaging rule of Eq. (25) on the three JTAs $A^{j_\alpha j_\beta} \subset A^{\alpha\beta}$ as subsets of $A^{\alpha\beta}$ we obtain

$$[\Delta^2(A^{\alpha\beta})]_{\text{no CI}} = [\Delta_1^2(A^{\alpha\beta})]_{\text{no CI}} + [\Delta_2^2(A^{\alpha\beta})]_{\text{no CI}}, \tag{34}$$

where

$$[\Delta_1^2(A^{\alpha\beta})]_{\text{no CI}} = \sum_{\mathbf{j}_\alpha \mathbf{j}_\beta} \overline{w_A^{j_\alpha j_\beta}} (E_A^{j_\alpha j_\beta})^2 - (E_A^{\alpha\beta})^2 \tag{35}$$

is the contribution of the JTA centers and

$$[\Delta_2^2(A^{\alpha\beta})]_{\text{no CI}} = \sum_{\mathbf{j}_\alpha \mathbf{j}_\beta} \overline{w_A^{j_\alpha j_\beta}} \Delta^2(A^{j_\alpha j_\beta}) \tag{36}$$

is the average of the JTA variances. Using the averaging rule of Eq. (25), now for the subsets $c^{j_\alpha j_\beta} \subset A^{j_\alpha j_\beta}$, the JTA variance has again two contributions arising from the nlj UTA centers and variances:

$$\Delta^2(A^{j_\alpha j_\beta}) = \Delta_1^2(A^{j_\alpha j_\beta}) + \Delta_2^2(A^{j_\alpha j_\beta}), \tag{37}$$

$$\Delta_1^2(A^{j_\alpha j_\beta}) = \sum_{c \in A} \overline{w_c^{j_\alpha j_\beta}} (E_c^{j_\alpha j_\beta})^2 - (E_A^{j_\alpha j_\beta})^2, \tag{38}$$

$$\Delta_2^2(A^{j_\alpha j_\beta}) \equiv \sum_{c \in A} \overline{w_c^{j_\alpha j_\beta}} \Delta^2(c^{j_\alpha j_\beta}). \tag{39}$$

3. The correspondence between JTA *and nl* UTAs *variances*

It is shown in Appendix B that the JTA variance $\Delta^2(A^{j_\alpha j_\beta})$ can be expressed in terms of the occupation numbers of the parent nl configuration A as

$$\Delta^2(A^{j_\alpha j_\beta}) = \sum_s (q_s - \delta_{s\alpha})(g_s - q_s - \delta_{s\beta}) P_s^{j_\alpha j_\beta}, \tag{40}$$

where $P_s^{j_\alpha j_\beta}$ is comprised of two contributions

$$P_s^{j_\alpha j_\beta} = P_{1,s}^{j_\alpha j_\beta} + P_{2,s}^{j_\alpha j_\beta} \tag{41}$$

originating from the respective terms of Eq. (37). The explicit expressions for $P_{1,s}^{j_\alpha j_\beta}, P_{2,s}^{j_\alpha j_\beta}$, and $P_s^{j_\alpha j_\beta}$ of Eq. (41) are given in Appendix B in terms of the quantities $\overline{w_A^{j_\alpha j_\beta}}$ of Eq. (B11), $D_o^{j_\alpha j_\beta}$, $D_{j_s}^{j_\alpha j_\beta}$ of Eq. (B12), and $\sigma(\mathbf{j}_s)$ of Eq. (20). These are "orbital quantities" that are common to all the nlj UTAs $c^{j_\alpha j_\beta} \in A^{\alpha\beta}$ (and in fact, for STAs, to all $c^{j_\alpha j_\beta} \in \Omega^{\alpha\beta}$). They originate from the radial parts of the matrix elements of the Hamiltonian and of the radiative transition operator and thus depend on the potential used. Since in our models we use a single potential for entire arrays they are simply constant numbers, even when we proceed to STAs. These orbital quantities do not depend on occupation numbers and play no role in the derivation that follows. Since their explicit expressions, are rather complex and lengthy, and were already published in detail [10,4], we will not repeat them here.

From Eqs. (40) and (36) we finally obtain

$$[\Delta_2^2(A^{\alpha\beta})]_{\text{no CI}} \equiv \sum_{\mathbf{j}_\alpha \mathbf{j}_\beta} \overline{w_A^{j_\alpha j_\beta}} \Delta^2(A^{j_\alpha j_\beta})$$

$$= \sum_s (q_s - \delta_{s\alpha})(g_s - q_s - \delta_{s\beta}) \overline{P}_s^{\alpha\beta} \tag{42}$$

where

$$\overline{P}_s^{\alpha\beta} \equiv \sum_{\mathbf{j}_\alpha \mathbf{j}_\beta} \overline{w}_A^{j_\alpha j_\beta} \; P_s^{j_\alpha j_\beta}. \quad (43)$$

The striking point of Eq. (42) that ignores CI, is that it has the same occupation number dependence, of the nl parent configuration, as in $\Delta^2_{\mathrm{ES}}(A^{\alpha\beta})$ of Eq. (12) that inherently includes CI. Therefore, in order to account for the CI effect on JTA widths, to fit $\Delta^2_{\mathrm{ES}}(A^{\alpha\beta})$, we make the substitution

$$P_s^{j_\alpha j_\beta} \rightarrow \sigma^2(s), \quad (44)$$

i.e., in Eq. (40) we replace $P_s^{j_\alpha j_\beta}$ by $\sigma^2(s)$.

As we shall see we can improve our results by the replacement

$$P_s^{j_\alpha j_\beta} \rightarrow x_{j_\alpha j_\beta} \sigma^2(s), \quad (45)$$

where $x_{j_\alpha j_\beta}$ are arbitrary weights obeying

$$\sum_{\mathbf{j}_\alpha \mathbf{j}_\beta} \overline{w}_A^{j_\alpha j_\beta} x_{j_\alpha j_\beta} = 1. \quad (46)$$

It is immediately seen that this replacement is equivalent to the replacement

$$\overline{P}_s^{\alpha\beta} \rightarrow \sigma^2(s) \quad (47)$$

in Eq. (42) leading to

$$[\Delta_2^2(A^{\alpha\beta})]^{\mathrm{modified}}_{\mathrm{no\ CI}} = \Delta^2_{\mathrm{ES}}(A^{\alpha\beta}), \quad (48)$$

where $[\Delta_2^2(A^{\alpha\beta})]^{\mathrm{modified}}_{\mathrm{no\ CI}}$ is the expression obtained from $[\Delta_2^2(A^{\alpha\beta})]_{\mathrm{no\ CI}}$ after the replacement of Eq. (45) in Eq. (40).

Equation (48) is important from the practical point of view since by making the constants replacements at the first stage of the calculation we can proceed with the j-j calculation ignoring CI and the result will now reconstruct the CI-corrected variance. As we shall see, this is particularly important for STAs where the partition function algebra [7] yields the same working formulas for the STA moments, in terms of the new set of constants. The explicit substitution that imposes the replacement (42) is shown in Appendix C.

In order to account for the entire CI effect, included in Eq. (10), it is required to modify $[\Delta_1^2(A^{\alpha\beta})]_{\mathrm{no\ CI}}$ of Eq. (34) as well such that

$$[\Delta_1^2(A^{\alpha\beta})]^{\mathrm{modified}}_{\mathrm{no\ CI}} = \Delta^2_{\mathrm{SO}}(A^{\alpha\beta}). \quad (49)$$

This leads to

$$[\Delta^2(A^{\alpha\beta})]^{\mathrm{modified}}_{\mathrm{no\ CI}} \equiv [\Delta_1^2(A^{\alpha\beta})]^{\mathrm{modified}}_{\mathrm{no\ CI}} + [\Delta_2^2(A^{\alpha\beta})]^{\mathrm{modified}}_{\mathrm{no\ CI}} \quad (50)$$

$$= [\Delta^2(A^{\alpha\beta})]_{\mathrm{CI}}. \quad (51)$$

Indeed, we have found that

$$[\Delta_1^2(A^{\alpha\beta})]_{\mathrm{no\ CI}} \approx [\Delta_1^2(A^{\alpha\beta})]_{\mathrm{CI}} \approx \Delta^2_{\mathrm{SO}}(A^{\alpha\beta}) \equiv \Delta_1^2, \quad (52)$$

i.e., the electrostatic interaction (with and without CI) affects the centers of j-j UTAs but not their contribution to the variance that is dominated by the spin orbit splitting. This approximation was validated by comparison with detailed calculations and will be used as well later in the determination of JTA shifts and intensity redistribution.

Although the substitutions (45) and (49) are approximations that reproduce the exact CI effect on the total variance, they do not guarantee the accuracy of the individual JTA variances. As shown later inaccuracies in these internal details become noticeable only when approaching the j-j limit where the CI effect becomes negligible. In this case we need to apply interpolation that imposes the proper limit. This point will be discussed further later in the results section.

For the weights $x_{j_\alpha j_\beta}$ in Eq. (45) we have found that assuming equal weights, i.e., $x_{j_\alpha j_\beta} = 1$ is quite satisfactory. A little improvement is achieved using the approximation that the ratios among the JTAs variances are not affected by CI, i.e.,

$$x_{j_\alpha j_\beta} = \frac{\overline{w}_A^{j_\alpha j_\beta} [\Delta^2(A^{j_\alpha j_\beta})]_{\mathrm{no\ CI}}}{\sum_{\mathbf{j}'_\alpha \mathbf{j}'_\beta} \overline{w}_A^{j'_\alpha j'_\beta} [\Delta^2(A^{j'_\alpha j'_\beta})]_{\mathrm{no\ CI}}}. \quad (53)$$

C. The CI correction to the JTA energy shifts and intensities

In addition to the broadening of JTAs, the CI affects JTAs by global shifts and intensity redistribution. These effects are coupled, yielding a total shift $\delta E_A^{\alpha\beta}$ to the average transition energy of $A^{\alpha\beta}$

$$\varepsilon_A^{\alpha\beta} = E_A^{\alpha\beta} + \delta E_A^{\alpha\beta}. \quad (54)$$

This shift is connected to the CI corrected JTA intensities $\overline{S}_A^{j_\alpha j_\beta}$ (normalized) and shifts $\delta E_A^{j_\alpha j_\beta}$ defined by

$$\varepsilon_A^{j_\alpha j_\beta} \equiv E_A^{j_\alpha j_\beta} + \delta E_A^{j_\alpha j_\beta}, \quad (55)$$

where $E_A^{j_\alpha j_\beta}$ is the JTA average energy, of Eqs. (32) and Eq. (B13), in the absence of CI. The expression for the total shift $\delta E_A^{\alpha\beta}$ was obtained analytically [4] as well, i.e.,

$$\delta E_A^{\alpha\beta} = \left\{ \frac{q_\alpha - 1 + \delta_{q_{l_\alpha},0}}{4l_\alpha + 1} - \frac{q_\beta}{4l_\beta + 1} \right\} \Gamma^{\alpha\beta}, \quad (56)$$

where $\Gamma^{\alpha\beta}$ is an ''orbital quantity'' given explicitly in Ref. [4] as a combination of the relativistic Slater integrals $F^k(\mathbf{j}_\alpha \mathbf{j}_\beta), G^1(\mathbf{j}_\alpha \mathbf{j}_\beta)$.

The equation

$$\delta E_A^{\alpha\beta} = \sum_{\mathbf{j}_\alpha \mathbf{j}_\beta} (\overline{S}_A^{j_\alpha j_\beta} \varepsilon_A^{j_\alpha j_\beta} - \overline{w}_A^{j_\alpha j_\beta} E_A^{j_\alpha j_\beta}) \quad (57)$$

by itself is still insufficient to solve for $\delta E_A^{j_\alpha j_\beta}$ and $\overline{S}_A^{j_\alpha j_\beta}$. An additional relation can be obtained from the contribution of the JTA global shifts to the total variance:

$$[\Delta_1^2(A^{\alpha\beta})]_{\mathrm{CI}} \equiv \sum_{\mathbf{j}_\alpha \mathbf{j}_\beta} \overline{S}_A^{j_\alpha j_\beta} (\varepsilon_A^{j_\alpha j_\beta})^2 - (\varepsilon_A^{\alpha\beta})^2. \quad (58)$$

For this purpose we use the approximation of Eq. (52) and substitute in Eq. (58)

$$[\Delta_1^2(A^{\alpha\beta})]_{\rm CI}\rightarrow\Delta_1^2\equiv[\Delta_1^2(A^{\alpha\beta})]_{\rm no\ CI} \qquad (59)$$

calculated directly from Eq. (38). This choice accounts for the relativistic wave functions that are used in our model but not in the derivation of Eq. (11).

The two coupled equations for the CI corrected JTA intensities $\overline{S_A^{j_\alpha j_\beta}}$ and the shifts $\delta E_A^{j_\alpha j_\beta}$ are now

$$\sum_{\mathbf{j}_\alpha\mathbf{j}_\beta}\overline{S_A^{j_\alpha j_\beta}}(E_A^{j_\alpha j_\beta}+\delta E_A^{j_\alpha j_\beta})=\varepsilon_A^{\alpha\beta}, \qquad (60)$$

$$\Delta_1^2=\sum_{\mathbf{j}_\alpha\mathbf{j}_\beta}\overline{S_A^{j_\alpha j_\beta}}(E_A^{j_\alpha j_\beta}+\delta E_A^{j_\alpha j_\beta})^2-(\varepsilon_A^{\alpha\beta})^2. \qquad (61)$$

Taking only the two significant JTAs [4] $--$ and $++$ [for s orbitals ($l=0$) there are only two arrays anyway] indexed by 1 and 2, respectively, and assuming $\delta E_1=-\delta E_2\equiv\delta E$ and $\overline{S_1}+\overline{S_2}=1$, we can write Eqs. (60) and (61) as

$$\overline{S_1}(E_1+2\,\delta E-E_2)+E_2-\delta E=\varepsilon_A^{\alpha\beta}, \qquad (62)$$

$$\Delta_1^2=\overline{S_1}(E_1+\delta E)^2+(1-\overline{S_1})(E_2-\delta E)^2-(\varepsilon_A^{\alpha\beta})^2. \qquad (63)$$

The solution of these two equations is

$$\overline{S_1}=\frac{\varepsilon_A^{\alpha\beta}-E_2+\delta E}{E_1+2\,\delta E-E_2} \qquad (64)$$

and

$$\delta E=-\frac{1}{2}(E_1-E_2)\pm\frac{1}{2}Q,$$

$$Q=\sqrt{(E_1+E_2)^2+4\Delta_1^2+4\varepsilon_A^{\alpha\beta}[\varepsilon_A^{\alpha\beta}-(E_1+E_2)]}. \qquad (65)$$

The denominator in Eq. (64) never vanishes since $E_2-E_1=2\,\delta E$ means that the two arrays centers coincide and lead to a zero variance.

It is easily seen that the two sets of solutions

$$\varepsilon_1\equiv E_1+\delta E=\frac{1}{2}(E_1+E_2)\pm\frac{1}{2}Q,$$

$$\varepsilon_2\equiv E_2-\delta E=\frac{1}{2}(E_1+E_2)\mp\frac{1}{2}Q, \qquad (66)$$

coincide. We therefore take the upper sign and obtain

$$\overline{S_1}=\frac{\varepsilon_A^{\alpha\beta}-\varepsilon_2}{E_1+2\,\delta E-E_2}=\frac{\varepsilon_A^{\alpha\beta}-\varepsilon_2}{\varepsilon_1-\varepsilon_2}=\frac{\varepsilon_A^{\alpha\beta}-\varepsilon_2}{Q}. \qquad (67)$$

Thus in addition to the replacements of Eq. (C3) we obtain the total CI effect on the spectrum by shifting JTAs and changing their intensities according to Eqs. (65) and (67).

IV. THE CI CORRECTION TO EXTENDED JTA SPECTRUM

The above derivation is identical for a STA $\Omega^{\alpha\beta}\equiv\Omega\rightarrow\Omega'$ between two nl superconfigurations assuming the same set of radial orbitals for the entire array. The same equations and solutions hold with the corresponding STA quantities.

The STA extensions of $[\Delta_2^2(A^{\alpha\beta})]_{\rm no\ CI}$ of Eq. (40) takes here the form

$$[\Delta_2^2(\Omega^{\alpha\beta})]_{\rm no\ CI}=\sum_s\langle(q_s-\delta_{s\alpha})(g_s-q_s-\delta_{s\beta})\rangle_\Omega\ \overline{P_s^{\alpha\beta}}, \qquad (68)$$

where the superconfiguration averages $\langle\rangle_\Omega$ are calculated in a straight forward manner by the partition function algebra [1,7] in the STA code. In order to account for the CI effect on the variances of extended JTAs we make the same substitution as in Eq. (45) defining $[\Delta_2^2(\Omega^{\alpha\beta})]_{\rm no\ CI}^{\rm modified}$. For STAs we take $x_{j_\alpha j_\beta}=1$. As will be shown in the results section this approximation is satisfactory. The specific modifications that impose this substitution in the STA code needs further clarification and is described in Appendix C.

It is important to note that the working formulas for STAs [1] involve the same constant orbital quantities as for UTAs. Thus with the replacements given above of the orbital quantities we can proceed with the same relativistic STA code. As we have shown the results will now include automatically the CI effect on STAs variances.

The results for the CI shifts and intensities are the same as in Eqs. (65)–(67), i.e.,

$$\delta E=-\frac{1}{2}(E_1-E_2)\pm\frac{1}{2}Q,$$

$$Q=\sqrt{(E_1+E_2)^2+4\Delta_1^2+4\varepsilon_\Omega^{\alpha\beta}[\varepsilon_\Omega^{\alpha\beta}-(E_1+E_2)]}, \qquad (69)$$

and

$$\overline{S_1}=\frac{\varepsilon_\Omega^{\alpha\beta}-\varepsilon_2}{E_1+2\,\delta E-E_2}=\frac{\varepsilon_\Omega^{\alpha\beta}-\varepsilon_2}{\varepsilon_1-\varepsilon_2}=\frac{\varepsilon_\Omega^{\alpha\beta}-\varepsilon_2}{Q}, \qquad (70)$$

where here

$$E_1=E_\Omega^{++},\quad E_2=E_\Omega^{--}, \qquad (71)$$

$$E_\Omega^{j_\alpha j_\beta}=D_0^{j_\alpha j_\beta}+\sum_s\langle(q_s-\delta_{s\alpha})\rangle_\Omega\overline{D_s^{j_\alpha j_\beta}}, \qquad (72)$$

$$\varepsilon_1=E_1+\delta E,\ \ \varepsilon_2=E_2-\delta E, \qquad (73)$$

$$\Delta_1^2=[\Delta_1^2(A^{\alpha\beta})]_{\rm no\ CI}=\sum_{\mathbf{j}_\alpha\mathbf{j}_\beta}\overline{w_\Omega^{j_\alpha j_\beta}}(E_\Omega^{j_\alpha j_\beta})^2-(E_\Omega^{\alpha\beta})^2, \qquad (74)$$

$$E_\Omega^{\alpha\beta}=\sum_t\overline{w_\Omega^{j_\alpha j_\beta}}E_\Omega^{j_\alpha j_\beta}, \qquad (75)$$

$$\overline{w_\Omega^{j_\alpha j_\beta}}=\overline{w_A^{j_\alpha j_\beta}}=\frac{1}{2}g_{j_\alpha}g_{j_\beta}\begin{Bmatrix} j_\alpha & j_\beta & \kappa\\ l_\alpha & l_\beta & \frac{1}{2}\end{Bmatrix}^2, \qquad (76)$$

and

$$\varepsilon_\Omega^{\alpha\beta}=E_\Omega^{\alpha\beta}+\delta E_\Omega^{\alpha\beta}, \qquad (77)$$

$$\delta E_{\Omega}^{\alpha\beta}=\left\{\frac{\langle q_{\alpha}-1+\delta_{q_{l_{\alpha}},0}\rangle_{\Omega}}{4l_{\alpha}+1}-\frac{\langle q_{\beta}\rangle_{\Omega}}{4l_{\beta}+1}\right\}\Gamma^{\alpha\beta}. \quad (78)$$

The total CI effect is completed by shifting extended JTAs and changing their intensities using Eqs. (69) and (70).

V. RESULTS

A. Testing the model assumptions by detailed calculations

The strength of the CI effect is dictated by the shift $\delta E_A^{\alpha\beta}$ of the average energy of $A^{\alpha\beta}$ given in Eq. (56). Clearly, the effect increases as the occupation number of the active shell α increases and that of β decreases. Further, since $\Gamma^{\alpha\beta}$ grows with increasing overlap between the active orbitals α and β, the CI effect is stronger for $\Delta n=0$ transitions and also for $\Delta n=1$ transitions where $l_{\alpha}<l_{\beta}$ for $n_{\alpha}\leqslant n_{\beta}$. Thus we have chosen examples for the following active orbitals: $4d\rightarrow 4f$, $3p\rightarrow 3d$, and $3d\rightarrow 4f$.

In order to test the model assumptions we have performed the following set of calculations on a series of specific $A^{\alpha\beta}$ arrays. (a) Detailed relativistic intermediate coupling level calculations (including CI), using the HULLAC code [12]. (b) Calculation of the nl UTAs $A^{\alpha\beta}$ spectra using the spectral moments calculated from the lines by detailed summation this line coincides with the one calculated from the analytical nl UTA moments [10] [Eqs. (10)–(12)]. (Bauche formulas are nonrelativistic except for the inclusion of the spin-orbit interaction, in order to make a fair comparison with the relativistic calculations we use in these formulas appropriate averages of relativistic Slater integrals for the nonrelativistic Slater integrals [4], and instead of using the spin-orbit contribution we take the full relativistic contributions to the JTAs' centers.) (c) Calculation of the JTAs $A^{j_{\alpha}j_{\beta}}$ spectra *without* CI, using the analytic JTA moments. (d) Calculation of the JTA spectra including CI using the present theory. Here we present two calculations d1 and d2.

d1 is the result of the theory as presented, while in d2 the array's widths are interpolated between LS and j-j in order to obtain the proper j-j limit. This point needs further explanation. As mentioned above the correspondence $[\Delta_1^2(A^{\alpha\beta})]_{\text{no CI}}\rightarrow\Delta_{\text{SO}}^2(A^{\alpha\beta})$ and $[\Delta_2^2(A^{\alpha\beta})]_{\text{no CI}}\rightarrow\Delta_{\text{ES}}^2(A^{\alpha\beta})$ ensures that the CI effect on the total variance of $A^{\alpha\beta}$ is correct, consistent with Bauche formulas. However, for atomic systems close to j-j, the first contribution dominates by far the second one, and a minor inaccuracy of this internal correspondence leads to excessively broad arrays. Therefore we have found it plausible to interpolate between LS and j-j to give the proper j-j limit (where CI effects vanish). The interpolated result dictated by the parameter $\delta=[\Delta_1^2(A^{\alpha\beta})]_{\text{no CI}}/\{[\Delta_1^2(A^{\alpha\beta})]_{\text{no CI}}+[\Delta_2^2(A^{\alpha\beta})]_{\text{no CI}}\}$, is presented in the d2 curves. The various cases are shown in the figures with the corresponding lines: (a) the dotted thin lines, (b) the solid thin lines, (c) the dashed heavy lines, (d1) the dashed thin lines, (d2) the solid heavy lines.

Since we are dealing, in these examples, with atomic systems (not plasma) we present the results for the pure atomic dimensionless oscillator strength, that up to a constant describes the absorption spectrum. The first case presented in Fig. 1 is the spectrum of $A^{\alpha\beta}$ with $\alpha=4d\rightarrow\beta=4f$ and $A=4d^9 4f$ of tungsten. This array participates in the spectrum of the NRL experiment discussed below. The reconstruction of the detailed line calculations by the present theory is obvious here. The CI shifts are very large as expected for $\Delta n=0$ transition array and since the $4d$ shell is almost full and the $4f$ shell is almost empty. As we can see in this case the nonrelativistic result (b) is a good approximation. This calculation demonstrates the importance of CI shifts and widths for these $\Delta n=0$ transitions, that are far away from j-j coupling, even though they originate from a heavy atom that requires relativistic treatment and has many other transition arrays closer to j-j. In this paper we have presented a theory that can account for both limits, while providing a systematic description of intermediate cases.

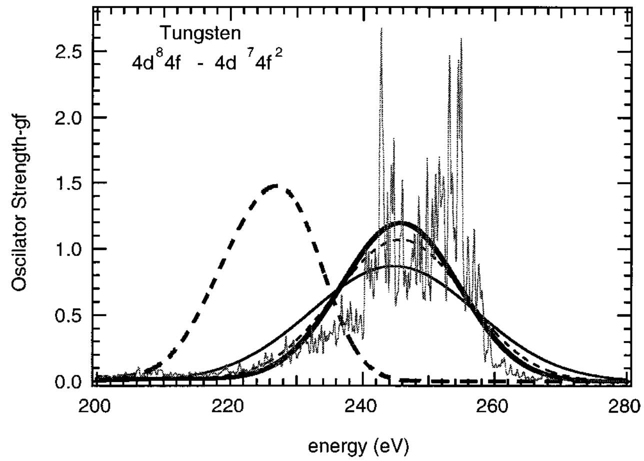

FIG. 1. The spectrum of $A^{\alpha\beta}=4d^8 4f-4d^7 4f^2$ of tungsten. (a) Dotted thin line: detailed relativistic intermediate coupling level calculations (including CI); (b) solid thin line: calculation of the nl UTAs $A^{\alpha\beta}$ spectra using the spectral moments; (c) dashed heavy lines: calculation of the JTAs $A^{j_{\alpha}j_{\beta}}$ spectra without CI, using the analytic JTA moments; (d1) dashed thin line: the result of the present theory–calculation of the JTA spectra including CI; (d2) solid heavy lines: interpolated calculation between LS and j-j.

A systematic shift from LS to j-j scheme, demonstrating the gradual decrease of CI as a function of Z is presented in Fig. 2. Here the $3p\rightarrow 3d$ transition array of $A=3p^4 3d^2$ is presented for Fe, Mo, Ag, Ba, and W. For all these cases the agreement of the corrected CI results to the detailed line calculations is very good. For iron and molybdenum we see that the CI-corrected spectrum actually coincide with the nl UTA result. The j-j result is not a good approximation here. In silver we already see a significant departure from LS but it is still far away from j-j. The barium spectrum is close to j-j but there is still a change in intensities. In tungsten the spectrum has almost complete j-j features. Figure 3 makes a similar investigation for $\Delta n=1$ transition arrays $A^{\alpha\beta}=3d^9 4f\rightarrow 3d^8 4f^2$ for Mo, Ba, Ga, and W. In this case the effect is strong mainly due to the condition on occupation numbers ($3d$ shell is almost full and the $4f$ shell is almost empty). In molybdenum and barium we see a single structure with a dominant shift effect, whereas for gadolinium and gold the j-j split becomes apparent but even for gold the CI effect is noticeable through intensity redistribution.

B. Comparison with experiments

In Figs. 4, 5 we present the two experimental results in comparison with the CI corrected STA calculations. These

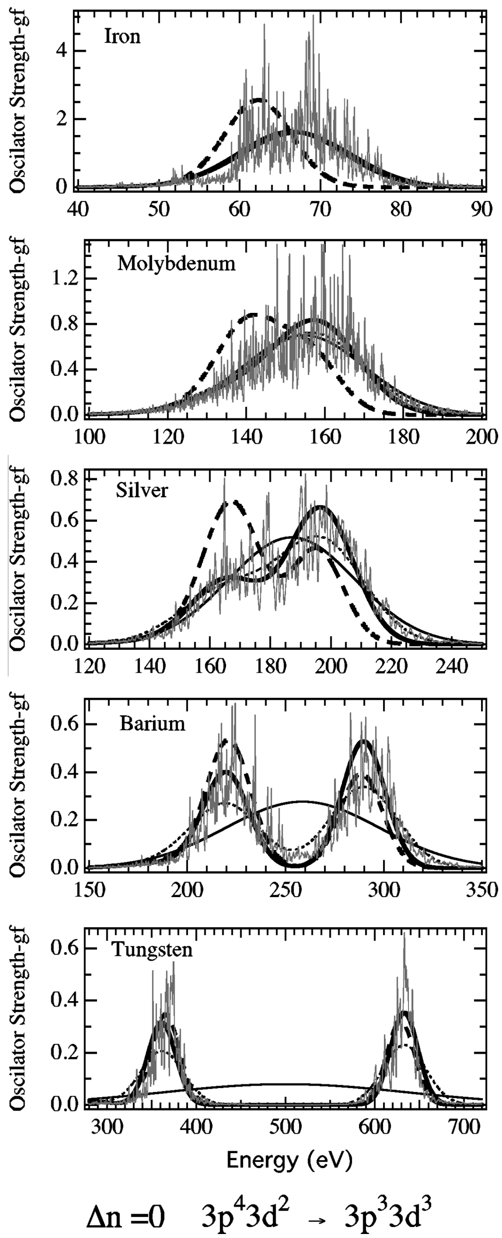

FIG. 2. The spectrum of $A^{\alpha\beta}=3p^4 3d^2 \rightarrow 3p^3 3d^3$ transition array for $Z=26,42,47,56$, and 74. The line identifications are as in Fig. 1.

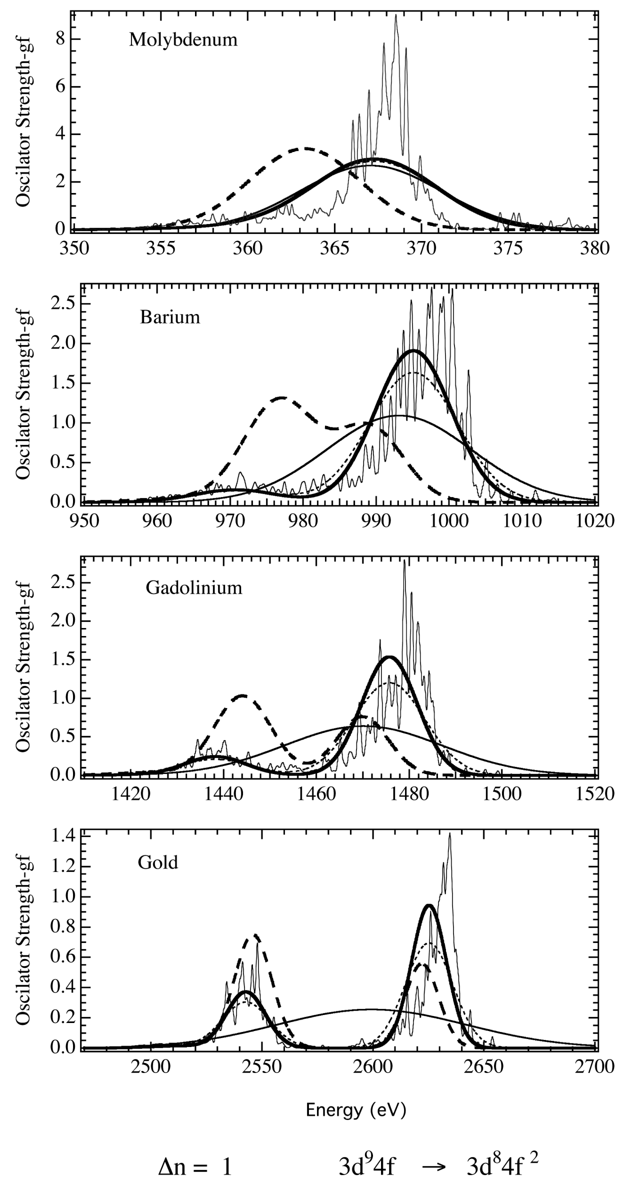

FIG. 3. The spectrum of the transition array of $A^{\alpha\beta}=3d^9 4f \rightarrow 3d^8 4f^2$ for $Z=42,56,31$, and 79. The line identifications are as in Fig. 1.

two experiments were the central motivation for the present work since they could not be simulated properly by the STA code without CI.

1. *The* NRL *tungsten experiment*

In Fig. 4 we see the result of an experiment performed recently at NRL and presented here. The NIKE KrF laser was shot at a CH target doped with 7% W (by atom). The intensity was 2.5×10^{12} W/cm^2. The spectrum was obtained with a grazing incident spectrometer, equipped with 1200 l/mm grating. The time integrated spectrum was recorded on Kodak 101 film. Some space resolution was obtained through the use of a slit perpendicular to the plasma. Hydrodynamic simulations [13] show that the tungsten radiation in the relevant spectral range is emitted during a relatively short time by a well localized region of the plasma. It is therefore sensible to assume one temperature ($T=80$ eV) and one density ($n_e=3\times 10^{20}$ cm^{-3}) for the calculations. Figure 4 presents the experimental results compared with the STA calculations. The experimental intensity is only relative and thus the peak intensity was set equal to the calculations. The dominant transitions here belong to the $4d\rightarrow 4f$ arrays producing a strong effect of CI shifts and widths that simulates the experimental result correctly.

2. *The* LLNL Fe *experiment*

Figure 5 presents the results of the Fe experiment performed recently at LLNL [11] to simulate astrophysical plasmas. The plasma conditions $Te=20$ eV and $\rho=10^{-4}$ gm/cc give rise to dominant $\Delta n=0$, $3p\rightarrow 3d$ arrays. It is clear that both CI shifts and width effects must be included to reproduce the experimental features. The lines resolution is not seen in the STA results that assumes unresolved UTAs and agrees with the OPAL UTA result [11].

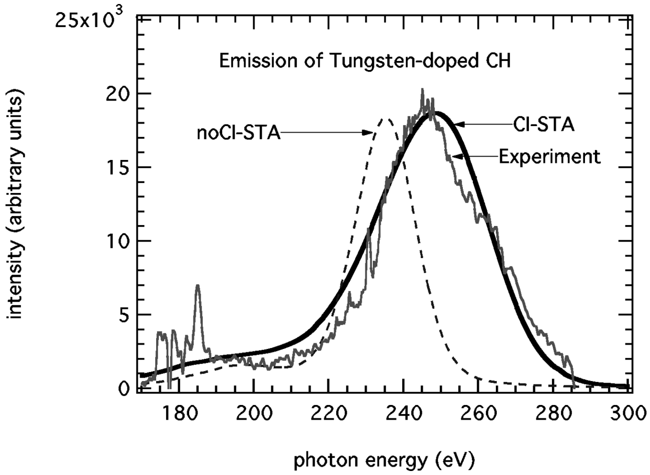

FIG. 4. The result of the NRL experiment compared with the STA calculations. The tungsten plasma conditions are $T = 80$ eV, $ne = 3\times10^{20}$ cm^{-3}.

VI. SUMMARY AND DISCUSSION

We have extended the STA model to include the entire CI effects among all nlj configurations belonging to the same parent nl configuration. Analytic expressions for the CI shifts, widths and intensity redistribution of both nlj UTAs and STAs are derived. These expressions extend our previous theoretical results [4] that dealt only with CI redistribution of the STA intensities. The extended model moves smoothly between LS and j-j conditions, accounting correctly for intermediate coupling as demonstrated in Figs. 2 and 3. The derivation was based on the assumption that the configuration independent spin orbit variances contribute almost solely to the spread of the JTA centers and that the contribution of the electrostatic interaction to this spread is negligible. These assumptions were tested and validated by detailed calculations. We have presented examples comparing the theoretical results with detailed calculations and with experiments showing the importance of the CI shifts and widths for various plasma conditions. In particular we have presented and discussed the results of a recent experiment performed at NRL on a tungsten plasma dominated by such $\Delta n = 0$ arrays. It is important to note that for an atom under specific conditions some of the transition arrays will be closer to the LS scheme while others will be closer to j-j scheme others maybe in intermediate coupling scheme. Thus there is a need for the above theory that accounts for all these possibilities automatically using a single general model. The remarkable achievement of the present approach is its success to account fully for a complex effect that usually requires matrix diagonalizations that in our case are impractical due to the enormous amount of nl configurations involved.

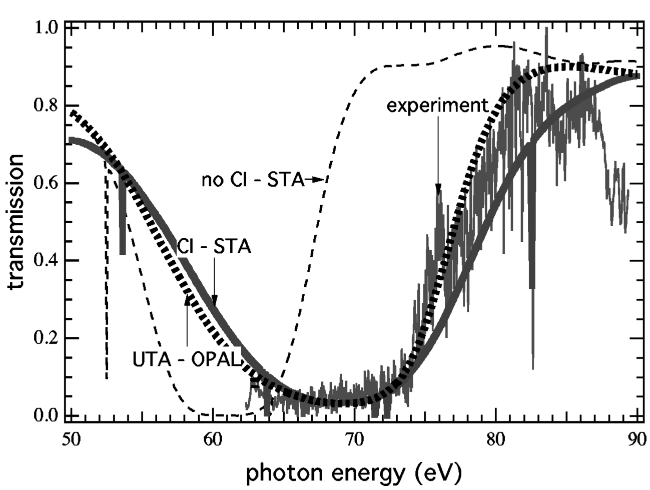

FIG. 5. The iron spectrum at $Te = 20$ eV and $\rho = 10^{-4}$ gm/cc; comparison among the LLNL experiment, the STA and the UTA-OPAL calculations.

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APPENDIX A: UTA WIDTH

The variance of a nl UTA $A^{\alpha\beta} \equiv A \to A'$,

$$A = \prod_s l_s^{q_s} l_\alpha^{q_\alpha} l_\beta^{q_\beta} \to A' = \prod_s l_s^{q_s} l_\alpha^{q_\alpha - 1} l_\beta^{q_\beta + 1}, \qquad \text{(A1)}$$

has the following two contributions [10]:

$$\Delta^2(A^{\alpha\beta}) = \Delta^2(l_\alpha^{q_\alpha} l_\beta^{q_\beta} \to l_\alpha^{q_\alpha - 1} l_\beta^{q_\beta + 1}) + \sum_{s \neq \alpha,\beta} \Delta^2(l_s^{q_s} l_\alpha \to l_s^{q_s} l_\beta). \qquad \text{(A2)}$$

Assuming that the states of both A and A' are calculated with the same potential the results are

$$\Delta^2(l_\alpha^{q_\alpha} l_\beta^{q_\beta} \to l_\alpha^{q_\alpha - 1} l_\beta^{q_\beta + 1}) \equiv \sum_{s=\alpha,\beta} (q_s - \delta_{s\alpha})(g_s - q_s - \delta_{s\beta}) \sigma_2^2(l_s l_\alpha \to l_s l_\beta), \qquad \text{(A3)}$$

$$\Delta^2(l_s^{q_s} l_\alpha \to l_s^{q_s} l_\beta) \equiv q_s(g_s - q_s)\sigma_1^2(l_s l_\alpha \to l_s l_\beta) \quad (s \neq \alpha,\beta). \qquad \text{(A4)}$$

Collecting terms yields

$$\Delta^2(A^{\alpha\beta}) = \sum_s (q_s - \delta_{s\alpha})(g_s - q_s - \delta_{s\beta}) \sigma^2(s), \qquad \text{(A5)}$$

where

$$\sigma^2(s) = \frac{\Delta^2(l_s l_\alpha \to l_s l_\beta)}{(g_s - 1 - \delta_{s\alpha} - \delta_{s\beta})} \qquad \text{(A6)}$$

and $\Delta^2(l_s l_\alpha \to l_s l_\beta)$ is specified [10a] for the two different cases $s = \alpha,\beta$ and $s \neq \alpha,\beta$. Similarly for nlj UTAs the variance is as in Eqs. (A5),(A6) with the replacement $a \equiv \mathbf{l}_a \to \mathbf{j}_a$ for $a = s,\alpha,\beta$.

APPENDIX B: THE JTA MOMENTS WITHOUT CI

1. Intensity

The configuration average multipole κ transition probability for orbital jump $\mathbf{j}_\alpha \to \mathbf{j}_\beta$ is given by [4]

$$w_c^{j_\alpha j_\beta} = g_c q_{\mathbf{j}_\alpha}(g_{\mathbf{j}_\beta} - q_{\mathbf{j}_\beta}) \begin{Bmatrix} j_\alpha & j_\beta & \kappa \\ l_\alpha & l_\beta & \frac{1}{2} \end{Bmatrix}^2 P_{\alpha\beta}^2, \tag{B1}$$

where

$$g_c = \prod_{\mathbf{j}_s \in c} \binom{g_{j_s}}{q_{\mathbf{j}_s}} \tag{B2}$$

and $P_{\alpha\beta}$ is the transition radial integral (multiplied by a factor) that is independent of the configuration c and is approximated here as an average over all $j_\alpha \in \alpha$ and $j_\beta \in \beta$. For convenience,when confusion can not arise, we use normal (instead of bold) j for the set nlj.

The normalized JTA intensity is

$$\overline{w}_A^{j_\alpha j_\beta} = \frac{w_A^{j_\alpha j_\beta}}{w_A^{\alpha\beta}}, \tag{B3}$$

where

$$w_A^{j_\alpha j_\beta} = \sum_{c \in A} w_c^{j_\alpha j_\beta}, \quad w_A^{\alpha\beta} = \sum_{j_\alpha j_\beta} w_A^{j_\alpha j_\beta}. \tag{B4}$$

Using the identities for any orbital $s \equiv n_s l_s$

$$\sum_{c \in A} g_{j_s} - \delta_{j_s j_a} - \delta_{j_s j_b} - \delta_{j_s j_c} \cdots = g_s - \delta_{sa} - \delta_{sb} - \delta_{sc} \cdots, \tag{B5}$$

$$\sum_{c \in A} q_{j_s} - \delta_{j_s j_a} - \delta_{j_s j_b} - \delta_{j_s j_c} \cdots = q_s - \delta_{sa} - \delta_{sb} - \delta_{sc} \cdots, \tag{B6}$$

and the binomial relations

$$\sum_{a+b=c} \binom{x}{a}\binom{y}{b} = \binom{x+y}{c}, \tag{B7}$$

$$a\binom{x}{a} = x\binom{x-1}{a-1}, \tag{B8}$$

$$(x-a)\binom{x}{a} = x\binom{x-1}{a}, \tag{B9}$$

we obtain

$$\overline{w}_c^{j_\alpha j_\beta} \equiv \frac{w_c^{j_\alpha j_\beta}}{\sum_{c \in A} w_c^{j_\alpha j_\beta}} = \frac{\prod_{j_s} \binom{g_{j_s} - \delta_{j_s, j_\alpha} - \delta_{j_s, j_\beta}}{q_{j_s} - \delta_{j_s, j_\alpha}}}{\prod_s \binom{g_s - \delta_{s,\alpha} - \delta_{s,\beta}}{q_s - \delta_{s,\alpha}}} \tag{B10}$$

and [4]

$$\overline{w}_A^{j_\alpha j_\beta} = \frac{1}{2} g_{j_\alpha} g_{j_\beta} \begin{Bmatrix} j_\alpha & j_\beta & \kappa \\ l_\alpha & l_\beta & \frac{1}{2} \end{Bmatrix}^2. \tag{B11}$$

independent of the occupation numbers of the configuration c. The denominator of Eq. (B10) never vanishes since for orbital jump $\alpha \to \beta$, $q_\alpha \geqslant 1$ and $q_\beta \leqslant g_\beta - 1$.

2. Average energy

The configuration average energies are [4]

$$E_c^{j_\alpha j_\beta} = D_o^{j_\alpha j_\beta} + \sum_{j_s} (q_{j_s} - \delta_{j_s j_\alpha}) D_{j_s}^{j_\alpha j_\beta}, \tag{B12}$$

where $D_o^{j_\alpha j_\beta}$ and $D_{j_s}^{j_\alpha j_\beta}$ are orbital quantities common for all $c^{j_\alpha j_\beta} \in A^{\alpha\beta}$, specified in Ref. [4]. The JTA average energy is thus

$$E_A^{j_\alpha j_\beta} = D_o^{j_\alpha j_\beta} + \sum_{c \in A} \overline{w}_c^{j_\alpha j_\beta} \sum_{j_s} (q_{j_s} - \delta_{j_s j_\alpha}) D_{j_s}^{j_\alpha j_\beta}. \tag{B13}$$

Substituting for $\overline{w}_c^{j_\alpha j_\beta}$ of Eq. (B10) and using Eqs. (B7)–(B9) we obtain

$$E_A^{j_\alpha j_\beta} - D_o^{j_\alpha j_\beta} = \frac{\sum_{c \in A} \prod_{j_t} \binom{g_{j_t} - \delta_{j_t j_\alpha} - \delta_{j_t j_\beta}}{q_{j_t} - \delta_{j_t j_\alpha}} \sum_{j_s} (q_{j_s} - \delta_{j_s j_\alpha}) D_{j_s}^{j_\alpha j_\beta}}{\prod_t \binom{g_t - \delta_{t\alpha} - \delta_{t\beta}}{q_t - \delta_{t\alpha}}} = \sum_s \overline{D}_s^{j_\alpha j_\beta} (q_s - \delta_{s\alpha}), \tag{B14}$$

where

$$\overline{D}_s^{j_\alpha j_\beta} = \sum_{j_s \in s} D_{j_s}^{j_\alpha j_\beta} \frac{(g_{j_s} - \delta_{j_s j_\alpha} - \delta_{j_s j_\beta})}{(g_s - \delta_{s\alpha} - \delta_{s\beta})}. \tag{B15}$$

3. Variance

The two contributions of Eq. (37) read

$$\Delta_1^2(A^{j_\alpha j_\beta}) = \sum_{c \in A} \overline{w}_c^{j_\alpha j_\beta} (E_c^{j_\alpha j_\beta} - E_A^{j_\alpha j_\beta})^2 = \Delta_{11}^2 - \Delta_{12}^2$$

and

$$\Delta_2^2(A^{j_\alpha j_\beta}) = \sum_{c \in A} \overline{w}_c^{j_\alpha j_\beta} \Delta^2(c^{j_\alpha j_\beta}), \tag{B16}$$

where

$$\Delta_{11}^2 = \sum_{c \in A} \overline{w}_c^{j_\alpha j_\beta} (E_c'^{j_\alpha j_\beta})^2, \tag{B17}$$

$$\Delta_{12}^2 = (E_A'^{j_\alpha j_\beta})^2, \tag{B18}$$

and $E_c'^{j_\alpha j_\beta}=E_c^{j_\alpha j_\beta}-D_o^{j_\alpha j_\beta}$, $E_A'^{j_\alpha j_\beta}=E_A^{j_\alpha j_\beta}-D_o^{j_\alpha j_\beta}$.

a. The expression for $\Delta_1^2(A^{j_\alpha j_\beta})$

The first term is obtained by substitution of the expressions (B10) and (B12), without $D_o^{j_\alpha j_\beta}$, for $\overline{w_c^{j_\alpha j_\beta}}$ and $E_c'^{j_\alpha j_\beta}$ in Eq. (B17). We obtain a double sum over nlj orbitals:

$$\Delta_{11}^2=\sum_{c\in A}\overline{w_c^{j_\alpha j_\beta}}(E_c'^{j_\alpha j_\beta})^2=\sum_{j_s j_{s'}}X(j_s,j_{s'}), \tag{B19}$$

where the contribution of a specific pair $j_s,j_{s'}$ is

$$X(j_s,j_{s'})=\frac{1}{\prod_d\binom{g_d-\delta_{d\alpha}-\delta_{d\beta}}{q_d-\delta_{d\alpha}}}\sum_{c\in A}\prod_{j_b}\binom{g_{j_b}-\delta_{j_bj_\alpha}-\delta_{j_bj_\beta}}{q_{j_b}-\delta_{j_bj_\alpha}}\times D_{j_s}^{j_\alpha j_\beta}D_{j_{s'}}^{j_\alpha j_\beta}(q_{j_s}-\delta_{j_sj_\alpha})(q_{j_{s'}}-\delta_{j_{s'}j_\alpha}). \tag{B20}$$

For $s=s'$ and $j_s=j_{s'}$ we use the binomial identities

$$\frac{\binom{g-1}{q-1}}{\binom{g}{q}}=\frac{q}{g}, \tag{B21}$$

$$\frac{\binom{g-2}{q-2}}{\binom{g}{q}}=\frac{q(q-1)}{g(g-1)}, \tag{B22}$$

and get

$$X(j_s,j_s)=[D_{j_s}^{j_\alpha j_\beta}]^2\left[\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta})(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta}-1)}{(g_s-\delta_{s\alpha}-\delta_{s\beta})(g_s-\delta_{s\alpha}-\delta_{s\beta}-1)}\times(q_s-\delta_{s\alpha})(q_s-\delta_{s\alpha}-1)+\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta})}{(g_s-\delta_{s\alpha}-\delta_{s\beta})}(q_s-\delta_{s\alpha})\right]. \tag{B23}$$

The denominator of Eq. (B23) for orbital jump $\alpha\to\beta$ vanishes only if α or β are s orbitals. In this case $g_s-\delta_{s\alpha}-\delta_{s\beta}-1=0$. However, it is seen from Eq. (12) that active $s(l=0)$ orbitals give zero contribution to the variance and are excluded from its calculation.

For the same reasons the denominators of the expressions below never vanish. For $s=s'$ and $j_s\neq j_{s'}=\overline{j_s}$, where

$$\overline{j}\equiv nlj' \quad \text{with} \quad j'=j\pm1 \quad \text{for} \quad j=l\mp1/2 \tag{B24}$$

we use Eq. (B22) and obtain

$$X(j_s,\overline{j_s})=D_{j_s}^{j_\alpha j_\beta}D_{\overline{j_s}}^{j_\alpha j_\beta}\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta})(g_{\overline{j_s}}-\delta_{\overline{j_s}j_\alpha}-\delta_{\overline{j_s}j_\beta})}{(g_s-\delta_{s\alpha}-\delta_{s\beta})(g_s-\delta_{s\alpha}-\delta_{s\beta}-1)}\times(q_s-\delta_{s\alpha})(q_s-\delta_{s\alpha}-1). \tag{B25}$$

and for $s\neq s'$ from Eq. (B21) we get

$$X(j_s,j_{s'})=D_{j_s}^{j_\alpha j_\beta}D_{j_{s'}}^{j_\alpha j_\beta}\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta})(g_{j_{s'}}-\delta_{j_{s'}j_\alpha}-\delta_{j_{s'}j_\beta})}{(g_s-\delta_{s\alpha}-\delta_{s\beta})(g_{s'}-\delta_{s'\alpha}-\delta_{s'\beta})}\times(q_s-\delta_{s\alpha})(q_{s'}-\delta_{s'\alpha}). \tag{B26}$$

For the second term of Eq. (B18) we obtain by taking the square of Eq. (B14), without $D_o^{j_\alpha j_\beta}$, a double sum over orbitals

$$\Delta_{12}^2\equiv(E_s'^{j_\alpha j_\beta})^2=\sum_{j_sj_{s'}}Y(j_s,j_{s'}), \tag{B27}$$

where again the identity (B21) is used giving for the contribution of the pair $(j_s,j_{s'})$ the expression

$$Y(j_s,j_{s'})=D_{j_s}^{j_\alpha j_\beta}D_{j_{s'}}^{j_\alpha j_\beta}\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta})}{(g_s-\delta_{s\alpha}-\delta_{s\beta})}\frac{(g_{j_{s'}}-\delta_{j_{s'}j_\alpha}-\delta_{j_{s'}j_\beta})}{(g_{s'}-\delta_{s'\alpha}-\delta_{s'\beta})}\times(q_s-\delta_{s\alpha})(q_{s'}-\delta_{s'\alpha}). \tag{B28}$$

Since for $s\neq s'$

$$X(j_s,j_{s'})=Y(j_s,j_{s'}), \tag{B29}$$

we have

$$\Delta_1^2(A^{j_\alpha j_\beta})=\Delta_{11}^2-\Delta_{12}^2=\sum_{j_sj_{s'}}[X(j_s,j_{s'})-Y(j_s,j_{s'})]=\sum_s\sum_{j_s\in s}\{[X(j_s,j_s)-Y(j_s,j_s)]+[X(j_s,\overline{j_s})-Y(j_s,\overline{j_s})]\}, \tag{B30}$$

where

$$[X(j_s,j_s)-Y(j_s,j_s)]=[D_{j_s}^{j_\alpha j_\beta}]^2\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta})}{(g_s-\delta_{s\alpha}-\delta_{s\beta})}(q_s-\delta_{s\alpha})\times\left\{\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta}-1)}{(g_s-\delta_{s\alpha}-\delta_{s\beta}-1)}(q_s-\delta_{s\alpha}-1)+1-\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta})}{(g_s-\delta_{s\alpha}-\delta_{s\beta})}(q_s-\delta_{s\alpha})\right\}$$
$$=[D_{j_s}^{j_\alpha j_\beta}]^2\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta})(g_{\bar{j}_s}-\delta_{\bar{j}_sj_\alpha}-\delta_{\bar{j}_sj_\beta})}{(g_s-\delta_{s\alpha}-\delta_{s\beta})^2(g_s-\delta_{s\alpha}-\delta_{s\beta}-1)}(q_s-\delta_{s\alpha})(g_s-q_s-\delta_{s\beta}) \quad \text{(B31)}$$

and

$$[X(j_s,\bar{j}_s)-Y(j_s,\bar{j}_s)]=-D_{j_s}^{j_\alpha j_\beta}D_{\bar{j}_s}^{j_\alpha j_\beta}\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta})(g_{\bar{j}_s}-\delta_{\bar{j}_sj_\alpha}-\delta_{\bar{j}_sj_\beta})}{(g_s-\delta_{s\alpha}-\delta_{s\beta})^2(g_s-\delta_{s\alpha}-\delta_{s\beta}-1)}\times(q_s-\delta_{s\alpha})(g_s-q_s-\delta_{s\beta}). \quad \text{(B32)}$$

Thus

$$\Delta_1^2(A^{j_\alpha j_\beta})=\sum_s (q_s-\delta_{s\alpha})(g_s-q_s-\delta_{s\beta})P_{1,s}^{j_\alpha j_\beta}, \quad \text{(B33)}$$

$$P_{1,s}^{j_\alpha j_\beta}=\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta})(g_{\bar{j}_s}-\delta_{\bar{j}_sj_\alpha}-\delta_{\bar{j}_sj_\beta})}{(g_s-\delta_{s\alpha}-\delta_{s\beta})^2(g_s-\delta_{s\alpha}-\delta_{s\beta}-1)}\times\sum_{j_s\in s}D_{j_s}^{j_\alpha j_\beta}(D_{j_s}^{j_\alpha j_\beta}-D_{\bar{j}_s}^{j_\alpha j_\beta}), \quad \text{(B34)}$$

and

$$\sum_{j_s\in s}D_{j_s}^{j_\alpha j_\beta}(D_{j_s}^{j_\alpha j_\beta}-D_{\bar{j}_s}^{j_\alpha j_\beta})=D_{s_+}^{j_\alpha j_\beta}(D_{s_+}^{j_\alpha j_\beta}-D_{s_-}^{j_\alpha j_\beta})+D_{s_-}^{j_\alpha j_\beta}(D_{s_-}^{j_\alpha j_\beta}-D_{s_+}^{j_\alpha j_\beta})=(D_{s_-}^{j_\alpha j_\beta}-D_{s_+}^{j_\alpha j_\beta})^2=(D_{j_s}^{j_\alpha j_\beta}-D_{\bar{j}_s}^{j_\alpha j_\beta})^2. \quad \text{(B35)}$$

b. The expression for $\mathbf{\Delta_2^2(A^{j_\alpha j_\beta})}$

$$\Delta_2^2(A^{j_\alpha j_\beta})\equiv\sum_{c\in A}\overline{w_c^{j_\alpha j_\beta}}\Delta^2(c^{j_\alpha j_\beta})=\sum_{c\in A}\overline{w_c^{j_\alpha j_\beta}}\sum_{\mathbf{j}_s}(q_{j_s}-\delta_{\mathbf{j}_s\mathbf{j}_\alpha})(g_{j_s}-q_{\mathbf{j}_s}-\delta_{\mathbf{j}_s\mathbf{j}_\beta})\sigma^2(\mathbf{j}_s)\equiv\sum_{\mathbf{j}_s}\Delta^2(j_\alpha j_\beta j_s)\sigma^2(\mathbf{j}_s), \quad \text{(B36)}$$

where from Eq. (B10) and

$$\frac{\binom{g-2}{q-1}}{\binom{g}{q}}=\frac{q(g-q)}{g(g-1)} \quad \text{(B37)}$$

we get

$$\Delta^2(j_\alpha j_\beta j_s)=\frac{1}{\prod_d\binom{g_d-\delta_{d\alpha}-\delta_{d\beta}}{q_d-\delta_{d\alpha}}}\times\sum_{c\in A}\prod_{j_t}\binom{g_{j_t}-\delta_{j_tj_\alpha}-\delta_{j_tj_\beta}}{q_{j_t}-\delta_{j_tj_\alpha}}\times(q_{j_s}-\delta_{j_sj_\alpha})(g_{j_s}-q_{j_s}-\delta_{j_sj_\beta})$$
$$=\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta})(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta}-1)}{(g_s-\delta_{s\alpha}-\delta_{s\beta})(g_s-\delta_{s\alpha}-\delta_{s\beta}-1)}\times(q_s-\delta_{s\alpha})(g_s-q_s-\delta_{s\beta}). \quad \text{(B38)}$$

The result for the variance is

$$\Delta_2^2(A^{j_\alpha j_\beta})\equiv\sum_{\mathbf{j}_s}\Delta^2(j_\alpha j_\beta j_s)\sigma^2(\mathbf{j}_s)=\sum_s(q_s-\delta_{s\alpha})(g_s-q_s-\delta_{s\beta})P_{2,s}^{j_\alpha j_\beta}, \quad \text{(B39)}$$

where

$$P_{2,s}^{j_\alpha j_\beta}=\sum_{j_s\in s}\sigma^2(j_s)\frac{(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta})(g_{j_s}-\delta_{j_sj_\alpha}-\delta_{j_sj_\beta}-1)}{(g_s-\delta_{s\alpha}-\delta_{s\beta})(g_s-\delta_{s\alpha}-\delta_{s\beta}-1)}.$$

Combining the results of Eqs. (B33) and (B39) the total JTA variance takes the form

$$\Delta^2(A^{j_\alpha j_\beta})=\Delta_1^2(A^{j_\alpha j_\beta})+\Delta_2^2(A^{j_\alpha j_\beta})=\sum_s(q_s-\delta_{s\alpha})(g_s-q_s-\delta_{s\beta})P_s^{j_\alpha j_\beta}, \quad \text{(B40)}$$

where

$$P_s^{j_\alpha j_\beta}=P_{1,s}^{j_\alpha j_\beta}+P_{2,s}^{j_\alpha j_\beta}, \tag{B41}$$

$$P_s^{j_\alpha j_\beta}=\frac{(g_{j_s}-\delta_{j_s j_\alpha}-\delta_{j_s j_\beta})}{(g_s-\delta_{s\alpha}-\delta_{s\beta})(g_s-\delta_{s\alpha}-\delta_{s\beta}-1)}\times\left[\frac{(g_{\bar{j}_s}-\delta_{\bar{j}_s j_\alpha}-\delta_{\bar{j}_s j_\beta})}{(g_s-\delta_{s\alpha}-\delta_{s\beta})}(D_{j_s}-D_{\bar{j}_s})^2+(g_{j_s}-\delta_{j_s j_\alpha}-\delta_{j_s j_\beta}-1)\sigma^2(j_s)\right]. \tag{B42}$$

APPENDIX C: THE EXPLICIT SUBSTITUTIONS REQUIRED FOR IMPOSING CI

1. UTAs

Equation (45) introduces the CI effect by the substitution

$$P_s^{j_\alpha j_\beta}\rightarrow x_{j_\alpha j_\beta}\sigma^2(s). \tag{C1}$$

This can be achieved easily by imposing

$$P_{2s}^{j_\alpha j_\beta}\rightarrow x_{j_\alpha j_\beta}\sigma^2(s),\quad P_{1s}^{j_\alpha j_\beta}\rightarrow 0 \tag{C2}$$

which is obtained explicitly by the replacement

$$\sigma^2(\mathbf{j}_s)\rightarrow\frac{1}{2-\delta_{l_s,0}}\frac{(g_s-\delta_{s\alpha}-\delta_{s\beta})(g_s-\delta_{s\alpha}-\delta_{s\beta}-1)}{(g_{j_s}-\delta_{j_s j_\alpha}-\delta_{j_s j_\beta})(g_{j_s}-\delta_{j_s j_\alpha}-\delta_{j_s j_\beta}-1)}\times\sigma^2(s) \tag{C3}$$

for both $j_s=l_s\pm1/2$ in Eq. (19). The denominator vanishes only for $j_s=j_\alpha=1/2$ or $j_s=j_\beta=1/2$; however, these cases are excluded, since as seen from Eq. (A5) with the replacement $a\equiv\mathbf{l}_a\rightarrow\mathbf{j}_a$ for $a=s,\alpha,\beta$, they do not contribute to the variance. With the substitution (C3) we can collect relativistic UTAs ignoring CI and obtain the CI corrected variance.

This becomes particularly efficient for STAs where the superposition of many relativistic UTAs is done analytically through manipulations on occupation numbers using the partition function algebra. The working formulas for STAs involve the constant orbital quantities and we have shown that all that is required to include the effect of CI of the STA spectrum is achieved by simply replacing these constants with explicitly defined new ones. The specific replacement for STAs is specified in the next section.

2. STAs

As in Eq. (37) the extended JTA variance has two contributions

$$[\Delta^2(\Omega^{j_\alpha j_\beta})]_{\text{no CI}}=[\Delta_1^2(\Omega^{j_\alpha j_\beta})]_{\text{no CI}}+[\Delta_2^2(\Omega^{j_\alpha j_\beta})]_{\text{no CI}}, \tag{C4}$$

$$[\Delta_1^2(\Omega^{j_\alpha j_\beta})]_{\text{no CI}}=\sum_{A\in\Omega}\sum_{c\in A}\bar{I}_{c\Omega}^{j_\alpha j_\beta}(E_c^{j_\alpha j_\beta}-E_\Omega^{j_\alpha j_\beta})^2, \tag{C5}$$

$$[\Delta_2^2(\Omega^{j_\alpha j_\beta})]_{\text{no CI}}=\sum_{A\in\Omega}\sum_{c\in A}\bar{I}_{c\Omega}^{j_\alpha j_\beta}\Delta^2(c^{j_\alpha j_\beta}). \tag{C6}$$

The normalized intensities

$$\bar{I}_{c\Omega}^{j_\alpha j_\beta}=\frac{I_c^{j_\alpha j_\beta}}{\sum_{c\in\Omega}I_c^{j_\alpha j_\beta}},\quad \bar{I}_{A\Omega}^{j_\alpha j_\beta}=\frac{I_A^{j_\alpha j_\beta}}{\sum_{A\in\Omega}I_A^{j_\alpha j_\beta}} \tag{C7}$$

include the Saha Boltzmann populations, given in terms of the corresponding partition functions [7]

$$\bar{I}_{c\Omega}^{j_\alpha j_\beta}=\frac{U_c^{j_\alpha j_\beta}}{U_\Omega^{j_\alpha j_\beta}},\quad \bar{I}_{A\Omega}^{j_\alpha j_\beta}=\frac{U_A^{j_\alpha j_\beta}}{U_\Omega^{j_\alpha j_\beta}}.$$

The second contribution in Eq. (C4) can be written as

$$[\Delta_2^2(\Omega^{j_\alpha j_\beta})]_{\text{no CI}}=\sum_{A\in\Omega}\bar{I}_{A\Omega}^{j_\alpha j_\beta}[\Delta_2^2(A^{j_\alpha j_\beta})]_{\text{no CI}} \tag{C8}$$

and the substitution (C3) introduces the CI effect that covers automatically also the contribution

$$[\Delta_{11}^2(\Omega^{j_\alpha j_\beta})]_{\text{no CI}}\equiv\sum_{A\in\Omega}\bar{I}_{A\Omega}^{j_\alpha j_\beta}[\Delta_1^2(A^{j_\alpha j_\beta})]_{\text{no CI}}$$

that is already included in the working formula of the STA variance [5]. This term must therefore be subtracted.

From Eqs. (B33), and (B34) it can be shown that this term can be written in terms of $j-j$ occupation numbers as

$$[\Delta_1^2(s^{j_\alpha j_\beta})]_{\text{no CI}}=\sum_{j_s}(\Delta'_{j_s})^2(q_{j_s}-\delta_{j_s j_\alpha})(g_{j_s}-q_{j_s}-\delta_{j_s j_\beta}), \tag{C9}$$

where

$$(\Delta'_{j_s})^2=[D_{j_s}^2-D_{j_s}D_{\bar{j}_s}]\times\frac{(g_{\bar{j}_s}-\delta_{\bar{j}_s j_\alpha}-\delta_{\bar{j}_s j_\beta})}{(g_s-\delta_{s\alpha}-\delta_{s\beta})(g_{j_s}-\delta_{j_s j_\alpha}-\delta_{j_s j_\beta}-1)}. \tag{C10}$$

Equation (C9) has exactly the same form as Eq. (19) that determines the working formulas of the STA moments. Therefore in addition to the substitution of Eq. (C3) we need also to subtract from $\sigma^2(\mathbf{j}_t)$the quantity $(\Delta'_{j_t})^2$, i.e., in practice, in the STA code the substitution is

$$\sigma^2(\mathbf{j}_s)\rightarrow\frac{1}{2-\delta_{l_s,0}}\frac{(g_s-\delta_{s\alpha}-\delta_{s\beta})(g_s-\delta_{s\alpha}-\delta_{s\beta}-1)}{(g_{j_s}-\delta_{\mathbf{j}_s\mathbf{j}_\alpha}-\delta_{\mathbf{j}_s\mathbf{j}_\beta})(g_{j_s}-\delta_{\mathbf{j}_s\mathbf{j}_\alpha}-\delta_{\mathbf{j}_s\mathbf{j}_\beta}-1)}\times\sigma^2(s)-(\Delta'_{j_s})^2. \tag{C11}$$

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