Photoelectric effect in the super transition array model

A. Bar-Shalom*
ARTEP Inc., Columbia, Maryland 21045

J. Oreg
Nuclear Research Center, P.O. Box 9001, Beer Sheva 84105, Israel

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In this work we present the super transition array (STA) approach for calculating the detailed photoelectric spectra under local thermodynamic equilibrium conditions. We define the bound-free STAs and obtain analytic expressions for their moments (total intensity, average energy, and variance). It is shown that the various STAs connected with a specific photoelectron can be combined first, and then integration over the continuum is carried out only once. The various initial superconfigurations give rise to the structure of the photoelectric spectrum near the ionization edges. The details of this structure are gradually revealed by the convergence procedure inherent in the STA model. The efficiency of the method is discussed. Results of a few examples are given in comparison with the average atom method and with detailed term accounting in cases where this approach is possible. [S1063-651X(96)09308-7]

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I. INTRODUCTION

In previous works [1–5] we have presented the super transition array (STA) method for calculating emission (absorption) line spectra emitted from plasma under local thermodynamic equilibrium (LTE) conditions. The number of populated levels contributing to the spectrum may be, under these conditions, enormously high so that detailed line accounting becomes impractical. The method is based on dividing the entire bulk of transitions to groups, STAs, whose moments (total intensity, average energy, and variance) could be calculated analytically, bypassing the need for direct summation over the individual lines one by one. Each STA is then represented by a Gaussian that is convoluted with the individual, collision, and Doppler broadened line shape $P(E-E')$. The STA Gaussians construct all together the entire spectrum. The fine details of the spectrum are revealed gradually by a convergence procedure obtained by splitting each STA in turn to a number of smaller STAs until the desired spectral resolution, defined by several criteria, is reached.

Much of the power of the STA method lies in the specific definition of a STA spectral group as a collection of all the level-to-level transitions originating from a superconfiguration Ξ (a well defined set of energetically neighboring configurations) and involving a specific one-electron jump $\alpha \equiv n_\alpha l_\alpha j_\alpha \Rightarrow \beta \equiv n_\beta l_\beta j_\beta$. A STA includes therefore all the transitions between two superconfigurations written symbolically as $\Xi \Rightarrow \Xi' = \Xi - \alpha + \beta$.

In this work we apply the same approach to the calculation of photoelectric spectrum where the final transition states belong to the continuum. We will show that the moments of the bound-free STAs are easily obtained using the same working formulas as in the bound-bound case with substitutions of the radial integrals only. Two bottlenecks exist in the calculation of the bound-free spectra. One is the calculation of the continuum orbitals. For this purpose we have developed a fast algorithm based on a phase-amplitude approach [6]. The second bottleneck is the superposition of each STA with the entire continuum range. As we will show, it is possible to first collect all the STAs connected to a specific photoelectron α and superpose the result with the entire continuum by only a single convolution.

In fact, results of the STA bound-free calculations have already been presented in Refs. [2,3] in comparison with other models. However, the theory and working formulas have not been published.

In Sec. II we review the basic STA concepts and quantities required in the following sections. In Sec. III we define the bound-free STAs and obtain the working formulas for their moments. We then show in this section how the superposition of the continuum is achieved. In Sec. IV we present examples comparing STA results with average atom and with detailed term accounting calculations. A summary and discussion are given in Sec. V.

II. BACKGROUND AND NOTATION

A detailed description of the STA model is given in Refs. [1,5]. For convenience, a brief summary is given here.

A. Spectral groups

The total bound-bound spectrum can be divided into groups G of transition lines

$$S(E) = \sum_G S_G(E), \tag{1}$$

where

$$S_G(E) = \sum_{i,j \in G} N_i w_{ij} P_{ij}(E - E_{ij}). \tag{2}$$

*Permanent address: Nuclear Research Center, P. O. Box 9001, Beer Sheva 84105, Israel.

In Eq. (2) the summation is over all the transitions $i \rightarrow j$ in G, where i,j indicate the corresponding initial and final levels, N_i is the population of the initial level, w_{ij} is the transition probability given in terms of the oscillator strength f_{ij},

$$w_{ij}=\frac{\pi e^2 h}{mc} f_{ij}, \tag{3}$$

and P_{ij} is the corresponding line shape centered on the transition energy E_{ij}.

The bound-free contribution has a similar form, but here the final level j belongs to the continuum and the summation over j should be replaced by integration. We will first discuss the bound-bound spectrum and later on we will analogously treat the bound-free spectrum.

B. Group spectral moments

For normalized symmetric line profiles we obtain, for the group moments, the following expressions: intensity

$$I_G \equiv \int S_G(E)dE = \sum_{i,j \in G} N_i w_{ij}, \tag{4}$$

average energy

$$E_G \equiv \frac{\int S_G(E)E\ dE}{I_G} = \frac{\sum_{i,j \in G} N_i w_{ij} E_{ij}}{I_G}, \tag{5}$$

and variance

$$(\Delta E_G)^2 \equiv \frac{\int S_G(E)(E-E_G)^2 dE}{I_G} = \Delta_G^2 + \Delta_P^2, \tag{6}$$

where

$$\Delta_G^2 = \frac{\sum_{i,j \in G} N_i w_{ij}(E_{ij}-E_G)^2}{I_G} \tag{7}$$

is the variance of the line centers in the group G and

$$\Delta_P^2 = \int P(E-\overline{E})(E-\overline{E})^2 dE \tag{8}$$

is the variance of the individual line shape assumed equal for all the lines in the group G. The central achievement of the STA theory is the ability to obtain, under LTE conditions, analytical working formulas for the moments, bypassing the impractical summations over the huge number of transitions one by one [1,5]. In order to account for the non-Gaussian nature of P we first construct a Gaussian distribution of the line centers from the moments I_G, E_G, and Δ_G^2,

$$\Gamma(E-E_G) = \frac{I_G}{\sqrt{2\pi}\Delta_G} \exp\left[-\frac{1}{2}\left(\frac{E-E_G}{\Delta_G}\right)^2\right], \tag{9}$$

and then construct the spectrum by the convolution with the individual line shape

$$\overline{S_G}(E) = \int \Gamma(E'-E_G)P(E-E')dE' \tag{10}$$

having the same moments as the original spectrum $S_G(E)$ defined by Eq. (2).

C. STA groups

In order to complete this brief review we now define a superconfiguration and a STA group. A superconfiguration Ξ is a collection of ordinary configurations defined symbolically by the product over supershells σ,

$$\Xi \equiv \prod_{\sigma} \sigma^{Q_\sigma}. \tag{11}$$

A supershell, in turn, is the union of energetically adjacent ordinary atomic subshells $s \equiv \mathbf{j}_s \equiv n_s l_s j_s$. In Eq. (11) the superconfigurations are constructed by distributing the Q_σ electrons occupying the supershell σ among the subshells s in all possible ways subject to $\{\Sigma_{s \in \sigma} q_s = Q_\sigma\}$,

$$\sigma^{Q_\sigma} \equiv \sum_{\left\{\sum_{s \in \sigma} q_s = Q_\sigma\right\}} \prod_s \mathbf{j}_s^{q_s}. \tag{12}$$

Clearly each partition of Q_σ is an ordinary configuration. The ionization lowering in the plasma limits the number of bound orbitals as described in Ref. [1]. A specific one-electron jump $\alpha \equiv n_\alpha l_\alpha j_\alpha \Rightarrow \beta \equiv n_\beta l_\beta j_\beta$ (e.g., $2p_{3/2} \rightarrow 3d_{5/2}$) transfers each configuration $c \in \Xi$ to the configuration c' with one less electron in the α shell and one additional electron in the β shell and leaving all the other shells untouched.

A STA characterized by $G \equiv \{\Xi, \alpha \Rightarrow \beta\}$ is defined as the level-to-level transition array between all the included pairs of configurations c and c'. The level-to-level transition array between two configurations constitutes an unresolved trasition array (UTA) [7,8] and a STA is thus a collection of energetically near lying UTAs and can be viewed as the array of transitions between two superconfigurations $\Xi \Rightarrow \Xi' = \Xi - \alpha + \beta$.

The convergence procedure mentioned above splits supershells to smaller supershells according to their energy spread. For each superconfiguration in its turn, at each step, supershells that give rise to relatively well-separated configurations are preferentially split. The detailed structure of the spectrum is thus gradually revealed, yielding a converging spectrum. This procedure converges to the UTA spectra where each UTA is completely unresolved. Finally, it is appropriate, and customary, to relate separately to a larger average atom (AA) array, unifying all the STAs involving the same one-electron jump $\alpha \Rightarrow \beta$, with all possible initial superconfigurations Ξ (containing at least one configuration having at least one α orbital and at least one hole in the β shell).

D. Partition functions and LTE level populations

The partition function of a group of levels L belonging to an atom or ion containing Q bound electrons, in thermal equilibrium with a surrounding plasma at temperature T and chemical potential μ is

$$U_Q(L)=\sum_{i\in L} g_i e^{-(E_i-Q\mu)/kT}, \tag{13}$$

where g_i and E_i are the statistical weight and energy of level i. The population of a particular level i belonging to this atom or ion under these LTE conditions is

$$N_i=\frac{N}{U} g_i e^{-(E_i-Q\mu)/kT}, \tag{14}$$

where N is the total density and U is the total partition function of all ions (Q) of the specific atom in the plasma

$$U=\sum_{Q,L} U_Q(L). \tag{15}$$

The second sum in Eq. (15) is over the groups of levels L that cover the entire collection of all the bound states for each of the charge states of the atom. In the STA model we use a particular way of dividing this collection to groups, i.e., superconfigurations $L\equiv\Xi$.

The partition function can be approximated by writing the first-order level energies as

$$E_i=E_i^{(0)}+E_\Xi^{(1)}, \tag{16}$$

where $E_i^{(0)}=\Sigma_s q_s\varepsilon_s$ is the zeroth-order level energy identical for all the states within a configuration and $E_\Xi^{(1)}$ is the first-order correction taken as an average, equal for all the levels within the initial superconfiguration Ξ [the analytic expression for $E_\Xi^{(1)}$ was given explicitly in Ref. [1], Eq. (B7)]. The result for the partition function of Ξ is

$$U_Q^{(1)}(\Xi)\equiv e^{-E_\Xi^{(1)}/kT}U_Q(\Xi)=e^{-E_\Xi^{(1)}/kT}\prod_\sigma U_{Q_\sigma}(\sigma), \tag{17}$$

where

$$U_{Q_\sigma}(\sigma)=\sum_{\left\{\begin{array}{c}\text{all partitions } q_s\\ \sum_{s\in\sigma} q_s=Q_\sigma\end{array}\right\}}\prod_s \binom{g_s}{q_s} X_s^{q_s},\quad X_s\equiv e^{-[(\varepsilon_s-\mu)/kT]}. \tag{18}$$

The representation (17) of the partition function is necessary in the derivation of the STA moments [1,5]. Clearly the convergence procedure yields the correct UTA result with first-order energies in the Boltzmann factors. Finally, when averages will be required, we will make use of the LTE Fermi-Dirac probabilities

$$n_r=\frac{1}{e^{(\varepsilon_r-\mu)/kT}+1}, \tag{19}$$

where $g_r n_r$ is the average occupation number of shell r.

III. THE BOUND-FREE STA SPECTRUM

A. Bound-free STA groups

Any bound-free transition is characterized by a single-electron jump from an initial bound orbital state $\alpha\equiv n_\alpha l_\alpha j_\alpha$ to a continuum orbital state $\tilde{\varepsilon}\equiv\varepsilon lj$, where ε is the continuum orbital energy. A bound-free STA group includes all the transitions, originating from a specific superconfiguration Ξ, that belong to a specific one-electron jump $\alpha\Rightarrow\tilde{\varepsilon}$, i.e., transitions between all the pairs of levels $i\in\Xi$ and $f\in\Xi'\equiv\Xi-\alpha$ belonging to the neighboring ion, constrained by energy requirement

$$\varepsilon=h\nu-E_{fi},\quad E_{fi}=E_f-E_i, \tag{20}$$

where E_f and E_i are the first-order energies of the final and initial levels, respectively. The spectral ''line'' $i\rightarrow[f\equiv f+\tilde{\varepsilon}]$, like a regular bound-bound transition line, is collision and Doppler broadened, yielding a similar line profile $P(E-E')$ centered on $E_{i\bar{f}}=E_{fi}+\varepsilon$, which is additively shifted with ε. For a given orbital jump $\alpha\Rightarrow\tilde{\varepsilon}$ the photon spectrum follows the detailed structure of the levels i,f. The intensity of superposition of the lines having the same pair i,f but different ε, weighted by the corresponding transition probabilities, is proportional to the one-electron matrix element connecting the active orbitals α and $\bar{\varepsilon}$. This intensity decreases with ε due to the decreasing overlap of the orbitals α and $\tilde{\varepsilon}$. The spectral structure is apparent near the edges (where the photon energy is exactly sufficient to ionize the bound orbital α). At this point the continuum orbital $\tilde{\varepsilon}$ (with $\varepsilon\approx 0$) has a relatively strong overlap with α. As in the case of the bound-bound spectrum, the huge multiplicity of initially populated levels and the individual line profiles P smear the spectrum. In the bound-free case additional smearing appears due to the superposition of the lines connecting the levels i,f over the continuum range of ε. Still, the result is a characteristic structure appearing near the edges in accordance with the plasma conditions. The convergence procedure described above is extended to include the photoelectric transitions, thus revealing these detailed structures of the spectrum.

B. Bound-free STA moments

It is easy to see [1,5] that as in the bound-bound case, the moments of a bound-free STA $G\equiv\{\Xi,\alpha\Rightarrow\tilde{\varepsilon}\}$ can be written, without any approximation, in terms of the following configuration average quantities: intensity

$$I_\Xi^{(\alpha\tilde{\varepsilon})}\equiv\sum_{i,f\in G} N_i w_{i\bar{f}}=\sum_{c\in\Xi} I_c^{(\alpha\tilde{\varepsilon})}, \tag{21}$$

average energy

$$E_\Xi^{(\alpha\tilde{\varepsilon})}I_\Xi^{(\alpha\tilde{\varepsilon})}\equiv\sum_{i,f\in G} N_i w_{i\bar{f}}E_{i\bar{f}}=\sum_{c\in\Xi} I_c^{(\alpha\tilde{\varepsilon})}E_c^{(\alpha\tilde{\varepsilon})}, \tag{22}$$

and variance

$$[\Delta_\Xi^{(\alpha\tilde{\varepsilon})}]^2 I_\Xi^{(\alpha\tilde{\varepsilon})}\equiv\sum_{i,f\in G} N_i w_{i\bar{f}}(E_{i\bar{f}}-E_G)^2=\sum_{c\in\Xi}\{I_c^{(\alpha\tilde{\varepsilon})}\times[(E_c^{(\alpha\tilde{\varepsilon})}-E_G)^2+[\Delta_c^{(\alpha\tilde{\varepsilon})}]^2]\}, \tag{23}$$

where

$$I_c^{(\alpha\tilde{\varepsilon})}\equiv\sum_{i\in c,f\in c'} N_i w_{i\bar{f}}=N_c w_c^{(\alpha\tilde{\varepsilon})}, \tag{24}$$

$$N_c \equiv \sum_{i \in c} N_i, \quad w_c^{(\alpha\tilde{\varepsilon})} \equiv \sum_{i \in c, f \in c'} \frac{N_i}{N_c} w_{i\bar{f}}, \tag{25}$$

$$E_c^{(\alpha\tilde{\varepsilon})} \equiv \frac{1}{w_c^{(\alpha\tilde{\varepsilon})}} \sum_{i \in c, f \in c'} \frac{N_i}{N_c} w_{i\bar{f}} \bar{E}_{i\bar{f}}, \tag{26}$$

$$[\Delta_c^{(\alpha\tilde{\varepsilon})}]^2 \equiv \frac{1}{w_c^{(\alpha\tilde{\varepsilon})}} \sum_{i \in c, f \in c'} \frac{N_i}{N_c} w_{i\bar{f}} (\bar{E}_{i\bar{f}} - E_c^{(\alpha\tilde{\varepsilon})})^2, \tag{27}$$

and $c' = c - \alpha$. Equations (24), (26), and (27) are analogous to the definitions of the bound-bound UTA moments. In the present case, each of these UTAs connect two configurations of two neighboring ions.

The STA model uses the assumption that for usual LTE plasmas the widths of relativistic configurations are much smaller than kT. This means that the populations of the levels within a configuration c are to a very good approximation distributed statistically. In this case, as in the UTA model, the population N_l of a single level $l \in c$ is proportional to the level's statistical weight

$$N_l / N_c = g_l / g_c, \tag{28}$$

where g_l and $g_c = \Sigma_{l \in c} g_l$ are the statistical weights of level l and of the configuration c, respectively.

C. Bound-free UTA moments

The moments of the usual bound-bound UTAs between two configurations c, c' belonging to the one electron jump $\alpha \Rightarrow \beta$,

$$c \equiv \prod_s \mathbf{j}_s^{q_s}, \quad c' \equiv \prod_s \mathbf{j}_s^{q_s'}, \quad q_\alpha' = q_\alpha - 1, \quad q_\beta' = q_\beta + 1, \tag{29}$$

were obtained by Bauche-Arnoult, Bauche, and Klapisch [7,8] assuming the statistical assumption of Eq. (28). The results are given in terms of the occupation number dependence and radial integrals as follows: the UTA intensity

$$I_c^{(\alpha\beta)} = b N_c \sum_\kappa (E_c^{(\alpha\beta)})^{2\kappa-1} q_\alpha (g_\beta - q_\beta) \times \begin{pmatrix} j_\alpha & \kappa & j_\beta \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix}^2 (r_{\alpha\beta}^\kappa)^2, \tag{30}$$

(as we will see, the summation over the multipoles κ will be important for the bound-free transitions), the average energy

$$E_c^{(\alpha\beta)} = D_0 + \sum_s (q_s - \delta_{s\alpha}) D_s^{(\alpha\beta)}, \tag{31}$$

and the variance

$$(\Delta_c^{(\alpha\beta)})^2 = \sum_s (q_s - \delta_{s\alpha})(g_s - q_s - \delta_{s\beta})(\Delta_s^{(\alpha\beta)})^2, \tag{32}$$

where

$$b = \frac{8\pi^2 e a_0}{3h^4 c^3}, \tag{33}$$

$r_{\alpha\beta}^\kappa$ is the radial integral of the electric or magnetic multipole transition (of rank κ) [9],

$$D_0 = \langle \beta | h | \beta \rangle - \langle \alpha | h | \alpha \rangle \equiv \langle \beta \rangle - \langle \alpha \rangle, \tag{34}$$

h is the single-electron Hamiltonian, and $D_s^{(\alpha\beta)}$ and $\Delta_s^{(\alpha\beta)}$ involve the radial part of electrostatic interaction between the orbital s and the active orbitals α and β. The expressions for these two quantities are rather lengthy (see Refs. [6,7,5]) and will not be needed explicitly here.

In the bound-free case the electrostatic interaction between the final orbital $\tilde{\varepsilon} \equiv \beta$ and any other shell (α or s) is assumed to be zero. Following Bauche-Arnoult, Bauche, and Klapisch [7,8] it is easy to see that the bound-free UTA moments of Eqs. (24)–(27) have exactly the same form as Bauche-Arnoult, Bauche, and Klapisch's results [Eqs. (30)–(32)] with the replacements

$$q_\varepsilon = 0, \quad D_0 = \varepsilon - \langle \alpha \rangle, \tag{35}$$

$$D_s^{(\alpha\beta)} \Rightarrow D_s^{(\alpha)}, \quad \Delta_s^{(\alpha\beta)} \Rightarrow \Delta_s^{(\alpha)} \tag{36}$$

where the expressions for the radial parts $D_s^{(\alpha)}$ and $\Delta_s^{(\alpha)}$ are obtained by simply eliminating any Slater integral involving interaction of the orbital $\beta \equiv \tilde{\varepsilon}$ with any other orbital. The expressions for these quantities are given explicitly in the Appendix.

In order to account for the Pauli principle for the continuum electrons in the transition probability $\alpha \Rightarrow \beta \equiv \tilde{\varepsilon}$ the number of ''holes'' in the final continuum state $g_\varepsilon' \equiv (g_\beta - q_\beta)$ of Eq. (28) must be considered. For the LTE plasma conditions this is taken into account by Fermi-Dirac statistics

$$g_\varepsilon' = 1 - n_\varepsilon = \frac{1}{e^{-[(\varepsilon-\mu)/kT]} + 1}. \tag{37}$$

D. Working formulas for the bound-free STA moments

By substitution of the UTA moment (30) in (21) using (37) we obtain the following expressions for STA intensity:

$$I_\Xi^{(\alpha\tilde{\varepsilon})} = \sum_\kappa M_{\alpha\tilde{\varepsilon}}^\kappa \sum_{c \in \Xi} N_c q_\alpha, \tag{38}$$

$$M_{\alpha\tilde{\varepsilon}}^\kappa = b g_\varepsilon' \begin{pmatrix} j_\alpha & \kappa & j_\varepsilon \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix}^2 (r_{\alpha\tilde{\varepsilon}}^\kappa)^2 \langle E_\alpha \rangle^{2\kappa-1}. \tag{39}$$

In the derivation of Eqs. (38) and (39) we have used the fact that the average transition energy of the one-electron jump $\alpha \Rightarrow \tilde{\varepsilon}$ is much greater than the width of all the significantly populated superconfigurations. We have therefore approximated (*only in the expressions for the intensity*)

$$E_c^{(\alpha\tilde{\varepsilon})} \approx \langle E_\alpha \rangle, \tag{40}$$

where $\langle E_\alpha \rangle$ is taken as the Fermi-Dirac average energy of the total one-electron jump array $\alpha \Rightarrow \tilde{\varepsilon}$, i.e.,

$$\langle E_\alpha \rangle = \varepsilon + \left[-\langle \alpha \rangle + \sum_r n_r \langle r, \alpha \rangle (g_r - \delta_{r\alpha}) \right], \quad (41)$$

where n_r is given by Eq. (19). In Eq. (39) we could have used $E_\Xi^{(\alpha\hat{\varepsilon})}$ [Eq. (22)] for each STA instead of the average quantity (40). However, this may improve the results only if the time-consuming quantity $r_{\alpha\hat{\varepsilon}}^{\kappa}$ is calculated for each STA as well. Since the approximation of Eq. (40) was found to be very satisfactory (for the intensity calculations only) we have chosen to adopt it in our model.

The derivation of the working formulas for the bound-free STA moments now follows exactly the same steps as in the bound-bound case of Refs. [1,5]. First we express the STA moments in terms of generalized partition functions using binomial manipulations over occupation numbers. In the second step we apply recursion formulas for these generalized partition functions to remove the direct summation over configurations. The results have exactly the same functional dependence as in the bound-bound case except that the variables are different due to the replacements mentioned above. Specifically, the results for the bound-free STA moments are the intensity

$$I_\Xi^{(\alpha\tilde{\varepsilon})} = A_\Xi^\alpha \sum_\kappa M_{\alpha\tilde{\varepsilon}}^\kappa, \quad (42)$$

where

$$A_\Xi^\alpha = \frac{N}{U} X_a g_\alpha \prod_\sigma U_{Q'_\sigma}(g^\alpha), \quad (43)$$

with

$$Q'_\alpha = Q_\alpha - \delta_{\alpha\sigma}, \quad \delta_{\alpha\sigma} = \begin{cases} 1, & \alpha \in \sigma \\ 0, & \alpha \notin \sigma, \end{cases} \quad (44)$$

and the average energy

$$E_\Xi^{(\alpha\tilde{\varepsilon})} = \varepsilon + E_\Xi^{(\alpha)}, \quad (45)$$

where

$$E_\Xi^{(\alpha)} \equiv -\langle \alpha \rangle + \sum_\sigma \varepsilon_\alpha^\sigma, \quad (46)$$

$$\varepsilon_\alpha^\sigma \equiv \sum_{n=1}^{Q_\sigma} \phi_n^{\sigma(\alpha)} U_{Q_\sigma - n}(g^\alpha) / U_{Q_\sigma}(g^\alpha), \quad (47)$$

$$\phi_n^{\sigma(\alpha)} = -\sum_{s \in \sigma} g_s^\alpha D_s^{(\alpha)} (-X_s)^n, \quad (48)$$

are independent of ε. The ε independent quantities $D_s^{(\alpha)}$ are given in the Appendix and the reduced weights g_s^α are defined in general by

$$g_s^{a,b,c,\cdots} = g_s - \delta_{sa} - \delta_{sb} - \delta_{sc} - \cdots . \quad (49)$$

Since the average energy of the bound-free STA depends on $\tilde{\varepsilon}$ only through an additive constant its variance by definition will not depend on it at all. The expression for the $\tilde{\varepsilon}$ independent STA variance is

$$[\Delta_\Xi^{(\alpha)}]^2 = \sum_\sigma \Delta_\alpha^\sigma, \quad (50)$$

where

$$\Delta_\alpha^\sigma = \sum_{n=1}^{Q_\sigma} \eta_n^{\sigma,(\alpha)} U_{Q_\sigma - n}(g^\alpha) / U_{Q_\sigma}(g^\alpha) - (\varepsilon_\alpha^\sigma)^2, \quad (51)$$

with

$$\eta_n^{\sigma,(\alpha)} \equiv \sum_{m=1}^{n-1} \phi_m^{\sigma,(\alpha)} \phi_{m-n}^{\sigma,(\alpha)} + n \Phi_n^{\sigma,(\alpha)}, \quad (52)$$

$$\Phi_n^{\sigma,(\alpha)} \equiv -\sum_{s \in \sigma} g_s^\alpha D_s^{(\alpha)} (-X_s)^n, \quad (53)$$

$$D_s^{(\alpha)} \equiv \{ [D_s^{(\alpha)}]^2 + (g_s^\alpha - 1) [\Delta_s^{(\alpha)}]^2 \}, \quad (54)$$

and $D_s^{(\alpha)}$ and $\Delta_s^{(\alpha)}$ are given explicitly in the Appendix.

E. Superposition of the bound-free STAs with continuum

We can now represent the bound-free STA $\{\Xi, \alpha \Rightarrow \tilde{\varepsilon}\}$ by the Gaussian

$$\Gamma_\Xi^{\alpha\tilde{\varepsilon}}(E - E_\Xi^{(\alpha\tilde{\varepsilon})}) \equiv \sum_\kappa M_{\alpha\tilde{\varepsilon}}^\kappa G_\Xi^\alpha (E - \varepsilon), \quad (55)$$

where

$$G_\Xi^\alpha (E - \varepsilon) \equiv \frac{A_\Xi^\alpha}{\sqrt{2\pi \Delta_\Xi^{(\alpha)}}} \exp\left\{ -\frac{1}{2} \left[\frac{E - (E_\Xi^{(\alpha)} + \varepsilon)}{\Delta_\Xi^{(\alpha)}} \right]^2 \right\}. \quad (56)$$

Since the STA average energy and variance do not depend on the continuum angular momentum j_ε, a single Gaussian will represent all the STAs $\{\Xi, \alpha \Rightarrow \tilde{\varepsilon}\}$ with fixed value of ε and all possible values of j_ε,

$$\Gamma_\Xi^{\alpha\varepsilon}(E - \varepsilon) \equiv M_{\alpha\varepsilon} G_\Xi^\alpha (E - \varepsilon), \quad (57)$$

where

$$M_{\alpha\varepsilon} = \sum_{\kappa, j_\varepsilon} M_{\alpha\varepsilon}^\kappa . \quad (58)$$

The summation over κ is crucial here since the transitions, as opposed to bound-bound transitions, can reach very high energies and its high powers appearing in higher multipoles compensate for the small size of the radial integrals. These radial integrals incidentally have an energy dependence as well, making the energy dependence $E^{2\kappa+1}$. Convolving $\Gamma_\Xi^\alpha(E - \varepsilon)$ with the individual line profile $P(E - E')$ (assuming the Voigt function to be equal for all the lines within a STA) we obtain

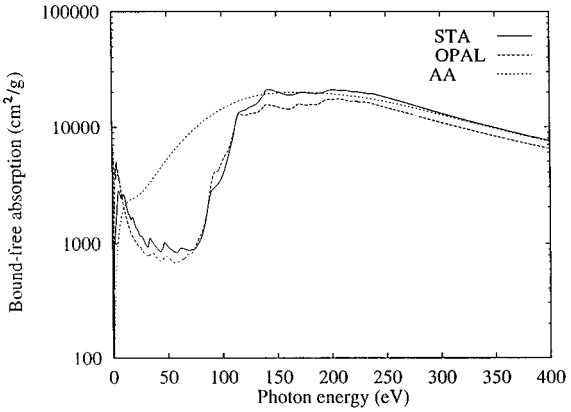

FIG. 1. Bound-free absorption of iron at $T=20$ eV and ion density $\rho=0.01$ g/cm^3. The solid, dotted, and dashed lines represent the STA, AA, and OPAL results, respectively.

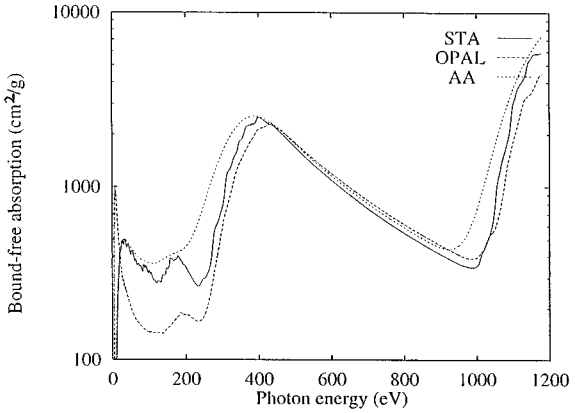

FIG. 2. Bound-free absorption of iron at $T=59$ eV and ion density $\rho=0.0127$ g/cm^3. The solid, dotted, and dashed lines represent the STA, AA, and OPAL results, respectively.

$$\overline{\Gamma}^{\alpha}_{\Xi}(E-\varepsilon)\equiv\int \Gamma^{\alpha}_{\Xi}(E'-\varepsilon)P(E-E')dE'=M_{\alpha\varepsilon}V^{\alpha}_{\Xi}(E-\varepsilon), \tag{59}$$

where

$$V^{\alpha}_{\Xi}(E-\varepsilon)\equiv\int G^{\alpha}_{\Xi}(E'-\varepsilon)P(E-E')dE' \tag{60}$$

is again a Voigt function. We can now assemble together all the $V^{\alpha}_{\Xi}(E-\varepsilon)$ connected with α and having continuum orbital energy ε:

$$\overline{\Gamma}^{\alpha}(E-\varepsilon)\equiv\sum_{\Xi}\overline{\Gamma}^{\alpha}_{\Xi}(E-\varepsilon)=M_{\alpha\varepsilon}V^{\alpha}(E-\varepsilon), \tag{61}$$

$$V^{\alpha}(E-\varepsilon)\equiv\sum_{\Xi}V^{\alpha}_{\Xi}(E-\varepsilon). \tag{62}$$

Finally, the contribution of the entire continuum to the total α array (ionizing the bound orbital α) is obtained again by the convolution

$$\Gamma^{\alpha}(E)\equiv\int V^{\alpha}(E-\varepsilon)M_{\alpha\varepsilon}d\varepsilon. \tag{63}$$

Equation (63) involves a single convolution for all the STAs involving ionization of orbital α. This procedure reduces drastically the computer time required compared to a direct approach where each STA is convolved with the continuum separately.

IV. EXAMPLES

In Fig. 1 we present the photoelectric absorption spectrum for iron at $T=20$ eV and ion density $\rho=0.01$ g/cm^3. The converged STA spectrum is compared with the AA result obtained as a special case of the STA model taking all the bound orbitals in a single supershell. It is obvious here that the AA result fails to produce the correct spectrum, whereas the converged STA spectrum reveals the detailed structure of the edges in remarkable agreement with the detailed term accounting spectrum of the OPAL computer code [10]. The bound-free absorption of iron at $T=59$ eV and ion density $\rho=0.0127$ g/cm^3 is presented in Fig. 2. The STA result here is compared again with both the AA and OPAL results. The differences between the STA and OPAL in this comparison are due to the different potentials used by the two methods, but the spectral structure agrees also here. Similar agreement is observed in the third example of Fig. 3, showing the bound-free absorption of Ge at $T=100$ eV and $\rho=0.01$ g/cm^3. It should be pointed out that similar quality of the spectral details is obtained easily by the STA method for complex spectra including a huge number of contributions far beyond the ability of the detailed term accounting approach.

V. SUMMARY AND DISCUSSION

In this work we have presented an extension of the STA model to the calculation of the bound-free spectrum. We have extended the definition of STAs to bound-free transition arrays and obtained the working formulas for calculating their moments. We have also shown that all the STAs connected with a specific photoorbital α and originating from all possible initial superconfigurations can be superposed first and thus the convolution with the continuum is done only once for each photoelectron α. This procedure, together with

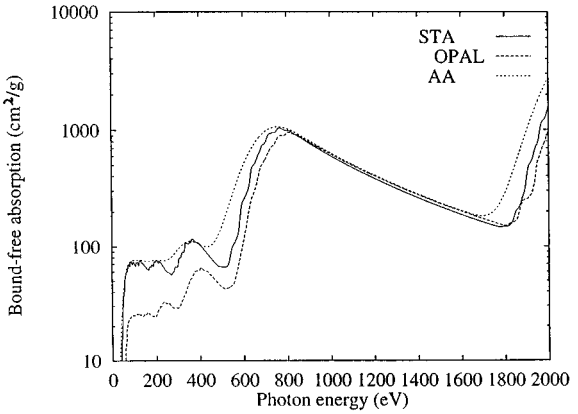

FIG. 3. Bound-free absorption of Ge at $T=100$ eV and ion density $\rho=0.01$ g/cm^3. The solid, dotted, and dashed lines represent the STA, AA, and OPAL results, respectively.

the phase-amplitude method [6] presented recently for the calculation of the continuum orbitals, combine to form a most efficient and accurate method for producing the bound-free spectrum. The convergence procedure inherent in the STA method produces also the detailed bound-free spectrum with the correct first-order energies in the Boltzmann factors for the level populations as well taking into account UTA widths and orbital relaxation (i.e., appropriate potential for each superconfiguration). Three examples are presented in which the STA spectra are compared with average atom results, which ignore the detailed structure near the ionization edges, and with detailed term accounting model implemented by the OPAL code. Clearly, as in the case of the bound-bound spectra [1,5], the STA method works as easily for much more complex bound-free cases, involving enormous amount of contributions, where the application of the detailed term accounting (the OPAL code) becomes impractical.

APPENDIX: MOMENTS OF THE BOUND-FREE UTAs

It is easy to see that the moments of the bound-free UTAs are obtained from the bound-bound expressions (29) and (30) for the average energy

$$E_c^{(\alpha\beta)}=D_0+\sum_s\,(q_s-\delta_{sa})D_s^{(\alpha\beta)} \tag{A1}$$

and the variance

$$(\Delta_c^{(\alpha\beta)})^2=\sum_s\,(q_s-\delta_{s\alpha})(g_s-q_s-\delta_{s\beta})(\Delta_s^{(\alpha\beta)})^2 \tag{A2}$$

by the substitution $\beta\Rightarrow\widetilde{\varepsilon}$, eliminating all the Slater integrals involving $\widetilde{\varepsilon}$. This is achieved by the replacements

$$D_s^{(\alpha\beta)}\Rightarrow D_s^{(\alpha)},\quad \Delta_s^{(\alpha\beta)}\Rightarrow\Delta_s^{(\alpha)}, \tag{A3}$$

where

$$D_s^{(\alpha)}\equiv-\langle s,\alpha\rangle,$$

$$\langle s,\alpha\rangle\equiv F^{\,0}(j_s,j_\alpha)-\frac{g_{j_s}}{g_{j_s}-\delta_{\alpha s}}\sum_k\begin{pmatrix} j_\alpha & k & j_s\\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}G^{\,k}(j_s,j_\alpha), \tag{A4}$$

given in terms of the direct and exchange Slater integrals $F^{\,k}(j_s,j_\alpha)$ and $G^{\,k}(j_s,j_\alpha)$, and

$$(\Delta_s^{(\alpha)})^2\equiv\mathscr{A}_s+\mathscr{B}_s+\mathscr{C}_s, \tag{A5}$$

$$\mathscr{A}_s=\sum_{k\ (\neq0)\ \text{even}}\frac{1}{(2k+1)(2j_s+1)(2j_\alpha+1)}\,[\overline{F^{\,k}}(j_s,j_\alpha)]^2, \tag{A6}$$

$$\mathscr{B}_s=\sum_{k,k'}\left[\frac{\delta_{kk'}}{(2k+1)}-\frac{1}{(2j_s+1)(2j_\alpha+1)}\right]\times\frac{1}{(2j_s+1)(2j_\alpha+1)}\,\overline{G^{\,k}}(j_s,j_\alpha)\overline{G^{\,k'}}(j_s,j_\alpha), \tag{A7}$$

$$\mathscr{C}_s=\sum_{k\ (\neq0)\ \text{even}}\sum_{k'}2\frac{(-1)^{k'}}{(2j_s+1)(2j_\alpha+1)}\times\begin{Bmatrix} j_\alpha & j_s & k'\\ j_s & j_\alpha & k\end{Bmatrix}\overline{F^{\,k}}(j_s,j_\alpha)\overline{G^{\,k}}'(j_s,j_\alpha), \tag{A8}$$

where $\overline{\mathcal{F}^k}(j_s,j_\alpha)$ and $\overline{\mathcal{G}^k}(j_s,j_\alpha)$ are the direct and exchange Slater integrals multiplied by the corresponding reduced matrix elements of the spherical harmonics C^k, as defined explicitly in the Appendix of Ref. [5].

[1] A. Bar-Shalom, J. Oreg, W. H. Goldstein, D. Shvarts, and A. Zigler, Phys. Rev. A **40**, 3183 (1989).

[2] A. Bar-Shalom, J. Oreg, and W. H. Goldstein, in *Proceedings of the IVth International Workshop on Radiative Properties of Hot Dense Matter, Sarasota, 1990*, edited by W. H. Goldstein, C. Hooper, J. Gauthier, J. Seely, and R. Lee (World Scientific, Singapore, 1990), p. 163.

[3] A. Bar-Shalom, J. Oreg, and W. H. Goldstein, in *Atomic Processes in Plasmas*, edited by Earl S. Marmar and James L. Terry, AIP Conf. Proc. No. 257, (AIP, New York, 1991).

[4] A. Bar-Shalom, J. Oreg, and W. H. Goldstein, J. Quant. Spectrosc. Radiat. Transfer **51**, 27 (1994).

[5] A. Bar-Shalom, J. Oreg, and W. H. Goldstein, Phys. Rev. E **51**, 4882 (1995).

[6] A. Bar-Shalom, J. Oreg, and M. Klapisch, Comput. Phys. Commun. **93**, 21 (1996).

[7] C. Bauche-Arnoult, J. Bauche, and M. Klapisch, Phys. Rev. A **25**, 2641 (1982).

[8] C. Bauche-Arnoult, J. Bauche, and M. Klapisch, Phys. Rev. A **31**, 2248 (1985).

[9] I. P. Grant, J. Phys. B **7**, 1459 (1974).

[10] C. A. Iglesias and F. J. Rogers, in *Proceedings of the IVth International Workshop on Radiative Properties of Hot Dense Matter, Sarasota, 1990* (Ref. [2]), p. 196.