Summation of the spectra of all partially resolved transition arrays in a supertransition array

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It is shown that the contributions of all partially resolved transition arrays (PRTAs) to the spectrum of a supertransition array (STA) may be summed by an efficient analytical method. The method is similar to the configurationally resolved super transition array method [G. Hazak and Y. Kurzweil, High Energy Density Phys. **8**, 290 (2012)] and avoids the Gaussianity assumption of the partially resolved super transition arrays method [B. G. Wilson, C. A. Iglesias, and M. H. Chen High Energy Density Phys. **14**, 67 (2015)], thus yielding an STA spectrum which is resolved down to the PRTA level.

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I. INTRODUCTION

The radiative opacity is an essential factor governing the structure and evolution of stars [1,2] as well as laboratory plasmas [3]. In plasmas containing medium to high-Z elements, at least some of the electrons remain bound to the ions even at very high temperatures and densities (e.g., iron at the center of the sun). In part of the spectral range, the opacity in these plasmas is dominated (e.g., Ref. [4]) by photoabsorption of dipolar radiative transitions between electronic states of the ions (line absorption).

The methods for evaluation of the line absorption coefficient, in hot dense plasmas, even in local thermodynamic equilibrium (LTE) conditions, which will be assumed throughout the present work, involve a compromise between the needed spectral resolution and the available computer resources. At one end stands the uncompromising method of detailed line accounting (DLA) [5], which produces a fully resolved spectrum, including all photoabsorption lines of all configuration-to-configuration transition arrays. For complex configurations with many states, the number of transitions becomes prohibitive for numerical calculations. In this case, one may turn to the unresolved transition arrays (UTA) method [6], which assumes that all lines in the spectrum of each configuration-to-configuration excitation merge into a single effective line of a Gaussian shape. The efficiency of the UTA method comes from the compact formulas for the three lowest energy moments (actually cumulants [7]) of the spectrum of each transition array [5,6], in terms of reduced matrix elements of the dipole operator, Slater integrals, and shell occupation numbers.

In some cases, the DLA resolution cannot be obtained by reasonable computer resources while the spectrum obtained by the UTA method is too crude. The method of partially resolved transition array (PRTA) [8,9] is suitable for these cases. The PRTA method allows the user to tune and balance between the computational cost and the obtained degree of resolution by choosing the mix between the DLA and UTA methods. The flexibility is obtained by applying the DLA approach to a limited subspace of chosen shells populated by "active" electrons. The effect of the electrons in the other shells ("spectators") on the spectrum of a transition array is accounted for through a Gaussian "dressing function" which broadens and shifts the lines obtained by the DLA calculation.

For heavy ions, the PRTA and UTA methods become unpractical due to the enormous number of possible configurations (and transition arrays). The supertransition-array (STA) method [5,10,11] is a powerful and efficient method which offers a further compromise allowing the summation over PRTA's or UTA's contribution to the spectrum with less computational effort at the cost of further spectral coarse graining. The efficiency of the STA method is obtained by grouping shells, with adjacent energies, into supershells, configurations into superconfigurations (SCs) and correspondingly transition arrays into STAs. The relative simplicity of the evaluation of the coarse-grained spectral absorption coefficient, in the STA method, is based on three assumptions (on top of the UTA assumptions) as follows:

(a) *The basic superconfiguration assumption.* All configurations which form a superconfiguration share the same radial potential with the same set of one-particle solutions.

(b) *The high-temperature approximation.* The spread of the energies of configurations within a superconfiguration is much smaller than the plasma temperature. In this limit, the energy in the Boltzmann factor, which determines the relative probability for a configuration within a superconfiguration, may be evaluated to zero order only, i.e., as the sum of single-electron energies in the mean potential. Electron-electron interaction energy adds a superconfigurational average factor common to all configurations within a superconfiguration. This corresponds to the use of the Gibbs-Bogoliubov-Feynman bound [12] as an estimate for the Boltzmann factor.

(c) *The unresolved Gaussian supertransition array assumption.* The spectra of all UTAs which form a STA merge into a single Gaussian shape.

With these three approximations the summation of contributions of all UTAs to a STA may be efficiently performed [5,10,11]. Explicitly, by the third approximation, one needs only to evaluate the three lowest energy cumulants of the STA spectrum. By the second approximation, the relative probabilities of configurations are the same as of those in a system of independent particles in a potential well [13]. This enables the derivation of explicit formulas for the moments (and cumulants) in terms of Slater integrals and partition functions [5,10,11] which may be evaluated by recursion relations [10] or other efficient stable methods [14–16].

The approximations in assumptions (a)–(c) are controlled by the choice of the degree of spectral coarse graining. In the extreme choice, one takes one shell in a supershell, and one configuration in a superconfiguration, and a different average radial potential with a different set of one-electron

states separately for each configuration. With this choice, the STA method coincides with the UTA method. Clearly, within the framework of the UTA model, assumptions (a)–(c) are exactly satisfied. The opposite extreme choice is that of one supershell consisting of all shells and one superconfiguration consisting of all configurations in all degrees of ionization. In Ref. [10] it was shown that with this choice, of maximum spectral coarse graining, the STA method yields the results of the average atom (AA) model.

The STA method for the summation over the UTA contributions to the spectrum was extended also to the summation over the PRTA contributions [17,18]. In this method, the effect of all "spectator" electrons in a superconfiguration on a spectral line which is obtained by the application of the DLA approach (to the limited subspace of "active" electrons) is lumped into a single Gaussian "dressing function."

Actually, the Gaussianity assumption, on which the STA method of summation is based [assumption (c) explained above], is not necessary for the summation over contributions of the UTAs spectra to an STA spectrum. As shown in Refs. [19,20] the mathematical machinery which is used for the summation of all UTA contributions to the moments of the supertransitional spectrum may be extended to allow the *direct efficient and exact* (within the framework of the high-temperature approximation explained above) summation of the spectra of all UTAs constituting the STA and sharing the same mean field.

This configurationally resolved super transition array (CRSTA) method [19,20] applies the direct summation and avoids the spectral coarse graining that comes with assumption (c). Yet it does not require any compromise beyond assumptions (a) and (b) of the STA method.

The purpose of the present work was to extend the CRSTA method by extending the method of summation of UTA's in an STA to the summation of the contribution of all PRTA's spectra to an STA spectrum. Unlike the PRSTA method [17,18] in which the dressing function is a single Gaussian, in our new method (which we call "PRCRSTA") the dressing function represents the exact summation of the contributions of all dressing functions of the PRTAs included in an STA. The result is a STA spectrum which is resolved down to the PRTA level.

The plan of the manuscript is as follows: Section II will be devoted to a brief review of the notations and some formulas of the UTA, STA, CRSTA, PRTA, and PRSTA methods, which are necessary for the rest of the presentation. In Sec. III, the derivation will be presented of the new formula for the STA spectrum which is a result of a direct summation of all PRTA's contained in the STA. The numerical implementation of the method is discussed in Sec. VI. Examples which demonstrate the capacity of the new method will be presented in Sec. IV. Section V will be devoted to summary of the paper.

II. THE UTA, STA, PRTA, AND PRSTA METHODS

Here we present a brief review of the notations and some formulas of the UTA, STA, CRSTA, PRTA, and PRSTA methods, which are necessary for the rest of the presentation.

A configuration is a many-electron atomic state in mean-field approximation. The state is described by the occupation numbers of the shells (single-electron states in the mean-field generated by all other electrons). It is customary to represent a (relativistic) configuration by the symbols $C = \prod_s (n_s l_s j_s)^{q_s^C}$, where a shell is characterized by the principal quantum number, n_s; the orbital angular momentum of the large component in the Dirac wave function, l_s; and the total orbital+spin angular momentum j_s; q_s^C is the occupation number of the s shell in the C configuration. The sum of q_s^C in all shells participating in a configuration is Q:

$$\sum_{s\in C} q_s^C = Q \tag{1}$$

(i.e., Q is the total number of bound electrons in the configuration).

The average configurational energy [21], E_C, is

$$E_C = E_C^{(0)} + \delta E_C^{(1)}, \tag{2}$$

where $E_C^{(0)}$ is the zero-order energy,

$$E_C^{(0)} = \sum_s q_s^C \varepsilon_s, \tag{3}$$

$\varepsilon_s \equiv \varepsilon_{n_s l_s j_s}$ is the eigenvalue of the single-particle equation with the radial mean field V and one-particle no-potential Dirac Hamiltonian, h_D,

$$[h_D + V]\phi_{nljm} = \varepsilon_{nlj}\phi_{nljm}, \tag{4}$$

and $\delta E_C^{(1)}$ is the first-order correction to the interaction energy, i.e., the difference between electron-electron interaction energy and the energy in the mean field,

$$\delta E_C^{(1)} = \frac{1}{2}\sum_s \sum_r q_s^C \left(q_r^C - \delta_{rs}\right)\Omega_{sr} + \sum_s q_s^C \left(\langle s| - V(r) - \frac{Z}{r}|s\rangle\right), \tag{5}$$

Configurations, being based on single-particle states, are degenerated. Different electron couplings lift the degeneracy and split the configurational energy. Consequently, each configuration-to-configuration excitation comprises many photoabsorption lines. In complex configurations the number of lines in a configuration-to-configuration transition array becomes formidable and the task of summing over the contributions of all these photoabsorption lines to the spectrum becomes unrealistic. The UTA model [5,6] avoids the task of summation by assuming that all lines in the spectrum of each configuration-to-configuration excitation merge into a single effective line of a Gaussian shape. With this assumption, the task of summing over all photoabsorption lines is replaced by the task of evaluating three energy-moments of the spectrum, from which the Gaussian shape is constructed. The approximation of the UTA model is in the assumption that the center of gravity, E_C^{ab}, and width, Δ_C^{ab}, fully represent the line shape. Explicitly, the approximation is in the assumption that the line shape of a dipole transition array C^{ab} from a configuration C to another configuration C' by electron jumping from the shell a to the shell b is of the form $\frac{1}{\sqrt{2\pi}\Delta_C^{ab}} \exp\left[-\frac{1}{2}\left(\frac{E-E_C^{ab}}{\Delta_C^{ab}}\right)^2\right]$, i.e., the spectral distribution of the UTA C^{ab} is proportional to the

function:

$$F^{ab}_{C,\mathrm{UTA}}(E) = q_a^C\left(g_b - q_b^C\right)\int \frac{1}{\sqrt{2\pi}\,\Delta^{ab}_C} \times \exp\left[-\frac{1}{2}\left(\frac{E' - E^{ab}_C}{\Delta^{ab}_C}\right)^2\right] P^{ab}_C(E - E')dE', \tag{6}$$

where P^{ab}_C represents the effective line shape which reflects the natural linewidth and the effect of broadening due to interaction with plasma microfield. q_a^C,q_b^C are the occupation numbers of the active shells a and b, and g_b is the degeneracy of the b shell. The specific form of the line shape P^{ab}_C may have a decisive effect on the measured spectrum. However, the present work focuses on a different aspect of spectrum evaluation; methods for summations of contributions of transition arrays to the spectrum, therefore in the rest of this paper, in order to simplify the presentation, we shall avoid the line shape issue [i.e., assume $P^{ab}_C(E - E') = \delta(E - E')$]; however, see some other possible line shapes described in Sec. IV.

The formulas for the center of gravity of the UTA, E^{ab}_C, and the UTA variance, $(\Delta^{ab}_C)^2$, may be represented in the following compact form [11]:

$$E^{ab}_C = (\langle b\rangle - \langle a\rangle) + \sum_s \left(q_s^C - \delta_{sa}\right) D^{ab}_s, \tag{7}$$

$$\left(\Delta^{ab}_C\right)^2 = \sum_s \left(q_s^C - \delta_{sa}\right)\left(g_s - q_s^C - \delta_{sb}\right)(\Delta^2)^{ab}_s, \tag{8}$$

where D^{ab}_s and $(\Delta^2)^{ab}_s$ coincide with the notation of Appendix A in Ref. [11].

In these formulas, q_s^C is the occupation number of the s shell in the initial configuration C. All other constants are independent of the occupation numbers.

In some cases the coarsening of the spectrum by the UTA approach is too extreme since the spectrum cannot be represented as a single Gaussian function, yet the large number of lines in a transition array prohibits summation of the contribution of all photoabsorption lines. The method of PRTA [8] is fitted to treat these cases.

In the PRTA method, one starts by the DLA solution of the isolated "active" transition, e.g., for two active shells the transition reads:

$$(n_a l_a j_a)^{q_a^C}(n_b l_b j_b)^{q_b^C} \rightarrow (n_a l_a j_a)^{q_a^C - 1}(n_b l_b j_b)^{q_b^C + 1}. \tag{9}$$

The DLA solution yields N^{ab}_{line} (q_a^C,q_b^C) transition lines. We denote the energy of the initial level by u_j, the transition energy by E^{ab}_j, the degeneracy by g^{ab}_j, and the (normalized) strength of a line in the DLA solution by s^{ab}_j. We also use the notation $\bar{C}_{ab} = \prod_{s\neq a,b}(n_s l_s j_s)^{q_s^C}$ for the "configuration" which does not include the active shells.

In the PRTA approach, one assumes that each of the N^{ab}_{line} lines is dressed by a function which represents the effect of all the spectator electrons, i.e., the spectrum of the PRTA is

$$F^{ab}_{C,\mathrm{PRTA}}(E) = \sum_{j=1}^{N^{ab}_{\mathrm{line}}} g^{ab}_j s^{ab}_j e^{-\beta u_j}\frac{1}{\sqrt{2\pi}\,\Delta^{ab}_{\bar{C}_{ab}}} \times \exp\left[-\frac{1}{2}\left(\frac{E - E^{ab}_{\bar{C}_{ab}} - E^{ab}_j}{\Delta^{ab}_{\bar{C}_{ab}}}\right)^2\right], \tag{10}$$

where $E^{ab}_{\bar{C}_{ab}}$, $\Delta^{ab}_{\bar{C}_{ab}}$ represent the effect of the spectators on the shift of the center of gravity of the UTA C^{ab} and on its variance, i.e.,

$$E^{ab}_{\bar{C}_{ab}} = E^{ab}_C - (\langle b\rangle - \langle a\rangle) + D^{ab}_a = \sum_{s\neq a,b} q_s D^{ab}_s, \tag{11}$$

$$\left(\Delta^{ab}_{\bar{C}_{ab}}\right)^2 = \sum_{s\neq a,b}\left(q_s^C - \delta_{sa}\right)\left(g_s - q_s^C - \delta_{sb}\right)(\Delta^2)^{ab}_s. \tag{12}$$

As mentioned in the Introduction, for many electron ions, the PRTA and UTA methods become unpractical due to the enormous number of possible configurations. These cases may be treated by the STA method, which is briefly reviewed below. A superconfiguration, Ξ, is defined by a specific partitioning of the bound electrons between supershells (a group of energetically adjacent atomic shells). Each specific partitioning of shell occupation within the supershells represents a configuration which is contained within the superconfiguration. The dipolar supertransition-array (denoted by Ξ^{ab}) is defined as the group of all the transition arrays in which an electron jumps from the shell a in all configurations C, contained in the superconfiguration Ξ, to a shell b. By this definition, Ξ^{ab} represents the group of all the transition arrays C^{ab} in which the initial configuration C is contained in the superconfiguration Ξ.

The specification of a superconfiguration, Ξ, is by the group of supershells, $\{s\}_\sigma$, denoted by $\{\{s\}_\sigma\}$ and by the group of numbers $\{Q_\sigma\}$ which assign to each supershell a total population, Q_σ.

The spectral distribution of the STA Ξ^{ab} is obtained by summing over contributions from all transition arrays each with the statistical weight which represents the probability for the initial configuration C of the transition array C^{ab}. Accepting the assumptions of the UTA approach and the basic assumption of the STA method described in the Introduction [namely assumption (a) that all configurations which form a superconfiguration share the same radial potential with the same set of one-particle solutions], the superconfigurational spectral distribution is proportional the function:

$$F^{ab}_{\Xi,\mathrm{UTA}}(E) = \frac{1}{Z_\Xi}\sum_{C\in\Xi} g_C \exp\left[-\beta(E_C - Q\mu)\right] q_a^C\left(g_b - q_b^C\right) \times \frac{1}{\sqrt{2\pi}\,\Delta^{ab}_C}\exp\left[-\frac{1}{2}\left(\frac{E' - E^{ab}_C}{\Delta^{ab}_C}\right)^2\right], \tag{13}$$

where

$$Z_\Xi = \sum_{C\in\Xi} g_C \exp\left[-\beta(E_C - Q\mu)\right] \tag{14}$$

is the superconfigurational grand-canonical partition function.

Further accepting also the high-temperature approximation, valid in the case that the spread of the energies of configurations within a superconfiguration is much smaller than the plasma temperature [assumption (b) of the STA and PRSTA approach described in the introduction] one can replace the statistical sum of an arbitrary configurational quantity, ξ_C:

$$\langle \xi_C \rangle = \sum_{C\in\Xi} \exp\left(-\beta E_C\right)\xi_C = \sum_{C\in\Xi} \exp\left[-\beta\left(E_C^{(0)} + \delta E_C^{(1)}\right)\right]\xi_C \tag{15}$$

by

$$\langle \xi_C \rangle \simeq \exp\left(-\beta\left\langle \delta E_C^{(1)}\right\rangle\right)\sum_{C\in\Xi} \exp\left(-\beta E_C^{(0)}\right)\xi_C, \tag{16}$$

where $\langle \delta E_C^{(1)} \rangle$ is the weighted average of $\delta E_C^{(1)}$[10]. Note that the approximation(16) just uses the Gibbs-Bogoliubov-Feynman bound [12,22] as an estimate for the Boltzmann factor.

With this approximation, the superconfigurational spectral distribution of Eq. (13) becomes

$$\begin{aligned} F^{ab}_{\Xi,\mathrm{UTA}}(E) \simeq F^{ab,HT}_{\Xi,\mathrm{UTA}}(E) &= \frac{\exp\left(-\beta\left\langle \delta E_C^{(1)}\right\rangle\right)}{\exp\left(-\beta\left\langle \delta E_C^{(1)}\right\rangle\right) Z^{(0)}_\Xi} \\ &\times \sum_{C\in\Xi} g_C \exp\left[-\beta\left(E_C^{(0)} - Q\mu\right)\right] q_a^C \left(g_b - q_b^C\right) \\ &\times \frac{1}{\sqrt{2\pi}\Delta^{ab}_C} \exp\left[-\frac{1}{2}\left(\frac{E' - E^{ab}_C}{\Delta^{ab}_C}\right)^2\right] \\ = \frac{1}{Z^{(0)}_\Xi}\sum_{C\in\Xi} g_C \exp\left[-\beta\left(E_C^{(0)} - Q\mu\right)\right] q_a^C \left(g_b - q_b^C\right) \\ &\times \frac{1}{\sqrt{2\pi}\Delta^{ab}_C} \exp\left[-\frac{1}{2}\left(\frac{E' - E^{ab}_C}{\Delta^{ab}_C}\right)^2\right], \end{aligned} \tag{17}$$

where $Z^{(0)}_\Xi$ is the the zero-order partition function:

$$Z^{(0)}_\Xi = \sum_{C\in\Xi} g_C \exp\left[-\beta\left(E_C^{(0)} - Q\mu\right)\right]. \tag{18}$$

The STA method reiterates the UTA assumption about the Gaussianity of the transition array and applies it also to the super-transition-array by assuming that the superconfigurational spectral distribution $F^{ab}_{\Xi,\mathrm{UTA}}(E)$ has a Gaussian form, i.e.,

$$F^{ab}_{\Xi,\mathrm{UTA}}(E) \approx A^{ab}_\Xi \exp\left[-\frac{1}{2}\left(\frac{E - E^{ab}_\Xi}{\Delta^{ab}_\Xi}\right)^2\right] \equiv F^{ab}_{\Xi,\mathrm{STA}}(E). \tag{19}$$

The formulas for the amplitude, center of gravity, and width of the superconfigurational spectrum A^{ab}_Ξ, E^{ab}_Ξ, Δ^{ab}_Ξ as sums over UTA contributions are described in Ref. [11]. These formulas may also be derived by Fourier transform of Eqs. (19) and (17) with respect to E and comparing the three lowest terms in the Taylor expansion around the origin of the transform variable τ. (For details, see Ref. [19].)

In Refs. [19,20], the mathematical machinery which is used for the summation of all UTA contributions to the moments of the supertransitional spectrum, was extended to allow the *direct efficient and exact* summation of the spectra of all UTAs constituting the STA and sharing the same mean field. In this method, called the CRSTA method, the summation in Eq. (17) is analytically performed without the aid of the Gaussianity assumption of Eq. (19), i.e., from the three assumptions (1)–(3) of the STA method described in the Introduction, one needs only assumptions (1) and (2). The result is a spectrum which reflects all the UTA details as in $F^{ab,HT}_{\Xi,\mathrm{UTA}}(E)$, i.e.,

$$F^{ab}_{\Xi,\mathrm{CRSTA}}(E) = F^{ab,HT}_{\Xi,\mathrm{UTA}}(E). \tag{20}$$

In Refs. [17,18], the method of PRTA was extended also to enable summation of the contribution of all PRTA to an STA. The result is called PRSTA. Here we describe a simple version of this method. Consider a superconfiguration

$$\Xi = (n_a l_a j_a)^{q_a^C} (n_b l_b j_b)^{q_b^C} \prod_k (\sigma_k)^{Q_k}, \tag{21}$$

(where σ_k is the k supershell and Q_k is the k supershell population) and a supertransition Ξ^{ab}:

$$\begin{aligned} &(n_a l_a j_a)^{q_a^C} (n_b l_b j_b)^{q_b^C} \prod_k (\sigma_k)^{Q_k} \\ &\quad\rightarrow (n_a l_a j_a)^{q_a^C - 1} (n_b l_b j_b)^{q_b^C + 1} \prod_k (\sigma_k)^{Q_k}. \end{aligned} \tag{22}$$

Start by the DLA solution of the isolated "active" transition:

$$(n_a l_a j_a)^{q_a^C} (n_b l_b j_b)^{q_b^C} \rightarrow (n_a l_a j_a)^{q_a^C - 1} (n_b l_b j_b)^{q_b^C + 1}. \tag{23}$$

The DLA solution yields $N^{ab}_{\mathrm{line}}\ (q_a^C, q_b^C)$ lines. Denote the energy of the initial level, the transition energy, degeneracy, and (normalized) strength of a line in the DLA solution by $u_j, E^{ab}_j, g^{ab}_j, s^{ab}_j$, respectively, and also $\bar{\Xi}_{ab} = \prod_k (\sigma_k)^{Q_k}$. As in the case of UTA summation [Equation (17)] one finds that the superconfigurational spectrum is proportional to the sum (in the high-temperature approximation) of contributions from all PRTA's,

$$\begin{aligned} F^{ab}_{\Xi,\mathrm{PRTA}}(E) &= \frac{1}{Z_\Xi} \sum_{\bar{C}_{ab}\in\bar{\Xi}_{ab}} g_{\bar{C}_{ab}} \exp[-\beta(E_{\bar{C}_{ab}} - Q_{\bar{C}_{ab}}\mu)] \\ F^{ab}_{C,\mathrm{PRTA}}(E) \simeq F^{ab,HT}_{\Xi,\mathrm{PRTA}}(E) &= \frac{1}{Z^{(0)}_{\bar{\Xi}_{ab}}} \sum_{\bar{C}_{ab}\in\bar{\Xi}_{ab}} g_{\bar{C}_{ab}} \\ &\times \exp\left[-\beta\left(E^{(0)}_{\bar{C}_{ab}} - Q_{\bar{C}_{ab}}\mu\right)\right] F^{ab}_{C,\mathrm{PRTA}}(E). \end{aligned} \tag{24}$$

By the explicit form of $F^{ab}_{C,\mathrm{PRTA}}(E)$ [Eq. (10)], the Gaussianity assumption reads:

$$\begin{aligned} F^{ab}_{\Xi,\mathrm{PRTA}}(E) \simeq F^{ab}_{\Xi,\mathrm{PRSTA}}(E) &= \sum_{j=1}^{N^{ab}_{\mathrm{line}}} g^{ab}_j s^{ab}_j e^{-\beta u_j} \\ &\times \phi_{\bar{\Xi}_{ab},\mathrm{STA}}\left(E - E^{ab}_{\bar{\Xi}_{ab}} - E^{ab}_j\right), \end{aligned} \tag{25}$$

$$\phi_{\bar{\Xi}_{ab},\mathrm{STA}}\left(E'\right) = A^{ab}_{\bar{\Xi}_{ab}} \exp\left[-\frac{1}{2}\left(\frac{E'}{\Delta^{ab}_{\bar{\Xi}_{ab}}}\right)^2\right]. \tag{26}$$

The formulas for the amplitude, center of gravity, and width of the superconfigurational dressing function, $A^{ab}_{\bar{\Xi}_{ab}}$, $E^{ab}_{\bar{\Xi}_{ab}}$, $\Delta^{ab}_{\bar{\Xi}_{ab}}$ as sums over UTA contributions may be obtained in a way similar to the derivation of the formulas for $A^{ab}_{\Xi_{ab}}$, $E^{ab}_{\Xi_{ab}}$, $\Delta^{ab}_{\Xi_{ab}}$, i.e., Fourier transform of Eqs. (26) and (25) with respect to E and comparing the three lowest terms in the Taylor expansion around the origin of the transform variable τ.

III. PR-CRSTA

As in the case of STA, the Gaussianity approximation [Eqs. (25) and (26)] (which is implicit in the derivation of the PRSTA method) is not necessary. The summation in Eq. (24) may be performed directly without this approximation, i.e., of the three assumptions (a)–(c) described in the Introduction, one needs only assumptions (a) and (b) and in parallel to formula (20) we have

$$F^{ab}_{\Xi,\text{PR-CRSTA}}(E) = F^{ab}_{\Xi,\text{PRTA}}(E). \tag{27}$$

Using this relation in Eq. (24) one gets:

$$\begin{aligned}
F^{ab}_{\Xi,\text{PR-CRSTA}}(E) &= F^{ab}_{\Xi,\text{PRTA}}(E) = \frac{1}{Z_{\bar{\Xi}_{ab}}} \sum_{\bar{C}_{ab}\in\bar{\Xi}_{ab}} g_{\bar{C}_{ab}} \exp\left[-\beta\left(E_{\bar{C}_{ab}} - Q_{\bar{C}_{ab}}\mu\right)\right] F^{ab}_{C,\text{PRTA}}(E) \\
&= \frac{1}{Z_{\bar{\Xi}_{ab}}} \sum_{j=1}^{N^{ab}_{\text{line}}} g^{ab}_j s^{ab}_j e^{-\beta u_j} \sum_{\bar{C}_{ab}\in\bar{\Xi}_{ab}} g_{\bar{C}_{ab}} \exp\left[-\beta\left(E_{\bar{C}_{ab}} - Q_{\bar{C}_{ab}}\mu\right)\right] \frac{1}{\sqrt{2\pi}\,\Delta^{ab}_{\bar{C}_{ab}}} \exp\left[-\frac{1}{2}\left(\frac{E - E^{ab}_{\bar{C}_{ab}} - E^{ab}_j}{\Delta^{ab}_{\bar{C}_{ab}}}\right)^2\right] \\
&\simeq \frac{\exp\left[-\beta\left(\left\langle\delta E^{(1)}_{\bar{C}_{ab}}\right\rangle\right)\right]}{\exp\left[-\beta\left(\left\langle\delta E^{(1)}_{\bar{C}_{ab}}\right\rangle\right)\right] Z^{(0)}_{\bar{\Xi}_{ab}}} \sum_{j=1}^{N^{ab}_{\text{line}}} g^{ab}_j s^{ab}_j e^{-\beta u_j} \sum_{\bar{C}_{ab}\in\bar{\Xi}_{ab}} g_{\bar{C}_{ab}} \exp\left[-\beta\left(E^{(0)}_{\bar{C}_{ab}} - Q_{\bar{C}_{ab}}\mu\right)\right] \\
&\quad \times \frac{1}{\sqrt{2\pi}\,\Delta^{ab}_{\bar{C}_{ab}}} \exp\left[-\frac{1}{2}\left(\frac{E - E^{ab}_{\bar{C}_{ab}} - E^{ab}_j}{\Delta^{ab}_{\bar{C}_{ab}}}\right)^2\right] \\
&= \frac{1}{Z^{(0)}_{\bar{\Xi}_{ab}}} \sum_{j=1}^{N^{ab}_{\text{line}}} g^{ab}_j s^{ab}_j e^{-\beta u_j} \sum_{\bar{C}_{ab}\in\bar{\Xi}_{ab}} g_{\bar{C}_{ab}} \exp\left[-\beta\left(E^{(0)}_{\bar{C}_{ab}} - Q_{\bar{C}_{ab}}\mu\right)\right] \frac{1}{\sqrt{2\pi}\,\Delta^{ab}_{\bar{C}_{ab}}} \exp\left[-\frac{1}{2}\left(\frac{E - E^{ab}_{\bar{C}_{ab}} - E^{ab}_j}{\Delta^{ab}_{\bar{C}_{ab}}}\right)^2\right].
\end{aligned} \tag{28}$$

In the third line of (28) we have used the high-temperature approximation. Using the Fourier transform to the Gaussian UTA, one gets:

$$\begin{aligned}
F^{ab}_{\Xi,\text{PR-CRSTA}}(E) &= \frac{1}{Z^{(0)}_{\bar{\Xi}_{ab}}} \sum_{j=1}^{N^{ab}_{\text{line}}} g^{ab}_j s^{ab}_j e^{-\beta u_j} \sum_{\bar{C}_{ab}\in\bar{\Xi}_{ab}} g_{\bar{C}_{ab}} \exp\left[-\beta\left(E^{(0)}_{\bar{C}_{ab}} - Q_{\bar{C}_{ab}}\mu\right)\right] \\
&\quad \times \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{2}\frac{1}{\hbar^2}\left(\Delta^{ab}_{\bar{C}_{ab}}\right)^2\tau^2 + i\frac{1}{\hbar}E^{ab}_{\bar{C}_{ab}}\tau - i\frac{1}{\hbar}\left(E - E^{ab}_j\right)\tau\right] d\tau \\
&= \sum_{j=1}^{N^{ab}_{\text{line}}} g^{ab}_j s^{ab}_j e^{-\beta u_j} \phi_{\bar{\Xi}_{ab},\text{PR-CRSTA}}\left(E - E^{ab}_j\right).
\end{aligned} \tag{29}$$

i.e., the line dressing function for the j line is as follows:

$$\phi_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(E') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(\tau) e^{-i\frac{1}{\hbar}E'\tau} d\tau, \tag{30}$$

where

$$\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(\tau) = \frac{1}{Z^{(0)}_{\bar{\Xi}_{ab}}} \sum_{\bar{C}_{ab}\in\bar{\Xi}_{ab}} g_{\bar{C}_{ab}} \exp\left[-\beta\left(E^{(0)}_{\bar{C}_{ab}} - Q_{\bar{C}_{ab}}\mu\right) - \frac{1}{2}\frac{1}{\hbar^2}\left(\Delta^{ab}_{\bar{C}_{ab}}\right)^2\tau^2 + i\frac{1}{\hbar}E^{ab}_{\bar{C}_{ab}}\tau\right]. \tag{31}$$

The quantities Q, $\left(\Delta^{ab}_{\bar{C}_{ab}}\right)^2$, $E^{(0)}_{\bar{C}_{ab}}$, and $E^{ab}_{\bar{C}_{ab}}$ in the exponent depend on the occupation, q^C_s, of the shells, s, participating in $\bar{C}_{ab}$ and are the sum over contributions from these shells. This property and the specific form of dependence on q^C_s simplifies the summation $\sum_{\bar{C}_{ab}\in\bar{\Xi}_{ab}}$ and the evaluation of the line dressing function $\phi_{\bar{\Xi}_{ab},\text{PR-CRSTA}}$ by the CRSTA method as described in Refs. [19,20] and already implemented in our CRSTA code. (Some details of the implementation are described in Appendix A).

Explicitly, using the formulas for $E^{(0)}_{\bar{C}_{ab}}, \Delta^{ab}_{\bar{C}_{ab}}$, and $E^{ab}_{\bar{C}_{ab}}$, the dressing function for the case of *single* supershell may be written as:

$$\begin{aligned}\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(\tau) &= \frac{1}{Z^{(0)}_{\bar{\Xi}_{ab}}}\tilde{\phi}_{\bar{Q}}(\tau) = \frac{1}{Z^{(0)}_{\bar{\Xi}_{ab}}}\sum_{\bar{C}_{ab}\in\bar{\Xi}_{ab}} g_{\bar{C}_{ab}} \exp\left[-\beta\left(E^{(0)}_{\bar{C}_{ab}} - Q_{\bar{C}_{ab}}\mu\right) - \frac{1}{2}\frac{1}{\hbar^2}\left(\Delta^{ab}_{\bar{C}_{ab}}\right)^2\tau^2 + i\frac{1}{\hbar}E^{ab}_{\bar{C}_{ab}}\tau\right] \\ &= \frac{1}{Z^{(0)}_{\bar{\Xi}_{ab}}}\left\{\sum_{\Sigma q_s = Q - q_a - q_b s\neq a,b}\prod_s \binom{g_s}{q_s^C}\left(X_s\left[\varepsilon_s - D^{ab}_s i\tau/\hbar\beta\right)\right]^{q_s^C} e^{-\frac{1}{2}\frac{1}{\hbar^2}\left(q_s^C-\delta_{sa}\right)\left(g_s-q_s^C-\delta_{sb}\right)\left(\Delta^2\right)^{ab}_s\tau^2}\right\} \\ &= \frac{1}{Z^{(0)}_{\bar{\Xi}_{ab}}}\left\{\sum_{\Sigma q_s^C = Q - q_a - q_b s\neq a,b}\prod_s f_s(g_s,q_s,\tau)\right\}, \end{aligned} \tag{32}$$

where, for a given set of shells, a configuration which belongs to a superconfiguration $\bar{\Xi}_{ab}$ with $\overline{Q} = Q - q_a - q_b$ bound electrons is determined by the condition $\sum q_s^C = \overline{Q}$ and we have used the shorthand

$$\begin{aligned} f_s\left(g_s,q_s^C,\tau\right) &= \binom{g_s}{q_s^C}\left[X_s\left(\varepsilon_s - D^{ab}_s i\tau/\hbar\beta\right)\right]^{q_s^C} \\ &\times e^{-\frac{1}{2}\frac{1}{\hbar^2}\left(q_s^C-\delta_{sa}\right)\left(g_s-q_s^C-\delta_{sb}\right)\left(\Delta^2\right)^{ab}_s\tau^2}. \end{aligned} \tag{33}$$

Note that f_s is a single-shell function.

The term in the curled brackets in Eq. (32), $\tilde{\phi}_{\overline{Q}} = \sum_{\Sigma q_s=\overline{Q}}\prod_{s\in\sigma} f_s(g_s,q_s^C,\tau)$, may be efficiently evaluated by a variation of the combinatorial methods developed for the STA method (see Appendix B).

Note that the single Gaussian form of the supertransitional dressing function as used in Ref. [17] is recovered by the short-time approximation of formula (31), i.e., by the expansion around $\tau = 0$, up to second order in τ (see Eqs. (22)– (27) in Ref. [19]). In the frequency domain this means that the Gaussian dressing function used in Ref. [17] may be obtained by applying a coarse-graining procedure to the full form in Eq. (31) which preserves the signature of all UTA's. The numerical effort required for its evaluation, and the Fourier transform to energy variable, is similar to the effort required for the coarse-grained Gaussian form of the supertransitional dressing function [Eq. (26)] [19].

IV. EXAMPLES

We have demonstrated the PR-CRSTA method for the evaluation of the spectra by two examples as follows:

Example 1:

The transition

$$\begin{aligned}&\text{Fe } X\ [Ne]3s^2 3p^3 3d^1(4s\ldots 6p)^1 \\ &\quad\rightarrow [Ne]3s^2 3p^2 3d^2(4s\ldots 6p)^1,\end{aligned}$$

in iron at temperature of 40 eV.

Example 2:

The transition

$$\begin{aligned}&\text{Fe } XI\ [Ne]3s^2 3p^1 3d^1(4s\ldots 6p)^2 \\ &\quad\rightarrow [Ne]3s^2 3p^0 3d^2(4s\ldots 6p)^2,\end{aligned}$$

in iron at temperature of 50 eV.

In these two examples, the spectator electrons are distributed in the Rydberg shells $4s\ldots 6p$. In Ref. [18], as well as in the present work, these shells are grouped into a single supershell.

For both examples, we have calculated the PR-CRSTA spectrum, $F^{ab}_{\Xi,\text{PR-CRSTA}}(E)$. The transition lines, in the spectrum, were synthetically broadened by a convolution with a Gaussian of full width at half maximum of 0.1 eV. In the time domain, this convolution operation turns into a multiplication of the function $\tilde{\phi}_{\overline{Q}}(\tau)$ by the factor $\exp\left(-\frac{1}{2}\frac{1}{\hbar^2}\alpha^2\tau^2\right)$.

As mentioned before, the treatment of various mechanisms for line broadening is out of the scope of the present work; nevertheless, a short comment is in order: The treatment in time domain, as applied in our new method, allows a convenient implementation of various line broadening. The simplest example is the Lorenzian broadening function, where in time domain $\tilde{\phi}_{\overline{Q}}(\tau)$ should be multiplied by the factor $\exp\left(-\frac{1}{\hbar}\gamma\tau\right)$. The result of the multiplication by the two factors $\exp\left(-\frac{1}{2}\frac{1}{\hbar^2}\alpha^2\tau^2\right)$ and $\exp\left(-\frac{1}{\hbar}\gamma\tau\right)$ leads, in frequency domain, to the Voigt line profile which is routinely used in opacity calculations [23]. The Voigt represents the combined effect of Doppler shifts due to thermal motion of the radiators and electron impact, in cases where the interval between impact events is longer then radiation wavelength and therefore these effects act independently. It is well known that the Voigt has an unphysical inverse-square asymptotic behavior. In the case where the separation between lines is large enough, this unphysical tail can lead to a significant error in the evaluated opacity. It was recently suggested that the cure for this problem would be by the use of various truncation methods, applied in the frequency domain [23]. The treatment in the time domain as applied in our new method opens the way to another convenient approach which does not suffer from the unphysical large-tail problem, by the application of collision narrowed line profiles which in the time domain have the form $\exp\left\{-\frac{1}{\hbar}\gamma\tau - \frac{1}{\hbar^2}\frac{1}{\beta^2}\alpha^2[\beta\tau - 1 + \exp(-\beta\tau)]\right\}$ [24]. We plan to investigate this approach in a future work.

The quantities E^{ab}_j, $g^{ab}_j s^{ab}_j e^{-\beta u_j}$ were calculated by use of the SCO-RCG code [18]. The dressing function $\phi_{\bar{\Xi}_{ab},\text{PR-CRSTA}}$ and the spectrum, $F^{ab}_{\Xi,\text{PR-CRSTA}}(E)$, were evaluated by the CRSTA code which was adapted for this task. Note that since $\phi_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(E - E^{ab}_j)$ is simply the shifted $\phi_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(E)$ function, it has to be calculated only once for all the lines. The combination of results from the two codes, SCO-RCG and CRSTA, should be done with some care since SCO-RCG

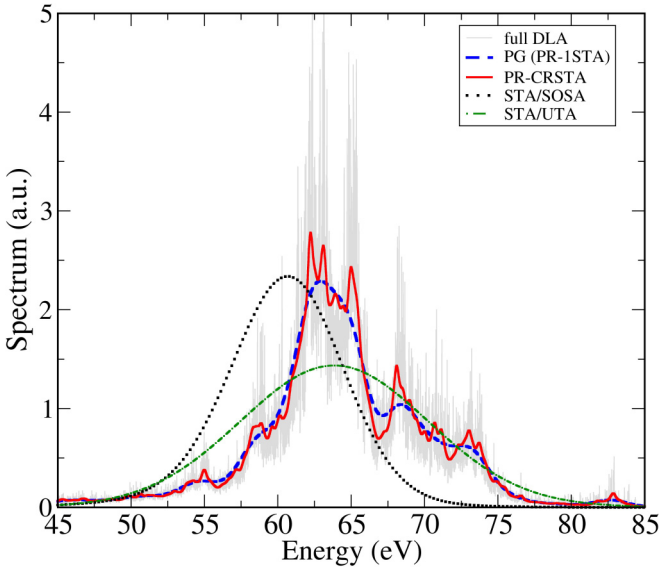

FIG. 1. Spectrum (a.u.) vs. energy (eV) of example 1, calculated by various methods.

is a nonrelativistic code, while CRSTA is a relativistic code. This means that the transition array $3p \to 3d$, as treated in the SCO-RCG code, when treated by the CRSTA code, comprises of three relativistic transitions: $3p_{1/2} \to 3d_{3/2}$, $3p_{3/2} \to 3d_{3/2}$, and $3p_{3/2} \to 3d_{5/2}$. In order to match the two descriptions, the function $\phi_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(E - E_j^{ab})$ is calculated using the following averaged relativistic quantities. The quantity $E^{ab}_{\bar{C}_{ab}}$ in Eq. (31) is replaced by the quantity $\langle E^{3p3d}_{\bar{C}_{ab}} \rangle = \sum_{s \neq a,b} q_s \langle D_s^{3p3d} \rangle$, where

$$\langle D_s^{3p3d} \rangle = \tfrac{1}{3}\left(D_s^{3p_{1/2}3d_{3/2}} + D_s^{3p_{3/2}3d_{3/2}} + D_s^{3p_{3/2}3d_{5/2}}\right).$$

Also, since the three relativistic transition lines statistics are independent, the UTA variance $(\Delta^{3p3d}_{\bar{C}_{ab}})^2$ is calculated by

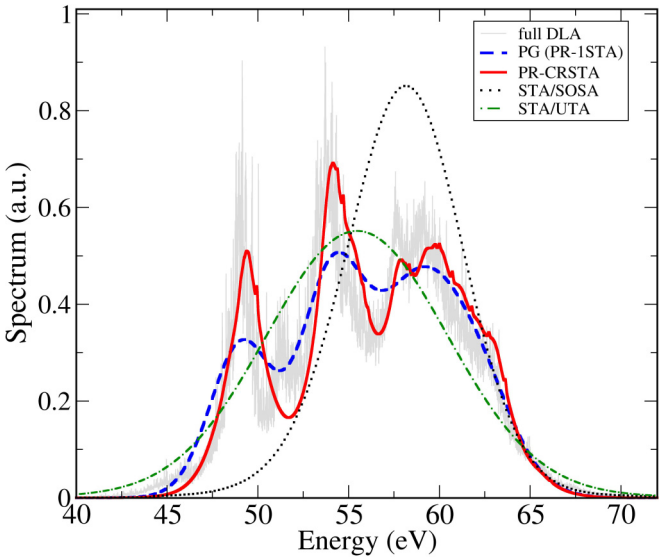

FIG. 2. Spectrum (a.u.) vs. energy (eV) of example 2, calculated by various methods.

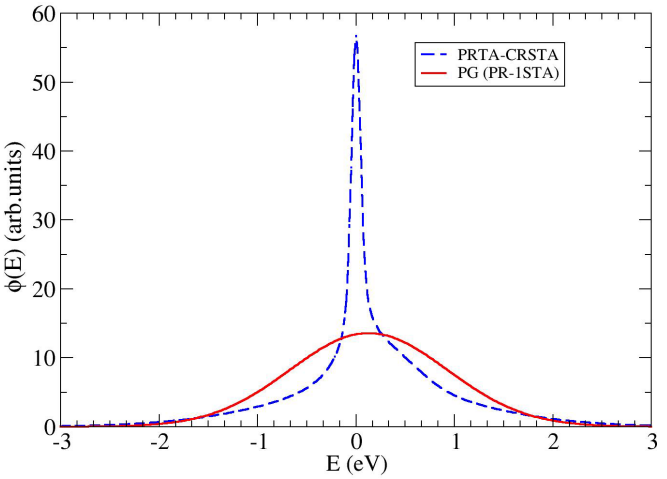

FIG. 3. Dressing function (arb. units) vs. energy(eV) for example 1. Comparison between the fully resolved dressind function (dashed-blue) and PG 1STA dressing function (solid-red).

the average variance

$$\begin{aligned}\left(\Delta^{3p3d}_{\bar{C}_{ab}}\right)^2 = {} & \tfrac{1}{3}\left[\left(\Delta^{3p_{1/2}3d_{3/2}}_{\bar{C}_{ab}}\right)^2 + \left(\Delta^{3p_{3/2}3d_{3/2}}_{\bar{C}_{ab}}\right)^2 + \left(\Delta^{3p_{3/2}3d_{5/2}}_{\bar{C}_{ab}}\right)^2\right] \\ & + \frac{1}{3}[(\delta E^{3p_{1/2}3d_{3/2}} - \delta\overline{E})^2 + (\delta E^{3p_{3/2}3d_{3/2}} - \delta\overline{E})^2 \\ & + (\delta E^{3p_{3/2}3d_{5/2}} - \delta\overline{E})^2],\end{aligned}$$

where δE^{ab} is the UTA shift of the transition $a \to b$ and $\delta\overline{E} = \frac{1}{3}[\delta E^{3p_{1/2}3d_{3/2}} + \delta E^{3p_{3/2}3d_{3/2}} + \delta E^{3p_{3/2}3d_{5/2}}]$.

The spectra of the two examples were evaluated by different methods as shown in Figs. 1 and 2. The methods relevant to the present discussion are the full DLA of all transition arrays which are compatible with the two examples (gray solid line), the Pain-Gilleron PRSTA calculation (dashed-blue line, denoted as "PG" in the figure), and the PRCRSTA calculation (solid red line). As expected, the PRCRSTA spectra are more detailed and closer to the DLA spectra. Figures 3 and 4 compare the Gaussian dressing functions used by the

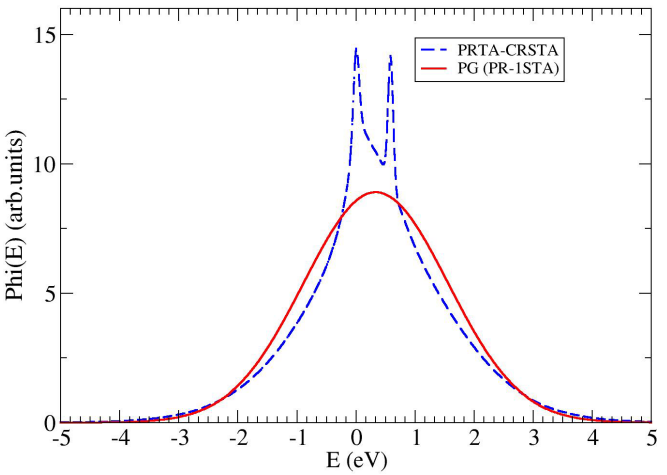

FIG. 4. The dressing function (arb. units) vs. energy(eV) for example 2. Comparison between the fully resolved dressind function (dashed-blue) and PG 1STA dressing function (solid-red).

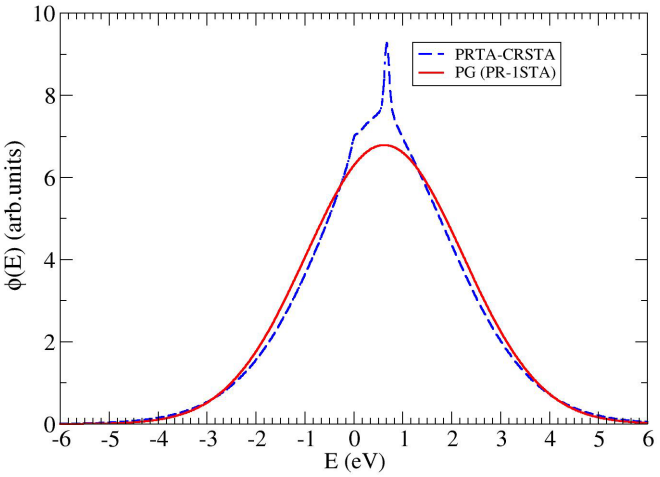

FIG. 5. Dressing function (arb. units) vs. energy (eV) for three spectator electrons calculated by PR-CRSTA (dashed-blue) and PG 1STA method (solid-red).

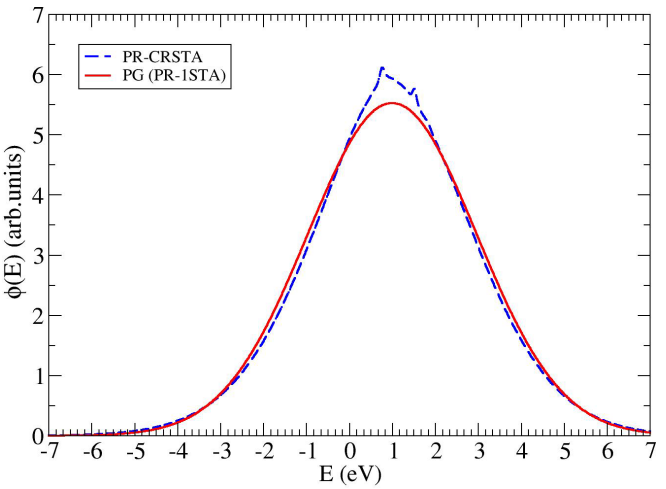

FIG. 6. Dressing function (arb. units) vs. energy (eV) for four spectator electrons calculated by PR-CRSTA (dashed-blue) and PG 1STA method (solid-red).

PRSTA method to the dressing functions of the PRCRSTA. The PRCRSTA dressing function, carries the signature of the separate effect of each spectator which explains the capability of this method to generate some of the details of the DLA spectrum which are not generated by the PRSTA method.

It is interesting to note that the PR-CRSTA dressing function becomes more close to a Gaussian shape, as the PG method assumes, as the number of electron spectators is increased, as shown in Figs. 5 and 6. Therefore, it seems that the PG method is a good approximation to the dressing function if there are more than three spectator electrons.

V. SUMMARY

The various existing tools for the theoretical evaluation of spectra in hot dense plasmas in LTE include the DLA [5], UTA [6], STA [5,10,11], PRTA [8], and PRSTA [17,18] methods. A skillful choice of tools from this rich list allows a well-balanced compromise between the needed resolution in the evaluated spectrum and the available computer resources. The UTA and PRTA are methods for evaluating the spectrum of a transition array, in cases where the DLA method is out of reach due to large number of lines in the transition array. These methods are based on a Gusssianity assumption. The UTA method assumes that the spectrum of the transition array has a functional form of a single Gaussian. The PRTA method assumes that the lines evaluated by DLA calculation accounting only for active electrons are dressed by a Gaussian broadening and shifting function which accounts for the effect of the spectator electrons. The STA is a method for summing over contributions of UTA's and the PRSTA is a method for summing over the contributions of all PRTA to the STA spectrum. The STA method assumes that the spectrum of the STA has a functional form of a single Gaussian, similarly, the PSRTA method assumes that the sum of the PRTA dressing functions of all PRTA's in a STA merge into a single Gaussian superconfigurational dressing function. The CRSTA method [19,20] relies on all the STA assumptions except for the Gaussianity assumption. Instead it applies a direct efficient method for the summation of all contributions of UTA's to the STA spectrum. The result is an STA spectrum which is resolved down to the UTA level.

The current work extends the CRSTA method and develops an efficient method for the summation of all PRTA's to the spectrum of the STA. The result is an STA spectrum which is resolved down to the PRTA level. The results shown in Figs. 1 and 2 demonstrate the capability of this method in following some of the spectral details of the fully resolved DLA calculations.

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APPENDIX A: NUMERICAL IMPLEMENTATION

The algorithm for calculating the PR-CRSTA spectrum, $F^{ab}_{\Xi,\text{PR-CRSTA}}(E)$ in Eq. (28), comprises of the following steps:

(1) Define a suitable temporal equimeshed grid $\{\tau_j = j\triangle\tau\}$, as is explained below.

(2) Calculate $\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(\tau_j)$ using the formulas of Eqs. (B4) and (B5) in Appendix B.

(3) Apply FFT to obtain the tabulated dressing function $\phi_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(E_j)$.

(4) Evaluate the sum: $\sum_{j=1}^{N^{ab}_{\text{line}}} g^{ab}_j s^{ab}_j e^{-\beta u_j} \phi_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(E - E^{ab}_j)$, for each required photon energy E, using the tabulated dressing function $\phi_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(E_j)$.

In step 2, of the abovementioned algorithm, $\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(\tau)$ should be evaluated on a temporal grid. We explain now how to choose, properly, the temporal grid parameters. The grid $\{\tau_j = j\triangle\tau\}$ is defined on the interval $[0, T_{\max}]$. $T_{\max}$ is estimated as the time where the function $\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(\tau)$ is already significantly decayed, i.e., $\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(T_{\max})/\ \tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(0) \leqslant \varepsilon \ll 1$. This condition is

ensured if

$$\prod_{s\in\sigma} e^{-\frac{1}{2\hbar^2}\min_{\Sigma q_s=\overline{Q}}\{(q_s^C-\delta_{sa})(g_s-q_s^C-\delta_{sb})(\Delta_s^{ab})^2\}T_{\max}^2} \leqslant \varepsilon.$$

Note that

$$\min\left\{(g_s-1)\left(\Delta_s^{ab}\right)^2\right\} \leqslant \min_{\Sigma q_s=\overline{Q}}\left\{\left(q_s^C-\delta_{sa}\right)\left(g_s-q_s^C-\delta_{sb}\right)\left(\Delta_s^{ab}\right)^2\right\},$$

therefore, a rough, but sufficient, estimation yields:

$$T_{\max}\approx\sqrt{|\ln\varepsilon|/\min\left\{(g_s-1)\left(\Delta_s^{ab}\right)^2\right\}}.$$

If there are included more broadening effects, like electron-impact, Doppler or synthetic broadening, then, $\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(\tau)$ includes more temporal decaying exponents, and $T_{\max}$ can be reduced correspondingly.

The temporal equimeshed gridpoints number, N_p, should be determined to cover the entire energy bandwidth of $\phi_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(E)$. The energy bandwidth of $\phi_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(E)$ is the energy range of the spectator electrons configurations transition energies:

$$E_{\bar{C}_{ab}}^{ab}=\sum_{s\neq a,b} q_s D_s^{ab}.$$

The corresponding *full* bandwidth, B_{full}^{ab}, is

$$B_{\text{full}}^{ab}=\max_{\Sigma q_s=\overline{Q}}\left\{\sum_{s\neq a,b} q_s D_s^{ab}\right\}-\min_{\Sigma q_s=\overline{Q}}\left\{\sum_{s\neq a,b} q_s D_s^{ab}\right\}. \quad \text{(A1)}$$

The bandwidth B_{full}^{ab} can be estimated in a simpler way than Eq. (A1), as

$$B_{\text{full}}^{ab}\approx\sum_{\overline{s}=1..\overline{n}_s} g_{\overline{s}} D_{\overline{s}}^{ab}-\sum_{\underline{s}=1..\underline{n}_s} g_{\underline{s}} D_{\underline{s}}^{ab},$$

where $\{g_{\overline{s}} D_{\overline{s}}^{ab}\}$ and $\{g_{\underline{s}} D_{\underline{s}}^{ab}\}$ are descending and ascending lists of the multiplications $\{q_s D_s^{ab}\}$ and $\overline{n}_s$ and $\underline{n}_s$ satisfy the conditions:

$$\sum_{\overline{s}=1..\overline{n}_s-1} g_{\overline{s}} \leqslant Q \leqslant \sum_{\overline{s}=1..\overline{n}_s} g_{\overline{s}},$$

$$\sum_{\underline{s}=1..\underline{n}_s} g_{\underline{s}} D_{\underline{s}}^{ab} \leqslant Q \leqslant \sum_{\underline{s}=1..\underline{n}_s+1} g_{\underline{s}} D_{\underline{s}}^{ab}.$$

The maximal time interval $\Delta\tau$ is estimated as

$$\Delta\tau=\frac{\pi}{B_{\text{full}}^{ab}}.$$

The full bandwidth is usually too large, since there are many configurations which barely contribute to the spectrum. It is therefore recommended to use an effective bandwidth which is as large as several times the STA variance of the transition energies $\{E_{\bar{C}_{ab}}^{ab}\}$. Recall that the STA cumulants can be obtained by the short time approximation of the function $\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(\tau)$ [19]:

$$\left(\Delta_{\Xi}^{ab}\right)^2=\left[\frac{\partial^2}{\partial(-i\tau)^2}\ln\left(\frac{\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(\tau)}{\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(0)}\right)\right]_{\tau=0}.$$

Numerically, we evaluate $\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(\tau)$ for n gridpoints, $\{\tau_i\}$, around $\tau=0$ and fit a polynomial $p(\tau)=\sum_{j=0..n-1} a_j(-i\tau)^j$ to the function $\ln[\frac{\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(\tau_j)}{\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(0)}]$. This fit yields the variance, i.e., $\left(\Delta_{\Xi}^{ab}\right)^2=a_2$. The effective bandwidth, B_{eff}^{ab}, is estimated as

$$B_{\text{eff}}^{ab}=m\Delta_{\Xi}^{ab},$$

where $m=4..8$. Correspondingly, the time interval is

$$\Delta\tau=\frac{\pi}{B_{\text{eff}}^{ab}}.$$

In summary, for both bandwidth estimations, the number of temporal gridpoints should satisfy:

$$N_p\geqslant T_{\max}/\Delta\tau.$$

We should note here that the above-mentioned choices of temporal grid parameters is not necessarily the optimal.

APPENDIX B: THE SUMMATION

The calculation of the function $\tilde{\phi}_{\bar{\Xi}_{ab},\text{PR-CRSTA}}(\tau)$, in Eq. (32), requires an efficient method to calculate the generalized partition functions:

$$U_Q(\tau)\equiv\sum_{\Sigma q_s^C=Q}\prod_{s=1}^{N} f_s\left(g_s,q_s^C,\tau\right). \quad \text{(B1)}$$

An analytical, efficient and numerically stable method to calculate this sum was proposed by Gilleron and Pain [15] for the special case of $\tau=0$. In this case, Gilleron and Pain proved that $U_Q(\tau=0)$ is the value of the coefficent Q of the generating polynomial :

$$G(z)=\prod_{s=1}^{N}(1+X_s(\varepsilon_s)z)^{g_s}=\prod_{s=1}^{N}\left(\sum_{j=0}^{g_s}\binom{g_s}{J}X_s(\varepsilon_s)^j z^j\right)$$
$$=\prod_{s=1}^{N}\left(\sum_{j=0}^{g_s} f_s(g_s,j,\tau=0)z^j\right)=\sum_{Q}U_Q(0)z^Q,$$

where

$$U_Q(0)=\frac{1}{Q!}\frac{\partial^Q}{\partial z^Q}G(z)\Big|_{z=0}=\sum_{\Sigma q_s^C=Q}\prod_{s=1}^{N} f_s\left(g_s,q_s^C,0\right). \quad \text{(B2)}$$

Using the same proof of Gilleron and Pain [15], it is easy to see that $U_Q(\tau)$ can be obtained from the generalized generating polynomial:

$$G(z,\tau)=\prod_{s=1}^{N}\left(\sum_{j=0}^{g_s} f_s(g_s,j,\tau)z^j\right)=\sum_{Q}U_Q(\tau)z^Q, \quad \text{(B3)}$$

where $U_Q(\tau)$ is obtained, similarly to $U_Q(0)$, as

$$U_Q(\tau)=\frac{1}{Q!}\frac{\partial^Q}{\partial z^Q}G(z,\tau)\Big|_{z=0}=\sum_{\Sigma q_s^C=Q}\prod_{s=1}^{N} f_s\left(g_s,q_s^C,\tau\right).$$

Therefore, $U_Q(\tau)$ can be efficiently calculated from the recursive fomula of Eq.(25) in Ref. [15], which originally derived for $U_Q(0)$, while substituting $\binom{g_N}{j}[X_N(\varepsilon_N)]^j \mapsto f_N(g_N,j,\tau)$, i.e.:

$$U_Q(\tau) \equiv u_{Q:N}(\tau) = \sum_{j=1..Q} u_{Q-j:N-1}(\tau) f_N(g_N,j,\tau)\Theta(g_N-Q),$$
$$u_{Q:0}(\tau) = \delta_{Q,0}, \tag{B4}$$

where Θ is the heavy side function.

Finally, for the case of a superconfiguration Ξ that contains electronic population $\{U_{Q_s}\}_{s=1..N_s}$, of N_s supershells, the generalized partition function, $U_\Xi(\tau)$, is obtained from the multiplication of the single supershell generalized partition functions:

$$U_\Xi(\tau) = \prod_{s=1}^{N_s} U_{Q_s}(\tau), \tag{B5}$$

where $U_{Q_s}(\tau)$ are calculated using Eq. (B4).

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