

# Operator technique for calculating superconfiguration-averaged quantities of atoms in plasmas

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An operator technique for performing superconfiguration averages is presented. This technique is applicable in the calculation of local thermodynamic equilibrium (LTE) spectral moments as well as average rates for the various atomic processes in non-LTE collisional radiative models. It is shown that for any moment or rate the configuration average polynomials, in the shell occupation numbers, can be regarded as derivative operators that average over superconfigurations when acting on their corresponding partition functions. The superconfiguration-averaged quantities are obtained as generalized partition functions for which a set of recursion formulas is presented allowing a short calculation path. Using this technique, analytic expressions for thermodynamical quantities, such as internal energy and specific heat, are obtained, taking into account orbital relaxation and first-order energies in the Boltzmann factors. This allows for the supertransition array code to yield accurate and consistent data for the equation of state used in hydrodynamic simulations, in addition to radiative properties. [S1063-651X(97)00305-X]

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## I. INTRODUCTION

In recent years we have developed the supertransition array (STA) model for the interpretation of bound-bound [1–5] and bound-free [6] spectra of local thermodynamic equilibrium (LTE) plasmas. The model divides the entire spectrum into STA's, between pairs of superconfigurations where each superconfiguration (SC) is a specific collection of near lying configurations. The spectrum of each STA is represented by a Gaussian constructed from the array moments, i.e., the total intensity, the average energy, and variance. The details of the total spectrum, obtained by superposition of all the STA's, are revealed gradually by splitting each SC to smaller SC's until convergence is reached.

In addition, in order to interpret non-LTE plasma regimes we have recently developed the non-LTE model SCROLL (superconfiguration radiative collisional) [7]. This model is aimed at including a high number of excited states in a collisional radiative model where detailed level or configuration accounting becomes impractical. Our approach is based on representing SC's as effective levels and solving rate equations for their populations. Again the details are revealed by splitting SC's until convergence is reached. The rates for the various atomic processes populating and depopulating the effective levels are calculated by averaging over the corresponding SC's assuming Boltzmann population *within SC's only*. This assumption is relaxed by the convergence procedure. The SC average rates are calculated for all the atomic processes: collisional and radiative excitations and ionizations and their inverse recombination and deexcitation processes, autoionization and spontaneous emission.

Much of the strength of the two models lies in the exact analytical expressions for the STA moments and for the SCROLL average rates. This point was discussed in some

detail in previous works [1–7] but the rigorous theory and the specific formulas and relations used in these models were not presented so far. In this work we present an operator technique for deriving analytic expressions for averages over a SC for any  $n$ -body scalar interaction. All the mentioned above quantities are special cases. We show that the configuration averages, which are polynomials in the shell occupation numbers, can be regarded as derivative operators that give the SC average when acting on the corresponding partition function. These operations are formulated as a "partition function algebra." The analytic expressions are obtained in terms of generalized partition functions (GPF's), for which a variety of recursion formulas are derived. These formulas allow a most efficient calculation path of the many required GPF's using other GPF's that had already been calculated in previous steps. The technique can be also applied to obtain analytic expressions for thermodynamical quantities taking into account orbital relaxation and first-order energies. As an example we obtain the analytic expressions for the internal energy, specific heat, and electronic pressure. The specific heat and electronic pressure involve derivatives of partition functions which, as will be shown, are expressed in terms of GPF's as well.

In Sec. II we introduce the required background and notations. In Sec. III we present the algebra for deriving SC averages as GPF's, and in Sec. IV we derive various useful relations between GPF's of different kinds that serve as shortcuts in their calculation. Finally, in Sec. V we apply this technique to obtain analytic expressions for the plasma optimized internal energy, specific heat, and pressure.

## II. DEFINITIONS AND NOTATIONS

### A. Supershell and superconfiguration

A supershell  $\sigma$ , is the union of energetically adjacent ordinary atomic subshells  $s \in \sigma$ ,  $s \equiv \mathbf{j}_s \equiv n_s l_s j_s$ . A SC,  $\Xi$  of a  $Q$  electron ion, is defined by its supershell occupation num-

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bers  $Q_\sigma$ . It is a collection of ordinary configurations written symbolically by the product over supershells,

$$\Xi \equiv \prod_\sigma \sigma^{Q_\sigma}, \quad \sum_\sigma Q_\sigma = Q. \quad (1)$$

In Eq. (1), the SC is constructed by distributing the  $Q_\sigma$  electrons occupying supershell  $\sigma$  among the subshells in all possible ways subject to  $\{\sum_{s \in \sigma} q_s = Q_\sigma\}$ :

$$\sigma^{Q_\sigma} \equiv \sum_{\left\{ \sum_{s \in \sigma} q_s = Q_\sigma \right\}} \prod_s \mathbf{j}_s^{q_s}. \quad (2)$$

Clearly, each partition of  $Q$  in Eqs. (1) and (2) is an ordinary configuration  $C$ ,

$$C \equiv \prod_s \mathbf{j}_s^{q_s} = \prod_\sigma \prod_{s \in \sigma} \mathbf{j}_s^{q_s}. \quad (3)$$

### B. SC partition function

The partition function (PF) of the SC,  $\Xi$ , occupied by  $Q$  electrons is defined [1] as a summation over all levels  $i$  of all configurations  $C \in \Xi$ :

$$U_\Xi \equiv \sum_{C \in \Xi} \sum_{i \in C} g_i e^{-(E_i - Q\mu)/kT} \equiv \sum_{C \in \Xi} U_C, \quad (4)$$

where  $g_i$  and  $E_i$  are the statistical weight and energy, respectively, of level  $i$ , and  $\mu$  is the chemical potential.

Using the zero-order energies and an average first-order energy correction [2]:

$$E_C^{(0)} = E_i^{(0)} = \sum_s q_s \epsilon_s, \quad (5)$$

$$E_C^1 = \sum_s q_s \epsilon_s + \Delta E_\Xi^1, \quad (6)$$

common to all  $i \in \Xi$ . The expression for  $\Delta E_\Xi^1$  will be given later [see Eq. (86)]. With these expressions we can write

$$U_C \equiv e^{-\Delta E_\Xi^1/kT} g_C e^{-(E_C^{(0)} - Q\mu)/kT}, \quad (7)$$

where the configuration statistical weight is given by the product of binomials

$$g_C \equiv \sum_{i \in C} g_i = \prod_{s \in C} \binom{g_s}{q_s} \quad (8)$$

and  $g_s = 2j_s + 1$ , are the statistical weights (degeneracies) of shells  $s$ . Equation (4) reduces then to

$$U_\Xi \equiv U_\Xi(g) = e^{-\Delta E_\Xi^1/kT} U_\Xi^{(0)}(g), \quad (9)$$

where

$$U_\Xi^{(0)}(g) \equiv \prod_{\sigma \in \Xi} U_\sigma(g), \quad (10)$$

$$U_\sigma(g) \equiv U_{Q_\sigma}(g) \equiv \sum_{\left\{ \sum_{s \in \sigma} q_s = Q_\sigma \right\}} \prod_{s \in \sigma} \binom{g_s}{q_s} X_s^{q_s}, \quad (11)$$

and

$$X_s \equiv e^{-(\epsilon_s - \mu)/kT}. \quad (12)$$

The notation  $(g)$  stands for the set of statistical weights  $\{g_s\}$  of the various shells. This set must be explicit, since as we will see later, the GPF's are defined formally as identical to Eqs. (9) and (10) but with a more general set of integers  $(g')$ , which are not necessarily the shells' statistical weights.

### C. SC-SC arrays and active orbitals

An array connecting two SC's,  $\Xi$  and  $\Xi'$ , can be identified solely by specifying the initial  $\Xi$  and the orbital jumps that lead to  $\Xi'$ . Each  $C' \in \Xi'$  is thus obtained from a specific  $C \in \Xi$  through these electron jumps.

## III. SUPERCONFIGURATION AVERAGES AS GENERALIZED PARTITIONS FUNCTIONS

### A. Configuration averages

It was shown [8] that the configuration average of any scalar  $n$ -body operator  $A$  is a polynomial of degree  $n$  in shell occupation numbers  $q_s$  of the initial configuration  $C$ . The polynomials of the configuration-averaged spectral moments [8–10] and of the configuration-averaged atomic processes rates [7] are all special case examples. The most general form of such polynomials is given in terms electrons and holes occupation numbers  $q_s$  and  $h_s \equiv (g_s - q_s)$ , respectively, as

$$\langle A \rangle_{CC'} = \sum_{\{m,n\}} e_{\{m,n\}} \prod_{r,s} q_r^{m_r} h_s^{n_s}, \quad (13)$$

where the curly brackets in  $\{m,n\} \equiv \{n\}, \{m\}$  denote two sets of exponents for all the various shells, with  $\{m\}_r = m_r$  for  $q_r$  and  $\{n\}_s = n_s$  for  $h_s = (g_s - q_s)$ . The coefficients  $e_{\{m,n\}}$  are independent of the  $q$ 's and are specific for each particular process, moment, and the specific active orbitals. In all practical cases, as in Refs. [1–10], only a few terms have non-zero coefficients. For the SC-rate averages, each initial configuration  $C$  is weighted by its partial Boltzmann population

$$\bar{N}_C = \frac{U_C(g)}{U_\Xi(g)} \quad (14)$$

so that the SC average of  $A$  is

$$\langle A \rangle_{\Xi\Xi'} = \frac{1}{U_\Xi(g)} \sum_{\substack{C \in \Xi \\ C' \in \Xi'}} \langle A \rangle_{CC'} U_C(g). \quad (15)$$

In the STA moments [1] the weights are the initial configuration populations and the radiative transition probabilities. For an  $a \rightarrow b$  orbital jump, this contributes the additional factor  $q_a(g_b - q_b)$  to the polynomial  $\langle A \rangle_{CC'}$ , and the normalization factor is changed accordingly.

### B. Shell averaging operators

The SC averages of the shell occupation numbers are defined by

$$\begin{aligned} \langle q_s \rangle_{\Xi} &\equiv \frac{1}{U_{\Xi}} \sum_{c \in \Xi} q_s U_C, \\ \langle q_r q_s \cdots \rangle_{\Xi} &\equiv \frac{1}{U_{\Xi}} \sum_{c \in \Xi} (q_r q_s \cdots) U_C. \end{aligned} \quad (16)$$

A similar definition holds for holes by the substitutions  $q \rightarrow h$ .

We define shell  $s$  electron and hole averaging operators  $\hat{q}_s$  and  $\hat{h}_s$  by

$$\hat{q}_s \equiv X_s \frac{\partial}{\partial X_s}, \quad \hat{h}_s \equiv g_s - X_s \frac{\partial}{\partial X_s}. \quad (17)$$

From Eqs. (11) and (12), it is easily recognized that

$$\begin{aligned} \hat{q}_s U_{\Xi}(g) &= \langle q_s \rangle_{\Xi} U_{\Xi}(g), \\ \hat{h}_s U_{\Xi}(g) &= \langle h_s \rangle_{\Xi} U_{\Xi}(g). \end{aligned} \quad (18)$$

As shown later, these relations between derivatives and averages play a role in the analytic derivation of thermodynamical quantities. From Eq. (10) we obtain

$$\begin{aligned} \langle q_s \rangle_{\Xi} &= \langle q_s \rangle_{\sigma_s} \equiv \frac{\hat{q}_s U_{\sigma_s}(g)}{U_{\sigma_s}(g)}, \\ \langle h_s \rangle_{\Xi} &= \langle h_s \rangle_{\sigma_s} \equiv \frac{\hat{h}_s U_{\sigma_s}(g)}{U_{\sigma_s}(g)}, \end{aligned} \quad (19)$$

where  $\sigma_s$  is the supershell containing the shell  $s$ .

The SC averages (15) can now be obtained by sequential operations of the shell operators  $\hat{q}_s$  and  $\hat{h}_s$  on  $U_{\Xi}(g)$  in any order since, from Eq. (17),

$$[\hat{q}_r, \hat{q}_s] = [\hat{q}_r, \hat{h}_s] = [\hat{h}_r, \hat{h}_s] = 0. \quad (20)$$

Thus the polynomial (13) can be regarded as an operator by the replacements  $q_s \rightarrow \hat{q}_s$  and  $h_s \rightarrow \hat{h}_s$ :

$$\hat{A} = \sum_{\{m,n\}} e_{\{m,n\}} \prod_{r,s} \hat{q}_r^{m_r} \hat{h}_s^{n_s}, \quad (21)$$

which averages the corresponding quantity over SC by operating on its PF:

$$\hat{A} U_{\Xi}(g) = \langle A \rangle_{\Xi} U_{\Xi}(g). \quad (22)$$

Note that when sequential operations are performed on Eqs. (17), the averages  $\langle q_s \rangle_{\Xi}$ ,  $\langle h_s \rangle_{\Xi}$  are not pure numbers since they are functions of the  $X_s$ 's.

In particular, it is easily seen from (16) and (17) that

$$\hat{q}_r \langle q_s \rangle = \hat{q}_s \langle q_r \rangle = \langle q_r q_s \rangle - \langle q_r \rangle \langle q_s \rangle, \quad (23)$$

$$\begin{aligned} \hat{q}_{s_{n+1}} \langle q_{s_1} q_{s_2} \cdots q_{s_n} \rangle &= \langle q_{s_1} q_{s_2} \cdots q_{s_{n+1}} \rangle - \langle q_{s_{n+1}} \rangle \\ &\quad \times \langle q_{s_1} q_{s_2} \cdots q_{s_n} \rangle, \end{aligned}$$

where  $s_k$  with different  $k$  may belong to the same or different shells. The appearance of Eqs. (18) and (22) as eigenvalue equations is therefore misleading. We will return to this point later.

As shown below, the operations defined above result in GPF's with modified statistical weights and/or number of electrons. The rules for making these modifications are simple and can be applied without any calculation. The final GPF's are then calculated using the recursion formulas of the various kinds.

### C. Averages as generalized partition functions (GPF's)

From the binomial relations

$$q \binom{g}{q} = g \binom{g-1}{q-1} \quad \text{and} \quad (g-q) \binom{g}{q} = g \binom{g-1}{q}, \quad (24)$$

it is seen that the operations  $\hat{q}_s$  and  $\hat{h}_s$  yield a common multiplicative factor for all the terms in the SC partition function sum. This factor can therefore be taken out of the sum yielding

$$\hat{q}_s U_{\Xi}(g) = g_s X_s U_{\Xi^s}(g^s), \quad (25)$$

$$\hat{h}_s U_{\Xi}(g) = g_s U_{\Xi}(g^s),$$

where  $U_{\Xi^s}(g^s)$ ,  $U_{\Xi}(g^s)$  are GPF's defined formally as identical to Eqs. (9), (10), and (11) with modified statistical weights and number of electrons: the set  $(g^s) \equiv \{g_1^s, g_2^s, \dots\}$  has the weight of shell  $s$  reduced by one. In general we use the notation for multiple reduction

$$g_t^{rs \cdots} \equiv g_t - \delta_{rt} - \delta_{st} - \cdots \quad (26)$$

and  $\Xi^{rs \cdots}$  is the SC defined by the supershell occupation numbers  $Q_{\sigma}^{rs \cdots}$ ,

$$Q_{\sigma}^{rs \cdots} \equiv Q_{\sigma} - \delta_{\sigma_r \sigma} - \delta_{\sigma_s \sigma} - \cdots, \quad (27)$$

where  $\delta_{\sigma_s \sigma}$  equals 1 if  $s \in \sigma$  and zero otherwise. Note that  $\hat{q}_s$  shifts both  $Q_{\sigma_s}$  and  $g_s$ , while  $\hat{h}_s$  shifts only the statistical weights  $g_s$ . Using Eq. (10) we obtain

$$\langle q_s \rangle_{\Xi} = \frac{g_s X_s U_{\Xi^s}(g^s)}{U_{\Xi}(g)} = \frac{g_s X_s U_{Q_{\sigma_s-1}}(g^s)}{U_{Q_{\sigma_s}}(g)} = \langle q_s \rangle_{\sigma_s}, \quad (28)$$

$$\langle h_s \rangle_{\Xi} = \langle h_s \rangle_{\sigma_s} = \frac{g_s U_{Q_{\sigma_s}}(g^s)}{U_{Q_{\sigma_s}}(g)}.$$

Because the result of  $\hat{q}_s$  and  $\hat{h}_s$  operations (25) is formally the same as an ordinary PF it can be subjected to a subse-

quent operation of the same type. Thus the averaging polynomial operators (13) can be applied by a succession of such elementary operations.

It was shown [1–10] that the configuration average polynomials (13) appearing in both STA moments and SCROLL rates can, in most cases, be rearranged in the form  $\cdots(q_r-1)q_r$  and  $\cdots(h_s-1)h_s$ . This is an “ordered form” where each step prepares exactly the required matching for the next one

$$\begin{aligned} \cdots(q-2)(q-1)q \binom{g}{q} &= \cdots(q-2)(q-1)g \binom{g-1}{q-1} \\ &= \cdots(g-1)g(q-2) \binom{g-2}{q-2} \\ &= \cdots(g-2)(g-1)g \binom{g-3}{q-3}. \end{aligned} \quad (29)$$

In this ordered form the SC averaging operators can be expressed as

$$\hat{A} \equiv \sum_{\{m,n\}} e'_{\{m,n\}} \prod_{r,s} P_{m_r}(\hat{q}_r) P_{n_s}(\hat{h}_s), \quad (30)$$

where

$$\begin{aligned} P_n(\hat{q}_s) &\equiv \prod_{k=0}^{n-1} (\hat{q}_s - k) = X_s^n \frac{\partial^n}{\partial X_s^n}, \\ P_n(\hat{h}_s) &\equiv \prod_{l=0}^{n-1} (\hat{h}_s - l), \\ P_0(\hat{q}_s) &\equiv P_0(\hat{h}_s) = 1. \end{aligned} \quad (31)$$

By sequential operations of Eq. (25) we obtain

$$\begin{aligned} P_{n_s}(\hat{q}_s) U_{\Xi}(g) &= \sum_{C \in \Xi} [(q_s - n_s + 1) \cdots (q_s - 1) q_s] U_C(g) \\ &= \langle (q_s - n_s + 1) \cdots (q_s - 1) q_s \rangle_{\Xi} U_{\Xi}(g) \\ &= \frac{g_s!}{(g_s - n_s)!} X_s^{n_s} U_{\Xi(n_s)}[g^{(n_s)}], \end{aligned} \quad (32)$$

where the GPF's  $U_{\Xi(n_s)}[g^{(n_s)}]$  have the modified statistical weights

$$g_t^{(n_s)} \equiv g_t - n_s \delta_{ts} \quad (33)$$

and  $\Xi^{(n_s)}$  is defined by the supershell occupation numbers

$$Q_{\sigma}^{(n_s)} \equiv Q_{\sigma} - n_s \delta_{\sigma,s}, \quad (34)$$

i.e., the occupation number of the supershell that includes  $s$  is reduced by  $n_s$ . Similarly for holes we have

$$P_{n_s}(\hat{h}_s) U_{\Xi}(g) = \frac{g_s!}{(g_s - n_s)!} U_{\Xi}[g^{(n_s)}]. \quad (35)$$

The elementary operations leading to Eqs. (32) and (35) could be performed in any order since they commute. However, following the sequential order (29) makes the derivation straightforward. Exceptional cases will be discussed later.

The SC averages (15), of any spectral moment or transition rate, can thus be expressed by means of Eqs. (30), (32), and (35) in terms of the GPF's,

$$\prod_{rs} P_{m_r}(\hat{q}_r) P_{n_s}(\hat{h}_s) U_{\Xi}(g) = B_{\{m,n\}} U_{\Xi\{m\}}(g^{\{m,n\}}), \quad (36)$$

where

$$B_{\{m,n\}} = \prod_{rs} \frac{g_r! X_r^{m_r}}{(g_r - m_r)! (g_s - n_s)!} \quad (37)$$

The curly brackets in Eq. (36) denote the set of polynomial degrees appearing on the left-hand side (lhs) product of the various shells, and the modified statistical weights here are

$$g_t^{\{m,n\}} \equiv g_t - \sum_r m_r \delta_{rt} - \sum_s n_s \delta_{st} \quad (38)$$

and the supershell occupation numbers in  $U_{\Xi\{m\}}$  are

$$Q_{\sigma}^{\{m\}} \equiv Q_{\sigma} - \sum_r m_r \delta_{\sigma,r}. \quad (39)$$

In Sec. IV we present a set of recursion relations connecting GPF's of different kind (different number of electrons, holes, and/or statistical weights). These relations enable us to calculate in turn each required GPF using previously calculated GPF's, thus reducing significantly the required computer time.

#### IV. EFFICIENT PATHS FOR CALCULATING GENERALIZED PARTITION FUNCTIONS

##### A. Recursion over electrons and holes

When a supershell is specified we omit the index  $\sigma$  in Eq. (11) and write the supershell partition function as  $U_Q(g) \equiv U_{Q_{\sigma}}(g)$ . It can be easily verified from Eq. (11) that for any shell  $a \in \sigma$  we have

$$\begin{aligned} \sum_{n=0}^G U_n(g) [-X_a]^{-n} &= \prod_{s \in \sigma} \sum_{q_s=0}^{g_s} \binom{g_s}{q_s} [-X_s/X_a]^{q_s} \\ &= \prod_s \left[ 1 - \frac{X_s}{X_a} \right]^{g_s} = 0, \end{aligned} \quad (40)$$

where

$$G = \sum_s g_s. \quad (41)$$

Note that for a specific supershell  $\sigma$  the sum in Eq. (41) is restricted to  $s \in \sigma$ .

Multiplying Eq. (40) by  $g_a X_a^Q$  with any  $Q$ , and summing over  $a$  leads to

$$\sum_{n=0}^G U_n(g)\chi_{Q-n}=0, \tag{42}$$

with

$$\chi_k \equiv \sum_s [-g_s(-X_s)^k]. \tag{43}$$

The sum in Eq. (42) can now be separated into three parts  $A_Q$ ,  $B_Q$ , and  $C_Q$  for  $n < Q$ ,  $n = Q$ , and  $n > Q$ , respectively.

An interesting and most useful fact is that for any  $Q$  all these three parts are proportional to  $U_Q(g)$ , specifically:

$$A_Q = QU_Q(g), \quad B_Q = -GU_Q(g), \quad C_Q = (G-Q)U_Q(g). \tag{44}$$

The first part ( $n < Q$ )

$$QU_Q(g) = \sum_{n=0}^{Q-1} U_n(g)\chi_{Q-n} \tag{45}$$

is the recursion formula for increasing  $Q$ , with  $U_0 = 1$ , obtained in [1] by taking derivatives of the generating function

$$F(z) \equiv \prod_s [1 + zX_s]^{g_s} = \sum_{\text{all } q_s} \prod_s \binom{g_s}{q_s} (zX_s)^{q_s} = \sum_Q U_Q(g)z^Q. \tag{46}$$

The third part ( $n > Q$ ) is similarly

$$(G-Q)U_Q(g) = \sum_{n=Q+1}^G U_n(g)\chi_{Q-n} \tag{47}$$

a recursion from full shells with  $U_G(g) = \prod_s X_s^{g_s}$ . This recursion can be obtained independently from the generating function

$$G(z) \equiv \prod_s [z + X_s]^{g_s} = \sum_n U_n(g)z^{G-n}. \tag{48}$$

Recursions from complete shells are used in both the STA and SCROLL codes to speed the calculations for cases where  $Q$  is closer to  $G$  than to 0.

**B. Shortcuts in the calculation of GPF's with shifted statistical weights**

The recursions (45) and (47) give  $U_Q(g)$  in terms of smaller or higher  $Q$  partition functions, but the statistical weights ( $g$ ) remain untouched. The averages (15), on the other hand, result in GPF's of the type (36), where ( $g$ ) is changed as well. Of course the recursions (45) and (47) work for any set ( $g'$ ), but instead of starting again from  $Q=0$  or  $Q=G$  we make use of the already calculated partition functions for ( $g$ ) as shown below.

Using the binomial identity

$$\binom{g}{q} = \binom{g-1}{q} + \binom{g-1}{q-1} \tag{49}$$

for any orbital  $a \in \sigma$  leads by substitution in Eq. (11) to

$$U_Q(g) = U_Q(g^a) + X_a U_{Q-1}(g^a), \tag{50}$$

where PF's of the set ( $g$ ) are obtained from those of ( $g^a$ ). The reverse relation is obtained by iterations on

$$U_Q(g^a) = X_a U_{Q-1}(g^a) - U_Q(g) \tag{51}$$

yielding  $U_Q(g^a)$  in terms of  $U_n(g)$   $n \leq Q$ :

$$U_Q(g^a) = \sum_{n=0}^Q U_n(g)(-X_a)^{Q-n} = \sum_{n=0}^Q U_{Q-n}(g)(-X_a)^n. \tag{52}$$

For holes we iterate starting from

$$U_Q(g^a) = \frac{1}{X_a} [U_{Q+1}(g) - U_{Q+1}(g^a)] \tag{53}$$

yielding

$$U_Q(g^a) = - \sum_{n=Q+1}^G U_n(g)(-X_a)^{Q-n} = - \sum_{n=1}^{G-Q} U_{n+Q}(g)(-X_a)^{-n} \tag{54}$$

consistent with Eq. (42).

The shift in statistical weights (52) and (54) can be generalized by successive operations to multiple shifts:

$$U_Q(g^{a_1 a_2 \dots a_p}) = \sum_{n_1=0}^Q (-X_{a_1})^{Q-n_1} \times \sum_{n_2=0}^{n_1} (-X_{a_2})^{n_1-n_2} \dots \times \sum_{n_p=0}^{n_{p-1}} (-X_{a_p})^{n_{p-1}-n_p} U_{n_p}(g), \tag{55}$$

where  $a_i$  may belong to the same or different shells.

Similarly for holes we get from Eq. (54)

$$U_Q(g^{a_1 a_2 \dots a_p}) = \sum_{n_1=Q+1}^G (-X_{a_1})^{Q-n_1} \times \sum_{n_2=n_1+1}^G (-X_{a_2})^{n_1-n_2} \dots \times \sum_{n_p=n_{p-1}+1}^G (-X_{a_p})^{n_{p-1}-n_p} U_{Q-\bar{n}_p}(g) \tag{56}$$

with

$$\bar{n}_p = \sum_{i=1}^{p-1} n_i. \tag{57}$$

These multiple shifts are used to eliminate shells completely when required as shown in the example of Sec. IV D.

### C. Eigenvectors as a source for additional useful GPF relations

From the definition of the averages (16) and (18) it is seen immediately that for any supershell or SC or entire ion, where the total number of electrons  $Q$  is constant, the PF's are eigenvectors of the corresponding operators

$$\hat{Q}_\sigma \equiv \sum_{s \in \sigma} \hat{q}_s, \quad \hat{H}_\sigma \equiv \sum_{s \in \sigma} \hat{h}_s, \quad (58)$$

$$\hat{Q} \equiv \sum_{\sigma} \hat{Q}_\sigma, \quad \hat{H} \equiv \sum_{\sigma} \hat{H}_\sigma$$

with the respective eigenvalues  $Q$  and  $(G-Q)$ ,

$$\hat{Q}U_Q(g) = QU_Q(g), \quad \hat{H}U_Q(g) = (G-Q)U_Q(g), \quad (59)$$

which holds for each supershell separately. The physical meaning of Eq. (59) is the obvious conservation laws

$$\sum_s \langle q_s \rangle_\sigma = Q_\sigma, \quad \sum_s \langle q_s \rangle_\Xi = Q \quad (60)$$

implying that by changing the binding energies and chemical potentials (changing the  $X_a$ 's) the average occupation numbers flow from one shell to the other with no loss.

By sequential operations we also obtain

$$\hat{Q}^n U_\sigma(g) = Q_\sigma^n U_\sigma(g), \quad (61)$$

$$\hat{Q}^n U_\Xi(g) = Q^n U_\Xi(g),$$

leading to an additional set of conservation laws:

$$\begin{aligned} \hat{Q}^n U_\Xi(g) &= \sum_{s_1 s_2 \dots s_n} \hat{q}_{s_1} \hat{q}_{s_2} \dots \hat{q}_{s_n} U_\Xi(g) \\ &= U_\Xi(g) \sum_{s_1 s_2 \dots s_n} \langle q_{s_1} q_{s_2} \dots q_{s_n} \rangle_\Xi \end{aligned} \quad (62)$$

so that

$$\sum_{s_1 s_2 \dots s_n} \langle q_{s_1} q_{s_2} \dots q_{s_n} \rangle = \sum_{s_1 s_2 \dots s_n} \langle q_{s_1} \rangle \langle q_{s_2} \rangle \dots \langle q_{s_n} \rangle = Q^n. \quad (63)$$

In addition, from Eq. (23) we obtain that for any  $s$ ,  $\langle q_s \rangle$  is an eigenvector of both  $\hat{Q}$  and  $\hat{H}$  with the eigenvalues zero and  $G$ , respectively,

$$\hat{Q}^n \langle q_s \rangle = \hat{Q} \langle q_s \rangle = 0, \quad (64)$$

$$\hat{H}^n \langle q_s \rangle = G^n \langle q_s \rangle.$$

Thus for any shell  $s_k$  the complementary operators

$$\hat{Q}_k^+ = \sum_{i=1}^k \hat{q}_i, \quad \hat{Q}_k^- = \sum_{i=k+1}^G \hat{q}_i \quad (65)$$

yield for any shell  $s$

$$\hat{Q}_k^+ \langle q_s \rangle = -\hat{Q}_k^- \langle q_s \rangle. \quad (66)$$

An example of Eq. (66) is the case  $k=1$ , with  $s_1=s$  ( $\hat{Q}_1^+ = \hat{q}_s$  and  $\hat{Q}_1^- = \sum_{r \neq s} \hat{q}_r$ ) connecting the variance of  $q_s$  (of any shell  $s$ ) to the two shell correlation with other shells:

$$\langle q_s^2 \rangle - \langle q_s \rangle^2 = - \sum_{r \neq s} \langle q_r q_s \rangle + \langle q_r \rangle \langle q_s \rangle. \quad (67)$$

All the above operations are a rich source for a variety of additional relations between GPF's of different types. For example, from Eq. (60) we obtain by means of Eq. (28) the useful relations

$$U_Q(g) = \frac{1}{G-Q} \sum_s g_s U_Q(g^s), \quad (68)$$

$$U_Q(g) = \frac{1}{Q} \sum_s g_s X_s U_{Q-1}(g^s). \quad (69)$$

An example of higher  $n$  relations obtained from Eq. (63) is the  $n=2$  case,

$$\sum_{rs} \langle q_r q_s \rangle = \sum_{rs} \langle q_r \rangle \langle q_s \rangle = Q^2 \quad (70)$$

leading to

$$U_{Q_\sigma}(g) = \frac{1}{Q_\sigma^2} \sum_{rs} g_r (g_s - \delta_{rs}) X_r X_s U_{Q_\sigma-2}(g^{rs}), \quad (71)$$

$$U_\Xi(g) = \frac{1}{Q^2} \sum_{rs} g_r (g_s - \delta_{rs}) X_r X_s U_{\Xi-2}(g^{rs}).$$

Finally it is clear that when operating on  $U(g)$ —the PF of the whole atomic system in the plasma—including several charge state ions we have

$$\hat{Q}U(g) = \sum_z Q_z U_z(g) \equiv \langle Q \rangle U(g), \quad (72)$$

where  $Q_z$  and  $U_z(g)$  are the average number of electron and partition function of ion  $z$  and  $U(g) = \sum_z U_z(g)$  and  $\langle Q \rangle$  are the total partition function and the average number of bound electrons in the plasma.

The various relations presented in the preceding sections are used in both the STA and SCROLL models to optimize the calculation of the many GPF's involved, thus reducing the computation time significantly.

### D. Averaging nonordered polynomials

Averaging a polynomial in  $q_a$ , which cannot be brought to an ordered form, requires a special attention. As an example, let us look at the SC average transition energy. In the SCROLL non-LTE model, the SC-average transition energy weighs transitions only by their initial population, similarly to the weights used for averaging the rates. For two SC's  $\Xi$  and  $\Xi'$  connected by the orbital jump  $a \rightarrow b$  the

configuration-average polynomial  $\langle A \rangle_{CC'}$  of Eq. (13) for the average transition energy is [9,1]

$$\langle A \rangle_{CC'} = D_0 + \sum_s (q_s - \delta_{sa}) D_s, \quad (73)$$

where the coefficients  $D_s$  are combinations of radial integrals. Clearly in the SC average (15), only configurations with  $q_a \neq 0$  contribute in this case.

The polynomial in  $q_a$  is not ordered since the  $s=a$  term cannot be ordered to start with  $q_a$  as a multiplicative factor. In the average of this term, configurations  $c \in \Xi$  with  $q_a = 0$  must be excluded:

$$\begin{aligned} \langle q_a - 1 \rangle_{\Xi} &\equiv \frac{1}{U_{\Xi}(g)} \sum_{c(q_a \neq 0) \in \Xi} (q_a - 1) U_c(g) \\ &= \frac{1}{U_{\Xi}(g)} \left[ \sum_{c \in \Xi} q_a U_c(g) - \sum_{c(q_a \neq 0) \in \Xi} U_c(g) \right], \end{aligned} \quad (74)$$

where

$$\sum_{c(q_a \neq 0) \in \Xi} U_c(g) = U_{\Xi}(g) - U_{\Xi}(g). \quad (75)$$

The second term in Eq. (75) is the PF of  $\Xi$  obtained from  $\Xi$  by omitting the shell  $a$ . It would have been possible to calculate it by the recursion on  $Q$  starting from scratch. However it is much more efficient and convenient to use the already calculated PF's eliminating the shell  $a$  through use of Eq. (55), restricted to shell  $a$ ,  $m_a = g_a$  times, i.e.,

$$\frac{1}{U_{\Xi}} \sum_{c \in \Xi} U_c(g) = \frac{1}{U_{\sigma_a}} U_{\sigma_a}(g^{m_a}), \quad (76)$$

with  $m_a = g_a$ .

The result for a general  $m_a = m$  is

$$\begin{aligned} U_{Q_{\sigma'}}(\bar{g}) &= \sum_{n_1=0}^{Q_{\sigma'}} \sum_{n_2=0}^{n_1} \cdots \sum_{n_m=0}^{n_{m-1}} (-X_a)^{Q_{\sigma'} - n_m} U_{n_m}(g) \\ &= \sum_{k=0}^{Q_{\sigma'}} N_k^{(m)} (-X_a)^{Q_{\sigma'} - k} U_k(g), \end{aligned} \quad (77)$$

where in  $(\bar{g})$  the shell  $a$  is excluded and  $N_k^{(m)}$  is the number of times  $U_k(g)$  appears in the sum over all the indices  $n_i$ . Clearly the specific value  $n_m = k$  appears exactly once for each set  $n_1 \geq n_2 \geq n_3 \geq \cdots \geq n_{m-1} \geq k$ . Thus

$$\begin{aligned} N_k^{(m)} &= \sum_{n_1=k}^{Q_{\sigma'}} \sum_{n_2=k}^{n_1} \cdots \sum_{n_{m-1}=k}^{n_{m-2}} 1 \\ &= \sum_{n_{m-1}=0}^{Q_{\sigma'} - k} \sum_{n_{m-2}=0}^{n_{m-1}} \cdots \sum_{n_2=0}^{n_3} \sum_{n_1=0}^{n_2} 1. \end{aligned} \quad (78)$$

These numbers were computed and tabulated using Bernoulli functions (Ref. [11], p. 804). Thus the result [Eq. (77)] is now substituted in Eq. (74) to obtain the correct averaging.

## V. ANALYTIC EXPRESSIONS FOR THERMODYNAMICAL QUANTITIES

In the previous developments of the STA model [1–6], the only concern was the calculation of radiative properties of hot dense matter. Indeed, the output of the STA code consists in tables of opacities that are read by the hydrodynamic codes. However, hydrodynamic codes could greatly benefit from a better atomic physics than what is commonly used for some key quantities, such as internal energy, specific heat, and electronic pressure. In many modern hydrodynamic codes, the evolution of the plasma is described in conservative form, and the code relies on the equation of state (EOS) tables to extract the temperatures and the pressure, which determine the plasma conditions at the next time step. Internal energy plays an important role, since it is that part of the total energy of the plasma cell that is not available to heat. More often than not, what is computed in the codes is only the so-called ‘‘ionization energy’’ that neglects the contribution of the excited states, and it is not consistent with the opacity tables. As a consequence its derivative, the specific heat, which is used to compute the temperature in the EOS subroutines, tends to be jerky, and this causes spurious oscillations and divergences.

In this section we apply the algebraic technique presented above to obtain analytic expressions for internal energy and derivatives of the SC partition functions with respect to temperature. Similar derivation holds for derivatives with respect to the density. Since the SC PF's include orbital relaxation (optimized potential for each SC) and first-order energies in the Boltzmann factors, we can construct an accurate derivative of the total PF of the atomic system by combining derivatives for each SC optimized separately. We plan to use the following formulas in STA to output additional tables that would be read in the hydrodynamic codes, thus improving greatly the quality of EOS and adding stability and consistency in the description of medium to high Z element plasmas.

### A. Internal energy

The total internal energy of an atomic plasma system is

$$E_{\text{total}} = \sum_C N_C E_C = \frac{N}{U_{\text{total}}} \sum_Q \sum_{\Xi} U_{\Xi}(g) E_{\Xi}, \quad (79)$$

where the summation over  $Q$  in Eq. (79) denotes the various charge states,

$$U_{\text{total}} \equiv \sum_Q \sum_{\Xi} U_{\Xi}(g) \quad (80)$$

and

$$E_{\Xi} \equiv \frac{1}{U_{\Xi}(g)} \sum_{c \in \Xi} U_c(g) E_C. \quad (81)$$

The ordered polynomial  $\langle A \rangle_{CC'}$  in Eq. (15) for the configuration average energy is [1]

$$\langle A \rangle_C = E_C = \sum_s q_s \langle s \rangle + \frac{1}{2} \sum_{rs} q_s (q_r - \delta_{rs}) \langle r, s \rangle, \quad (82)$$

where  $\langle r, s \rangle$  and  $\langle s \rangle$  are radial integrals defined explicitly in Appendix B of [1]. This notation should not be confused with the averages  $\langle q_s \rangle$  defined previously.

Using Eq. (16) the SC-average internal energy takes the form

$$E_{\Xi} = \frac{1}{U_{\Xi}(g)} \left[ \sum_s \langle s \rangle \langle q_s \rangle_{\Xi} + \frac{1}{2} \sum_{rs} \langle r, s \rangle \langle q_s (q_r - \delta_{rs}) \rangle_{\Xi} \right], \quad (83)$$

which we may calculate with optimized potentials for each SC. The ordered polynomials in Eq. (82) are special cases of Eq. (30) with the coefficients

$$e'_{\{m, n\}} = \delta_{\{n\}, \{n\}^{(0)}} [\langle s \rangle \delta_{\{m\}, \{m\}^{(s)}} + \frac{1}{2} \langle r, s \rangle \delta_{\{m\}, \{m\}^{(rs)}}], \quad (84)$$

where the exponent sets  $\{m\}^{(r)}, \{m\}^{(rs)}$  are defined by  $\{m\}_t^{(r)} \equiv \delta_{tr}$  and  $\{m\}_t^{(rs)} = \delta_{tr} + \delta_{ts}$  and  $\{n\}_t^{(0)} = 0$  (no hole dependence) for all shells  $t$ . In Eq. (84) the  $\delta_{\{m\}, \{m\}^{(r)}}$  are 1 for equal sets and zero otherwise.

Equation (32) gives the expression for the SC-average energy in terms of GPF's:

$$E_{\Xi} \equiv \frac{1}{U_{\Xi}(g)} \left[ \sum_s g_s X_s \langle s \rangle U_{\Xi s}(g^s) + \frac{1}{2} \sum_{rs} g_r (g_s - \delta_{rs}) X_r X_s \langle r, s \rangle U_{\Xi rs}(g^{rs}) \right]. \quad (85)$$

It should be pointed out that the second term on the rhs of Eq. (85) is the two electron contribution to  $\Delta E_{\Xi}^1$  of Eq. (9):

$$\Delta E_{\Xi}^1 = [\langle s \rangle - \epsilon_s] + \frac{1}{2U_{\Xi}^{(0)}(g)} \sum_{rs} g_r (g_s - \delta_{rs}) X_r X_s \times \langle r, s \rangle U_{\Xi rs}^{(0)}(g^{rs}). \quad (86)$$

### B. Specific heat

The specific heat is obtained by differentiation  $E_{\text{total}}$  of Eqs. (83) and (85) with respect to the temperature. Numerical differentiation may not be accurate enough because of well-known local irregularities of  $E_{\text{total}}$  in the  $(\rho, T)$  plane, due to the ionic shell structure.

For analytic differentiation we rearrange Eq. (83) in the form

$$\begin{aligned} E_{\text{total}} &= \frac{N}{U_{\text{total}}} \sum_Q \sum_{\Xi} U_{\Xi}(Q, g) E_{\Xi} \\ &= \frac{N}{U_{\text{total}}} \sum_Q \sum_{\Xi} \left\{ \sum_s [s]_{\Xi} \langle q_s \rangle_{\Xi} + \frac{1}{2} \sum_{r,s} [\langle r, s \rangle]_{\Xi} \langle q_s q_r \rangle_{\Xi} \right\} \end{aligned} \quad (87)$$

with

$$[s]_{\Xi} \equiv [\langle s \rangle - \frac{1}{2} \langle s, s \rangle]_{\Xi}, \quad (88)$$

where the subscript  $\Xi$  denotes that a specific potential is used in the calculation of  $\langle r, s \rangle$  and  $\langle s \rangle$  for each SC:

$$\begin{aligned} C_{\nu} &= \frac{\partial E_{\text{total}}}{\partial T} = - \frac{E_{\text{total}}}{U_{\text{total}}} \frac{\partial U_{\text{total}}}{\partial T} \\ &+ \frac{N}{U_{\text{total}}} \sum_Q \sum_{\Xi} \left[ \sum_s \left\{ [s]_{\Xi} \frac{\partial}{\partial T} \langle q_s \rangle + \langle q_s \rangle \frac{\partial}{\partial T} [s]_{\Xi} \right\} + \frac{1}{2} \sum_{r,s} \left\{ [\langle r, s \rangle]_{\Xi} \frac{\partial}{\partial T} \langle q_r q_s \rangle_{\Xi} + \langle q_r q_s \rangle_{\Xi} \frac{\partial}{\partial T} [\langle r, s \rangle]_{\Xi} \right\} \right]. \end{aligned} \quad (89)$$

From Eq. (9) we obtain

$$\begin{aligned} \frac{\partial U_{\text{total}}}{\partial T} &= \sum_{\Xi} \frac{U_{\Xi}(g)}{kT} \left[ \frac{\Delta E_{\Xi}^1}{T} - \frac{\partial \Delta E_{\Xi}^1}{\partial T} \right] \\ &+ \sum_{\Xi} e^{-\Delta E_{\Xi}^1/kT} \frac{\partial}{\partial T} U_{\Xi}^{(0)}(g). \end{aligned} \quad (90)$$

It is seen from Eqs. (89), (90), and (86) that the specific heat depends in addition to GPF's on derivatives of the types

$$\frac{\partial}{\partial T} \langle r, s \rangle, \quad \frac{\partial}{\partial T} \langle r \rangle, \quad \text{and} \quad \frac{\partial}{\partial T} U_{\Xi}^{(0)}(g). \quad (91)$$

The first two quantities depend on  $T$  indirectly through the free electron potential, which in our model is common to all the SC's of all ions in the plasma. For direct application of Eq. (89) these quantities can be calculated numerically, or modeled analytically. This, however, is beyond the scope of the present work. The analytic derivative  $(\partial/\partial T)U_{\Xi}^{(0)}(g)$ , which contains the SC dependence, can, on the other hand, be easily obtained, for any modified values of  $Q$  and/or  $(g)$ , since  $U_{\Xi}^{(0)}(g)$  depends on the plasma temperature only through the quantities  $X_s$  of Eq. (12). As shown above the derivatives with respect to these variables are given in terms of the average occupation number of the corresponding shell. Specifically, from Eq. (10) the derivative with respect to  $T$  is written as

$$\frac{1}{U_{\Xi}^{(0)}(g)} \frac{\partial}{\partial T} U_{\Xi}^{(0)}(g) = \sum_{\sigma \in \Xi} \frac{1}{U_{\sigma}(g)} \frac{\partial}{\partial T} U_{\sigma}(g) \quad (92)$$

and from Eqs. (17) and (25) we have

$$\frac{\partial}{\partial T} U_{\sigma}(g) = \sum_{a \in \sigma} \frac{\partial}{\partial X_a} U_{\sigma}(g) \frac{\partial X_a}{\partial T} = \sum_{a \in \sigma} \eta_a(T) U_{Q_{\sigma-1}}(g^a), \quad (93)$$

where

$$\eta_a(T) = \frac{g_a}{kT} \left[ \frac{(\epsilon_a - \mu)}{T} - \frac{\partial}{\partial T} (\epsilon_a - \mu) \right]. \quad (94)$$



Equation (51) expresses  $U_\sigma(g^a)$  for any  $a \in \sigma$  in terms of the same  $U_\sigma(g)$  and thus we obtain finally

$$\frac{\partial}{\partial T} U_\sigma(g) = \sum_{n=0}^{Q_\sigma-1} \zeta_\sigma^n(T) U_{Q_\sigma-n-1}(g) \quad (95)$$

with

$$\zeta_\sigma^n(T) = \sum_{a \in \sigma} g_a \eta_a(T) (-X_a)^n. \quad (96)$$

The quantity  $(\partial/\partial T)\epsilon_a$  is included in  $(\partial/\partial T)\langle a \rangle$  of Eq. (89) [1]. The chemical potential  $\mu(\rho, T)$ , on the other hand, behaves like [12]  $e^{-\mu/kT} = a(\rho, T)T^{3/2}/\rho$ , where  $a(\rho, T)$  varies smoothly; its derivatives can therefore be easily calculated.

For evaluating the *pressure* we require the derivative  $\partial E_{\text{total}}/\partial \rho$  that has the same form as Eq. (89) with the replacements  $T \rightarrow \rho$ . In addition to GPF's, it depends likewise on

$$\frac{\partial}{\partial \rho} \langle r, s \rangle, \quad \frac{\partial}{\partial \rho} \langle r \rangle, \quad \text{and} \quad \frac{\partial}{\partial \rho} U_{\Xi}^{(0)}(g). \quad (97)$$

Again the important SC dependence appears in  $(\partial/\partial \rho)U_{\Xi}^{(0)}(g)$ , which is obtained in terms of GPF's and has the same form as Eqs. (92) and (95) with the replacements  $T \rightarrow \rho$  and where

$$\eta_a(\rho) = -\frac{g_a}{kT} \frac{\partial}{\partial \rho} (\epsilon_a - \mu). \quad (98)$$

## VI. SUMMARY

In this work we have presented the elementary algebra for performing SC averages over any polynomial in the shell occupation numbers. The LTE spectral moments as well as SC average rates in non-LTE models are special cases. The analytic expressions for the averaged quantities are obtained by a succession of elementary operations where each step results in a GPF with reduced number of electrons and/or a shell's statistical weight by unity. The calculation of the obtained GPF's becomes very efficient using a set of relations that allow short calculation paths. Each GPF in turn is obtained from GPF's of neighboring systems (with respect to the number of electrons and statistical weights) that are calculated in previous steps. These paths thus reduce significantly the required computer time. Using this technique we have also obtained analytic expressions for derivatives of GPF's which are required to calculate accurately thermodynamical quantities such as specific heat and electronic pressure including orbital relaxation and first-order energies in the Boltzmann factors. This allows the STA code to yield consistent data for the equation of state in addition to opacities.

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