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Statistical treatment of radiative transitions in local thermodynamic equilibrium plasmas

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The fluctuations of the electronic configurations around the average-atom configuration are estimated using classical statistical mechanics. This method allows the spectral opacities to be rapidly calculated without explicit recourse to detailed configuration accounting. Coupled to a screened-hydrogenic average-atom model, it can be implemented into the atomic physics package of a hydrodynamic code. We compare our results to numerical spectra constructed with more detailed codes or experimental spectra. [S1063-651X(97)12106-7]

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I. INTRODUCTION

In both astrophysics and laboratory plasma physics, an essential contribution to energy transport in hot and dense plasmas comes from radiation. Radiative opacity [1] is the key parameter that rules radiative transfer. Its difficult evaluation requires methods with increasing degrees of complexity. One can consider transitions between configurations (detailed configuration accounting or DCA) or, at a more accurate level, between spectroscopic terms resulting from configurations (detailed term accounting or DTA). However, the number of term-to-term transitions becomes prohibitively large with increasing complexity of configurations, though they can be included in DCA calculations as a broadening of the configuration-to-configuration transitions [2,3].

In a laser-plasma simulation, the opacity has to be known because radiation effects may be important and can substantially modify the hydrodynamic evolution of the system. For computer time reasons, a balance has to be reached between accuracy and rapidity. This is why approximate models are needed to perform in-line computations. The screened-hydrogenic average-atom model with fractional shell populations (see Ref. [4], and references therein) is well suited to describe multicharged-ion plasmas in such studies. For given temperature T and density ρ, the average-atom populations, the free-free, bound-free, and bound-bound photoabsorption cross sections are determined and a first approximate spectrum can easily be constructed. Nevertheless, the quality of opacities deduced from this average-atom spectrum is known to be poor, even taking into account the line profiles [5] or ℓ splitting [4,6,7]. The reason for this is that each one-electron transition depends on the total electronic configuration, which is generally different from the average configuration. Consequently, the contribution of a large number of configurations tends to split an average-atom transition in many components. As an explicit DCA cannot be rapidly calculated, a statistical approach is needed to estimate the distribution of the configurations that substantially contribute to the opacity around the average-atom configuration [8], in order to increase the quality of the average-atom spectrum. For local thermodynamic equilibrium (LTE) plasmas, an approximate photoabsorption spectrum can be obtained without explicitly considering all the different configurations. The main effect is a statistical broadening of each average-atom line [9–11], which is a direct consequence of the evaluation of the statistical distribution of the dominant configurations around the average atom configuration. Each individual line is additionally broadened by usual physical effects, such natural broadening, Doppler, Stark broadening, . . . [5]. Replacing the average-atom line with a statistically broadened line may then be a good approximation when the number of lines is large and the lines are so closely spaced that a strong overlapping takes place.

The outline of the paper is as follows. In Sec. II, we recall how an approximate expression of the grand canonical partition function Z_G of the bound electrons can be found using the classical theory of fluctuations. This expression is important because it allows a fast computation of the mean value of any physical quantity (like radiative opacity) which is an explicit function of the electron shell populations. Furthermore, a method to evaluate average-atom bound-bound and bound-free oscillator strengths is proposed. It ensures that one-electron sum rules are preserved and that the discrete spectrum and the continuum series are continuously connected. In Sec. III, the aforementioned expression of Z_G is used to statistically broaden the average-atom bound-bound and bound-free one-electron transitions. It is shown that the splitting in integer ion stages can be easily included. In Sec. IV, we perform comparisons between results obtained using this formalism, more elaborate calculations, and experimental data.

II. THE SCREENED-HYDROGENIC AVERAGE-ATOM MODEL

A. Statistical mechanics

Different methods exist to describe highly charged LTE ion plasmas. The screened-hydrogenic atom model is simple, frequently used, reasonably accurate, and has been proven to be properly defined and thermodynamically consistent [4]. Within this formalism, fast computations are possible in a hydrodynamic code. All developments start from the grand canonical partition function Z_G of bound electrons

$$Z_G=\sum_{(P_i)} \mathcal{D}_{(P_i)}e^{-\beta\left(E[(P_i)]-\mu\sum_{i=1}^{K_{\max}} P_i\right)}. \tag{1}$$

$E[(P_i)]$ and $\mathcal{D}_{(P_i)}$ are the energy and the statistical weight of an electronic configuration (P_i). Introducing the binomial coefficient $\binom{n}{p}\{\binom{n}{p}=n!/[p!(n-p)!]\}$ and the shell degeneracies (D_i),$\mathcal{D}_{(P_i)}$ is equal to $\mathcal{D}_{(P_i)}=\Pi_{i=1}^{K_{\max}}\binom{D_i}{P_i}$. μ is the chemical potential and β is the inverse temperature ($\beta=1/k_BT$, k_B is the Boltzmann constant), whereas the sum $\Sigma_{(P_i)}$ runs over the set of all configurations that can be constructed from the $K_{\max}$ bound shells. So $\Sigma_{(P_i)}$ means $\Sigma_{P_1=0}^{D_1}\cdots\Sigma_{P_i=0}^{D_i}\cdots\Sigma_{P_{K_{\max}}=0}^{D_{K_{\max}}}$.

The exact value of Z_G is known only in a few cases. A brute force computation of the discrete sum $\Sigma_{(P_i)}$ is difficult due to the large number of configurations. Furthermore, a closed form is in general impossible to obtain when the configuration energy $E[(P_i)]$ is a nonlinear function of the configurations (P_i). The basic idea to evaluate Z_G consists in replacing $\Sigma_{(P_i)}$ by an integral using auxiliary variables (X_i). The integral representation of Z_G is not unique. We do not discuss this detail since it is beyond the scope of the paper [4,12]. It is sufficient to keep in mind that Z_G can be written as follows:

$$Z_G=\int [dX_i]e^{-\beta S[(X_i)]}. \tag{2}$$

$[dX_i]$ and $S[(X_i)]$ are, respectively, an integration measure and a function that depends explicitly on (X_i).

Since we are dealing with the partition function of a system at thermodynamic equilibrium, only a limited group of configurations notably contribute to the discrete sum in Eq. (1). In consequence, the saddle-point method can be used to estimate Z_G in Eq. (2). $S[(X_i)]$ is expanded around its minimum up to second order

$$\begin{aligned}S[(X_i)]=S[(X_i^0)]&+\sum_j \left.\frac{\partial S}{\partial X_j}\right|_{(X_i^0)}(X_j-X_j^0)\\&+\frac{1}{2}\sum_{j,k}(X_j-X_j^0)\left.\frac{\partial^2 S}{\partial X_j\partial X_k}\right|_{(X_i^0)}\\&\times(X_k-X_k^0)+\cdots .\end{aligned}\tag{3}$$

The quantities (X_i^0) satisfy the equations

$$\left.\frac{\partial S}{\partial X_j}\right|_{(X_i^0)}=0. \tag{4}$$

After some algebraic manipulations, one finds that Eqs. (4) are identical to the coupled-nonlinear Fermi-Dirac equations, which define the fractional occupations (N_i^0) of the bound orbitals of the screened-hydrogenic average-atom model

$$\overline{N_i^0}=\frac{D_i}{1+e^{\beta e_i^0}}$$

$$e_i^0=\left.\frac{\partial E}{\partial P_i}\right|_{(\overline{N_i^0})}-\mu. \tag{5}$$

These equations have been proposed by More and Zimmerman [13] starting from an *ad hoc* free energy. (N_i^0) are roughly equal to the statistical mean shell occupations (P_i) [4]

$$\overline{N_j^0}\approx\overline{P_j}=\frac{1}{Z_G}\sum_{(P_i)}\mathcal{D}_{(P_i)}P_je^{-\beta(E[(P_i)]-\mu\Sigma_{i=1}^{K_{\max}}P_i)}. \tag{6}$$

The chemical potential μ is calculated by imposing the average neutrality of the ion cell. Z, Z, and $F_\alpha(\eta)$ are, respectively, the ion charge number, the average ionization, and the Fermi-Dirac function $[F_\alpha(\eta)=\int_0^\infty x^\alpha/(1+e^{x-\eta})dx]$, μ obeys the equations ($\eta=\beta\mu$)

$$\sum_{i=1}^{K_{\max}}\overline{N_i^0}+\overline{Z}=Z$$

$$\overline{Z}=4\pi\frac{A}{\rho\mathcal{N}}\left(\frac{2m}{\beta h^2}\right)^{3/2}F_{1/2}(\eta). \tag{7}$$

A is the molar mass of the element, $\mathcal{N}$ the Avogadro number, ρ the mass density, m the electron mass, and h the Planck constant.

The grand canonical partition function Z_G ensures the thermodynamic consistency of the model and allows the screened-hydrogenic average-atom model to be clearly established. Moreover, Z_G is the fundamental quantity to calculate the statistical average ζ of any physical quantity ζ which depends explicitly on the electronic configuration (P_i)

$$\overline{\zeta}=\frac{1}{Z_G}\sum_{(P_i)}\mathcal{D}_{(P_i)}\zeta[(P_i)]e^{-\beta(E[(P_i)]-\mu\Sigma_{i=1}^{K_{\max}}P_i)}. \tag{8}$$

We face again the original problem raised by the calculation of Z_G using Eq. (1). One solution could consist in finding an integral representation of ζ in Eq. (8) and evaluating it with the saddle-point technique. One writes ζ as follows:

$$\begin{aligned}\overline{\zeta}=\frac{1}{Z_G}\sum_{(P_i)}&\left[\prod_{i=1}^{K_{\max}}\binom{D_i}{P_i}e^{\eta P_i}\right]\\&\times\int\left[\prod_{i=1}^{K_{\max}}dX_i\delta(X_i-P_i)\right]\zeta[(X_i)]e^{-\beta E[(X_i)]}.\end{aligned}\tag{9}$$

δ is the Dirac distribution. The factorization of $\Sigma_{(P_i)}$ can be done by using the Fourier transformation of δ and by expressing $\zeta[(X_i)]$ as $\zeta[(X_i)]=e^{\ln\{\zeta[(X_i)]\}}$. ζ is equal to the ratio of two partition functions

$$\overline{\zeta}=\frac{Z_G(\zeta)}{Z_G}. \tag{10}$$

Z_G is the partition function in Eq. (1) which can be written as an integral [Eq. (2)]. $Z_G(\zeta)$ is a partition function where the configuration energy $E[(P_i)]$ has been replaced by $E[(P_i)]-1/\beta\ \ln\{\zeta[(P_i)]\}$. A saddle-point evaluation of Z_G and $Z_G(\zeta)$ gives an approximate value of ζ [Eq. (4)]. Nevertheless, this method is inadequate for fast calculations, especially when spectral opacities are considered. For example, LTE photoabsorption bound-bound opacity $\overline{\kappa^{\mathrm{bb}}}$ can be formally written as the ratio of two partition functions as in Eq. (10), with $\overline{\kappa^{\mathrm{bb}}}$ depending explicitly on photon energy $h\nu$. In consequence, a saddle-point evaluation needs to be performed at each step $h\nu$ [12] because the quantities (X_i^0), which are solutions of Eqs. (4), are now frequency dependent. In other words, Eq. (9) has to be evaluated using a frequency-dependent saddle-point method.

This difficulty may be overcome by using the classical theory of fluctuations [14]. The underlying idea consists in calculating ζ with only the average-atom populations defined by Eqs. (5) and (7). A Taylor expansion of ζ around the mean shell occupations (P_i) defined by Eq. (6) is performed

$$\zeta[(P_i)]=\zeta[(\overline{P_i})]+\sum_{i=1}^{K_{\max}}\left.\frac{\partial\zeta}{\partial P_i}\right|_{(\overline{P_i})}\Delta P_i+\cdots, \tag{11}$$

with $\Delta P_i=P_i-\overline{P_i}$. Since LTE is assumed, the fluctuations of ζ around $\overline{\zeta}$ are small; so a first-order Taylor expansion with respect to the (ΔP_i) is sufficient to get the mean and the variance of ζ

$$\overline{\zeta}\approx\zeta[(\overline{P_i})]$$

$$\sigma_\zeta^2\approx\sum_{i,j=1}^{K_{\max}}\left.\frac{\partial\zeta}{\partial P_i}\right|_{(\overline{P_i})}\left.\frac{\partial\zeta}{\partial P_j}\right|_{(\overline{P_i})}\overline{\Delta P_i\Delta P_j}. \tag{12}$$

From Eq. (6), we know that $(\overline{P_i})$ are approximately given by $(\overline{N_i^0})$. The correlations $\overline{\Delta P_i\Delta P_j}$ can be obtained as follows. In Eq. (1), the statistical weight $\mathcal{D}_{(P_i)}$ of a configuration is written as $e^{S[(P_i)]/k_B}$. Each binomial factor can be computed with the Stirling formula

$$S[(P_i)]=-k_B\sum_{i=1}^{K_{\max}}\left[P_i\ln\left(\frac{P_i}{D_i}\right)+(D_i-P_i)\ln\left(\frac{D_i-P_i}{D_i}\right)\right]. \tag{13}$$

Now, populations (P_i) are supposed to be real and can take all the possible values from $-\infty$ to $+\infty$. The discrete sum $\Sigma_{(P_i)}$ is replaced by a multidimensional integral. Z_G becomes proportional to

$$\int d^{K_{\max}}P e^{-\beta\Omega[(P_i)]}, \tag{14}$$

with $d^{K_{\max}}P=\Pi_{i=1}^{K_{\max}}dP_i$ and $\Omega[(P_i)]=E[(P_i)]-TS[(P_i)]-\mu\Sigma_{i=1}^{K_{\max}}P_i$. The former integral is evaluated with the saddle-point method. The grand potential Ω is developed around its minimum up to second order. The populations that extremize Ω are the average-atom populations. Let us introduce the matrix ω whose components are

$$\omega_{ij}=\beta\left.\frac{\partial^2\Omega}{\partial P_i\partial P_j}\right|_{(\overline{N_i^0})}. \tag{15}$$

Using Eq. (6), easy algebraic calculations show that

$$\omega_{ij}=\beta V_{ij}+\frac{\delta_{ij}}{\overline{\omega_1^2}}, \tag{16}$$

with

$$V_{ij}=\left.\frac{\partial^2 E}{\partial P_i\partial P_j}\right|_{(\overline{N_i^0})} \tag{17}$$

and

$$\overline{\omega_i^2}=\frac{\overline{N_i^0}(D_i-\overline{N_i^0})}{D_i}. \tag{18}$$

We find that the probability $d\mathcal{P}$ (normalized to unity) of an electronic configuration (P_i) boils down to

$$d\mathcal{P}=\left(\frac{\det(\omega)}{(2\pi)^{K_{\max}}}\right)^{1/2}d^{K_{\max}}\Delta P e^{-1/2\Delta P^T\omega\Delta P}, \tag{19}$$

with $\Delta P^T\omega\Delta P=\Sigma_{i,j=1}^{K_{\max}}\Delta P_i\omega_{ij}\Delta P_j$. From Eq. (19), it is now quite easy to show [14] that

$$\overline{\Delta P_i\Delta P_j}\approx(\omega^{-1})_{ij}. \tag{20}$$

The last step is to consider the integer charge stage splitting which has been lost by going from Eq. (1) to Eq. (19). This detail is important because the spectral features of various ionization stages can be seen on experimental photoabsorption spectra [15,16]. To do so, a constraint is included in Eq. (19). The populations (P_i) are still fractional but their sum is necessarily an integer: $\Sigma_{i=1}^{K_{\max}}P_i+Z'=Z$. Z' is a particular charge stage. With $\Sigma_{i=1}^{K_{\max}}\overline{P_i}+\overline{Z}=Z$ and $\Delta Z'=\overline{Z}-Z'$, it seems therefore natural to consider the probability $d\widetilde{\mathcal{P}}$ (normalized to unity)

$$d\widetilde{\mathcal{P}}=\sum_{Z'}\frac{1}{\mathcal{Z}}d^{K_{\max}}\Delta P e^{-1/2\Delta P^T\omega\Delta P}\delta\left(\sum_{i=1}^{K_{\max}}\Delta P_i-\Delta Z'\right)$$

$$\mathcal{Z}=\sum_{Z'}\left(\frac{(2\pi)^{K_{\max}}}{\det(\omega)}\right)^{1/2}\frac{\exp(-\frac{1}{2}(\Delta Z'/\sigma_{\overline{Z}})^2)}{\sqrt{2\pi\sigma_{\overline{Z}}^2}}. \tag{21}$$

$\sigma_{\overline{Z}}^2$ is the variance of ionization. Using Eqs. (12), (16), and (20), it is simply equal to

$$\sigma_{\overline{Z}}^2=\sum_{i,j=1}^{K_{\max}}(\omega^{-1})_{ij}. \tag{22}$$

Eq. (21) can be established properly from Eq. (1) [4]. It should be noted that both expressions of $d\mathcal{P}$ and $d\widetilde{\mathcal{P}}$ are simple and allows to calculate analytically a wide set of integrals.

B. Calculation of bound-bound and bound-free oscillator strengths

Once the average-atom populations are determined, one needs oscillator strengths to study the spectral properties of the plasmas. In this paper, only one-electron radiative dipolar electric transitions are considered. The initial and final states of the optical electron allows the processes to be distinguished; mainly free free (diffusion and inverse bremsstrahlung), bound free (photoionization), and bound bound (line absorption). The radiative opacities are proportional to the related cross sections. In the framework of the new screened-hydrogenic model (NSHM) [4], the free-free part of the spectrum raises no new problem [17,18]. The situation is different for bound-bound and bound-free transitions because we do not have any wave functions to calculate the matrix elements and get the oscillator strengths, nor any rapid semiclassical solution [19] due to ℓ splitting [4]. To overcome this difficulty, the key idea consists in connecting the discrete spectrum and the continuum series by continuity [18,20–22] while satisfying the one-electron sum rules [23,24].

Let us consider the following bound-bound and bound-free transitions, formally written as $n\ell \rightarrow n'\ell'(n<n')$ and $n\ell \rightarrow E\ell'$, and the related oscillator strengths $f_{n\ell,n'\ell'}$ and $df_{n\ell,E\ell'}/dE$. When the wave functions $\Psi_{n'\ell'}$ and $\Psi_{E\ell'}$ are both normalized in energy, the final states merge smoothly into the continuous form at the threshold $E=I_{n\ell}$ [21,25]. $I_{n\ell}$ is the continuum threshold of $n\ell$ level. Furthermore, a power law in energy is observed for $df_{n\ell,E\ell'}/dE$. These remarks are useful in proposing a fast evaluation of bound-bound and bound-free oscillator strengths for multicharged ions.

It seems natural to approximate the one-electron photoionization differential oscillator strength $df_{n\ell,E\ell'}/dE$ as $A_{n\ell,E\ell'}(I_{n\ell}/E)^{\alpha_{n\ell,E\ell'}}$. The exponent depends on $n\ell$, the partial wave $(\ell \rightarrow \ell \pm 1)$, and on the atomic system. Rose [26] proposed to use $\alpha_{1s,Ep}=\frac{8}{3}$ for $1s$ subshell and $\alpha_{n\ell,E\ell'}=3$ in the other cases. At the present time, we prefer to keep the value 3 for any $\alpha_{n\ell,E\ell'}$, following Kramers [19] and More [18] and waiting for more intensive comparisons with sophisticated atomic calculations. When $n<n'$, $f_{n\ell,n'\ell'}$ is linked to $df_{n\ell,E\ell'}/dE$ by continuity leading to: $f_{nl,n'l'}=Z^2_{n'\ell'}/n'^3 A_{n\ell,E\ell'}(I_{n\ell}/[\Delta E_{n\ell,n'\ell'}])^{\alpha_{n\ell,E\ell'}}$. $\Delta E_{n\ell,n'\ell'}$ is the transition energy and $Z^2_{n'\ell'}$ the screened charge calculated with the NSHM. When $n>n'$, $f_{n\ell,n'\ell'}$ is deduced from $f_{n'\ell',n\ell}$ using the relation: $-(2\ell'+1)f_{n'\ell',n\ell}=(2\ell+1)f_{n\ell,n'\ell'}$. For $\Delta n=0$ transitions, no general behavior or continuity rules are accessible. In consequence, as only two unknowns for each partial wave are remaining, namely, $f_{n\ell,n\ell'}$ and $A_{n\ell,E\ell'}$, we choose to close the system using the one-electron sum rules satisfied by oscillator strengths and dipolar matrix elements in any many-electron atom in the nonrelativistic regime [20,22,23]. The unknown quantities are then solutions of a first-order linear system which can be solved rapidly. In many-electron ion, $f_{n\ell,n\ell'}$ and $df_{n\ell,E\ell'}/dE$ have to be multiplied by the $n\ell$ shell occupancy $P_{n\ell}$ and by a degeneracy factor which corrects for possible occupation of the final state, $(1-P_{n'\ell'}/D_{n'\ell'})$ and $1/(1+e^{\mu-\varepsilon/k_BT})$ respectively, $(\varepsilon=h\nu-I_{n\ell})$ [4,18].

III. STATISTICAL BROADENING OF RADIATIVE TRANSITIONS

A. Opacity calculation

By definition, the opacity $\overline{\kappa}$ for LTE one-component plasmas at photon energy $h\nu$ is equal to [1]

$$\overline{\kappa(h\nu)}=[\overline{\kappa^{\mathrm{bb}}}(h\nu)+\overline{\kappa^{\mathrm{bf}}}(h\nu)+\overline{\kappa^{\mathrm{ff}}}(h\nu)](1-e^{-h\nu/k_BT})+\overline{\kappa^{\mathrm{scat}}}(h\nu). \tag{23}$$

The parentheses $(1-e^{-h\nu/k_BT})$ represents the stimulated emission. The terms $\overline{\kappa^{\mathrm{bb}}}$, $\overline{\kappa^{\mathrm{bf}}}$, and $\overline{\kappa^{\mathrm{ff}}}$ are bound-bound, bound-free, and free-free opacities, respectively. In the last one, pure scattering is excluded but taken into account via $\overline{\kappa^{\mathrm{scat}}}$. $\overline{\kappa}$ has the dimension of an area divided by a mass; it is commonly expressed in cm^2/g. We use this choice throughout this paper. For $\overline{\kappa^{\mathrm{ff}}}$, we choose the Kramers cross section for inverse bremsstrahlung. This cross section is averaged using a Maxwell distribution for electrons. Numerically, we find [18]

$$\overline{\kappa^{\mathrm{ff}}}=87.9\times 10^9\left(\frac{\overline{Z}}{A}\right)^2\frac{\overline{Z}\rho}{(h\nu)^3}\frac{g_{bi}}{\sqrt{k_BT}}. \tag{24}$$

g_{bi} is the Gaunt factor. It is kept to unity in our calculations. Energies (k_BT and $h\nu$) are in eV. The molar mass A is in g and the mass density in g/cm^3. As mentioned, inverse bremsstrahlung is not the only process between free electrons. Thomson diffusion is included too [18]

$$\overline{\kappa^{\mathrm{scat}}}(h\nu)=0.4\,\frac{\overline{Z}}{A}. \tag{25}$$

Note that $\overline{\kappa^{\mathrm{scat}}}$ and $\overline{\kappa^{\mathrm{ff}}}$ involve free-free transitions but their nature are deeply different. $\overline{\kappa^{\mathrm{ff}}}$ really corresponds to an absorption process whereas $\overline{\kappa^{\mathrm{scat}}}$ is a scattering process. In radiative transfer, the scattered photons do not belong to a beam but have not physically disappeared from the medium. Scattering has to be considered in the Rosseland opacity calculation because it describes the propagation of a radiation beam inside a medium but not in Planck opacity calculation which describes a radiation emission process. $\overline{\kappa^{\mathrm{bb}}}$ and $\overline{\kappa^{\mathrm{bf}}}$ are the most difficult to obtain.

B. Line broadening

1. Sharp line

Let us consider a one-electron transition between two configurations α and β. The LTE photoabsorption bound-bound opacity $\overline{\kappa^{\mathrm{bb}}}$ without the correction due to stimulated emission is equal to [4]

$$\overline{\kappa^{\mathrm{bb}}}(h\nu)=\frac{C_\kappa}{A}\sum_{\substack{\alpha,\beta\\ E(\alpha)<E(\beta)}}\mathcal{P}(\alpha)f_{\alpha,\beta}\Psi_{\alpha,\beta}(h\nu), \tag{26}$$

where $\mathcal{P}(\alpha)$ is the probability of the initial configuration α, $f_{\alpha,\beta}$ is the transition oscillator strength, and $\Psi_{\alpha,\beta}$ is the line profile [5] normalized to unity, C_κ is a numerical coefficient equal to $\mathcal{R}\mathcal{N}4\pi^2\alpha a_0^2$, with $\mathcal{R}$, α, and a_0 being, respectively, the Rydberg constant, the fine structure constant (that should not be confused with the configuration index), and the Bohr radius for hydrogen atom with infinite nuclear mass. When the photon energy is expressed in eV, C_κ is equal to 6.67×10^7 cm^2 eV. By introducing the populations $[P_k(\alpha)]$

of the $K_{\max}$ bound subshells of the ion with configuration α, its energy $E(\alpha)$, and degeneracy $\mathcal{D}(\alpha)$, $\mathcal{P}(\alpha)$ is given by the expression

$$\mathcal{P}(\alpha)=\frac{1}{Z_G}\,\mathcal{D}(\alpha)e^{-\beta[E(\alpha)-\mu\Sigma_{i=1}^{K_{\max}}P_i(\alpha)]}$$

$$Z_G=\sum_{\alpha}\,\mathcal{D}(\alpha)e^{-\beta[E(\alpha)-\mu\Sigma_{i=1}^{K_{\max}}P_i(\alpha)]}. \qquad (27)$$

For convenience, an explicit reference (through the variable α) to a particular configuration is now made. As mentioned, the major drawback of this technique is the calculation time due to the large number of configurations that must be chosen. One is easily convinced that the treatment of high-Z ions cannot be handled such a way, even keeping only the most probable configurations (the choice of which is anyway somewhat arbitrary).

A crude solution would consist in approximating $\overline{\kappa}^{\mathrm{bb}}$ with the average-atom spectrum. Whereas this assumption is useful to describe the statistical properties of a plasma (mean ionization, electron pressure . . .), it gives only a rough guess of its spectral properties [11] because many configurations can contribute to the total spectrum for a given transition. The absence of lines can have dramatic consequences on the Rosseland mean opacity estimation which is very sensitive to the number and line profile.

We have developed a technique to improve the average-atom spectrum without explicitly considering every individual configuration α. We now estimate the contribution of configurations for a specific one-electron transition $k\rightarrow k'$. Doing so, we will obtain the value of $\overline{\kappa^{\mathrm{bb}}}(h\nu)$ for an energy $h\nu$ without performing the summation in Eq. (26). For simplicity, $\Psi_{\alpha,\beta}$ is chosen to be a Dirac distribution centered at the $k\rightarrow k'$ transition energy $\Delta E_{k,k'}(\alpha)$. Equation (26) is rewritten as

$$\overline{\kappa^{\mathrm{bb}}}(h\nu)=\frac{C_\kappa}{A}\sum_{k\rightarrow k'}\,\sum_{\alpha}\,f_{k,k'}(\alpha)\mathcal{P}(\alpha)\,\delta(h\nu-\Delta E_{k,k'}(\alpha)). \qquad (28)$$

As the plasma is in LTE only configurations close to the average-atom configuration will significantly contribute to $\overline{\kappa^{\mathrm{bb}}}(h\nu)$ in Eq. (28). Due to the presence of the Boltzmann factor, $f_{k,k'}(\alpha)$ is close to the average-atom oscillator strength $\widetilde{f}_{k,k'}$ [1]. Equation (28) is then written as

$$\overline{\kappa^{\mathrm{bb}}}(h\nu)=\frac{C_\kappa}{A}\sum_{k\rightarrow k'}\,\overline{f_{k,k'}}\sum_{\alpha}\,\mathcal{P}(\alpha)\,\delta(h\nu-\Delta E_{k,k'}(\alpha)). \qquad (29)$$

At this point, it is particularly attractive to use the classical theory of fluctuations [14]. This approach is justified when many lines overlap. The original discrete splitting tends to be smeared out to produce a quasicontinuous broadening. Of course, each individual line is broadened by various mechanisms (Doppler, collisions, . . .) [5] which enhance the quasicontinuous broadening originating from the statistics (hence, the name of statistical broadening for this phenomenon [9,11]).

We then use the ideas developed in Sec. II. The electron populations are allowed to vary continuously and the discrete summation becomes a multidimensional integral [27]. In the framework of the screened-hydrogenic average-atom model (although the method can be applied to any average-atom model), we have observed that $\mathcal{P}(\alpha)$ is equal to a Gaussian probability density defined by Eq. (19). $\overline{\kappa^{\mathrm{bb}}}$ is equal to

$$\overline{\kappa^{\mathrm{bb}}}(h\nu)=\frac{C_\kappa}{A}\sum_{k\rightarrow k'}\,\overline{f_{k,k'}}\left(\frac{\det(\omega)}{(2\pi)^{K_{\max}}}\right)^{1/2}$$
$$\times\int d^{K_{\max}}\Delta P e^{-1/2\Delta P^T\omega\Delta P}$$
$$\times\,\delta(h\nu-\Delta E_{k,k'}(\Delta P_i)). \qquad (30)$$

The transition energy $\Delta E_{k,k'}[(\Delta P_i)]$ is expressed as a first-order Taylor expansion in occupation numbers around the average-atom configuration:

$$\Delta E_{k,k'}[(\Delta P_i)]=\Delta E_{k,k'}(0)+\sum_{i=1}^{K_{\max}}\left.\frac{\partial\Delta E_{k,k'}}{\partial P_i}\right|_0\Delta P_i+\cdots\;.$$

Due to the form of the density probability $d\mathcal{P}$ in Eq. (19), the natural variables are the deviations (ΔP_i) with respect to the average-atom populations. It is useful to introduce the notations

$$\overline{\Delta E}_{k,k'}=\Delta E_{k,k'}(0)$$

$$\varepsilon_{k,k'}^{i}=\left.\frac{\partial\Delta E_{k,k'}}{\partial P_i}\right|_0$$

$$\sigma_{k,k'}=\sqrt{\varepsilon_{k,k'}^{T}\omega^{-1}\varepsilon_{k,k'}}=\sqrt{\mathrm{var}(\Delta E_{k,k'})}. \qquad (31)$$

Using the Fourier transformation of the Dirac distribution, the constraint in Eq. (30) which prevents any calculation of the Gaussian integral disappears. By using the identity [28]

$$\int_{\mathbb{R}^N}d^Nxe^{-(1/2x^TUx+b^Tx)}=\left(\frac{(2\pi)^N}{\det(U)}\right)^{1/2}e^{1/2b^TU^{-1}b}, \qquad (32)$$

where U is a $N\times N$ symmetric definite positive matrix and x and b are N-dimensional vectors, a simpler expression for $\overline{\kappa^{\mathrm{bb}}}$ is obtained

$$\overline{\kappa^{\mathrm{bb}}}(h\nu)=\frac{C_\kappa}{A}\sum_{k\rightarrow k'}\,\widetilde{f}_{k\rightarrow k'}\int du\;\;\delta(h\nu-\overline{\Delta E}_{k,k'}-u)$$
$$\times\frac{e^{-u^2/(2\sigma_{k,k'}^2)}}{\sqrt{2\pi\sigma_{k,k'}^2}}. \qquad (33)$$

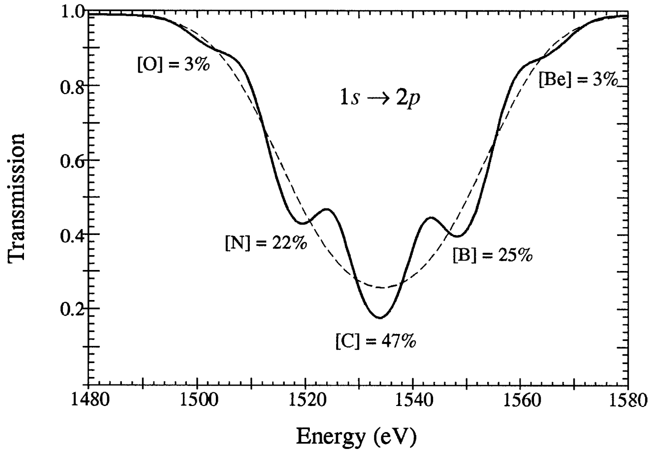

FIG. 1. Transmission spectrum of a LTE aluminum plasma ($T = 40$ eV, $\rho = 1.35\times 10^{-2}$ g/cm^3) deduced from the NSHM with (solid line) and without (dashed line) the splitting in integer charge stages. The energy domain corresponds to $1s\rightarrow 2p$ transitions. The energy resolution is equal to 0.7 eV. Ion fractions are estimated; [O] means [O]-like ions, etc.,... .

This convolution product can be calculated analytically but we prefer to leave it in this particular form in order to keep an expression that can be compared to forthcoming results. To sum up, the initial summation, which can contain a huge number of configuration [Eq. (26)], involves finally a limited number of terms.

It is important to note that $\overline{\Delta E}_{k,k'}$ is not the mean energy $\widetilde{\Delta E}_{k,k'}$ of the cluster of lines corresponding to a particular transition energy [10]. As in UTA (unresolved transition arrays) [2] or STA (super transition arrays) [3] frameworks, $\widetilde{\Delta E}_{k,k'}$ must be calculated by weighting the Gaussian probability law by the oscillator strengths $f_{k,k'}:f_{k,k'} = f^{\mathrm{one}}_{k,k'}(\{P_i\})P_k(D_{k'}-P_{k'})$. $f^{\mathrm{one}}_{k,k'}$ is the one-electron oscillator strength averaged with respect to initial (k) and final (k') states. An error can appear when, for a given transition $k\rightarrow k'$, the product $P_k(D_{k'}-P_{k'})$ is close to zero.

2. *Broad line*

Going back to Eq. (26), each line width is a function of $[h\nu - \Delta E_{k,k'}(\alpha)]$ and depends implicitly on configuration α. In order to generalize Eq. (33), the amplitude but also the shape of each individual line, for a transition $k\rightarrow k'$, are close to the average-atom one $\widetilde{\Psi}_{k,k'}$. Only the transition energy depends on the configuration of interest. The calculation becomes feasible by changing $f_{k,k'}(\alpha)$ in $\widetilde{f}_{k,k'}$ in Eq. (28). $\overline{\kappa^{\mathrm{bb}}}$ is then approximately given by

$$\overline{\kappa^{\mathrm{bb}}}(h\nu) = \frac{C_\kappa}{A}\sum_{k\rightarrow k'}\widetilde{f}_{k,k'}\left(\frac{\det(\omega)}{(2\pi)^{K_{\max}}}\right)^{1/2}\int d^{K_{\max}}\Delta P \times e^{-1/2\Delta P^T\omega\Delta P}\widetilde{\Psi}_{k,k'}(h\nu - \Delta E_{k,k'}(\Delta P_i)). \tag{34}$$

Taking the Fourier transformation of $\widetilde{\Psi}_{k,k'}$, $\overline{\kappa^{\mathrm{bb}}}$ is equal to

$$\overline{\kappa^{\mathrm{bb}}}(h\nu) = \frac{C_\kappa}{A}\sum_{k\rightarrow k'}\widetilde{f}_{k\rightarrow k'}\int du\ \widetilde{\Psi}_{k,k'}(h\nu - \overline{\Delta E}_{k,k'} - u) \times \frac{e^{-u^2/(2\sigma^2_{k,k'})}}{\sqrt{2\pi\sigma^2_{k,k'}}}. \tag{35}$$

Contrasting with the last result, the convolution cannot be analytically reduced for any line shape and must be computed numerically (except for a Gaussian profile). In practice, the variance $\sigma^2_{k,k'}$ is moderate and the convolution has to be performed by considering only a small energy interval.

C. Photoionization threshold broadening

The statistical method to broaden the broad lines is kept to treat the photoionization thresholds. The bound-free cross sections of the configurations (α), involved in a particular photoionization process of the subshell k, are assumed to have the same shape but different threshold energies $[I_k(\alpha)]$. Starting from [4]

$$\overline{\kappa^{\mathrm{bf}}}(h\nu) = \frac{C_\kappa}{A}\sum_{k,\alpha}\mathcal{P}(\alpha)\varphi_{\alpha,k}(h\nu - I_k(\alpha)), \tag{36}$$

where $\overline{\kappa^{\mathrm{bf}}}$ is the bound-free mean opacity without stimulated emission, $\mathcal{P}(\alpha)$ is the probability of the initial configuration α seen above, and $\varphi_{\alpha,k}$ is the bound-free threshold profile. We easily find an approximate expression for $\overline{\kappa^{\mathrm{bf}}}$. The same units as in Eq. (26) have been kept. Replacing $\widetilde{\Psi}_{k,k'}$ by $\widetilde{\varphi}_k$ and introducing

$$\overline{I_k} = I_k(0),$$

$$\varepsilon^i_k = \left.\frac{\partial I_k}{\partial P_i}\right|_0,$$

$$\varrho_k = \sqrt{\varepsilon^T_k\omega^{-1}\varepsilon_k} = \sqrt{\mathrm{var}(I_k)} \tag{37}$$

in Eq. (35), we get the final result

$$\overline{\kappa^{\mathrm{bf}}}(h\nu) = \frac{C_\kappa}{A}\sum_k\int du\ \widetilde{\varphi}_k(h\nu - \overline{I_k} - u)\ \frac{e^{-u^2/2\varrho^2_k}}{\sqrt{2\pi\varrho^2_k}}. \tag{38}$$

D. Splitting in integer ion stages

Starting from a grand canonical description of a LTE plasma, a definite meaning can be given to the notion of screened-hydrogenic average-atom model, which enables to build a method of splitting in integer charge stages that can be extended to any average-atom model [4]. In order to improve the former radiative-transition statistical broadening, we can include the detailed integer stage accounting by using both the classical theory of fluctuations and the average-atom model. We have seen in Sec. II that it is sufficient to replace the initial Gaussian density probability $d\mathcal{P}$ [Eq. (19)] by $d\widetilde{\mathcal{P}}$ defined by Eq. (21).

In consequence, by keeping the notations of Eq. (34), $\overline{\kappa^{\mathrm{bb}}}$ can be expressed as

$$\overline{\kappa^{\mathrm{bb}}}(h\nu)=\frac{C_\kappa}{A}\sum_{k\to k'}\sum_{Z'}\tilde{f}_{k,k'}\frac{1}{\mathcal{Z}}\int d^{K_{\max}}\Delta P e^{-1/2\Delta P^T\omega\Delta P}\times\tilde{\Psi}_{k,k'}(h\nu-\Delta E_{k,k'}(\Delta P_i))\times\delta\left(\Delta Z'-\sum_{k=1}^{K_{\max}}\Delta P_k\right). \tag{39}$$

By introducing the notations [Eq. (31)]

$$\mathcal{A}_{\mathcal{N}}=\begin{pmatrix}\mathrm{var}(\Delta E_{k,k'}) & \mathrm{cor}(\overline{Z},\Delta E_{k,k'})\\ \mathrm{cor}(\overline{Z},\Delta E_{k,k'}) & \mathrm{var}(\overline{Z})\end{pmatrix}$$

$$\mathrm{cor}(\overline{Z},\Delta E_{k,k'})=\sum_{i,j=1}^{K_{\max}}(\omega^{-1})_{i,j}\varepsilon^i_{k,k'} \tag{40}$$

$$a_b(u)=\begin{pmatrix}u\\ \Delta Z'\end{pmatrix}$$

and by using the Fourier transformation of the Dirac distribution and of the line profile $\tilde{\Psi}_{k,k'}$ in Eq. (39), we obtain a closed expression for $\overline{\kappa^{\mathrm{bb}}}$, namely,

$$\overline{\kappa^{\mathrm{bb}}}(h\nu)=C_\kappa A\,\frac{\displaystyle\sum_{k\to k'}\sum_{Z'}\tilde{f}_{k,k'}\int du\;\tilde{\Psi}_{k,k'}(h\nu-\overline{\Delta E}_{k,k'}-u)\,\frac{e^{-1/2a_b^T(u)\mathcal{A}_{\mathcal{N}}^{-1}a_b(u)}}{2\pi\sqrt{\det(\mathcal{A}_{\mathcal{N}})}}}{\displaystyle\sum_{Z'}\frac{e^{-(\Delta Z')^2/(2\sigma_Z^2)}}{\sqrt{2\pi\sigma_Z^2}}}. \tag{41}$$

As for the statistical broadening of photoionization thresholds, the way to incorporate the splitting in integer charge stages in $\overline{\kappa^{\mathrm{bf}}}$ is similar to what has been previously done. By keeping in mind Eqs. (37) and by introducing the following useful variables:

$$\mathcal{E}_{\mathcal{L}}=\begin{pmatrix}\mathrm{var}(I_k) & \mathrm{cor}(\overline{Z},I_k)\\ \mathrm{cor}(\overline{Z},I_k) & \mathrm{var}(\overline{Z})\end{pmatrix}$$

$$\mathrm{cor}(\overline{Z},I_k)=\sum_{i,j=1}^{K_{\max}}(\omega^{-1})_{i,j}\varepsilon^i_k$$

$$\ell_e(u)=\begin{pmatrix}u\\ \Delta Z'\end{pmatrix}, \tag{42}$$

$\overline{\kappa^{\mathrm{bf}}}$ is equal to

$$\overline{\kappa^{\mathrm{bf}}}(h\nu)=\frac{C_\kappa}{A}\,\frac{\displaystyle\sum_k\sum_{Z'}\int du\;\tilde{\phi}_k(h\nu-\overline{I_k}-u)\,\frac{e^{-1/2\ell_e^T(u)\mathcal{E}_{\mathcal{L}}^{-1}\ell_e(u)}}{2\pi\sqrt{\det(\mathcal{E}_{\mathcal{L}})}}}{\displaystyle\sum_{Z'}\frac{e^{-(\Delta Z')^2/(2\sigma_Z^2)}}{\sqrt{2\pi\sigma_Z^2}}}. \tag{43}$$

Eqs. (35), (38), (41), and (43) are the basic formulas that allow a fast estimation of radiative opacities for in-line calculations.

E. Consistency between bound-bound and bound-free opacities

Our method of oscillator strength calculation uses the one-electron sum rules and the consistent treatment of bound-bound and bound-free transitions. It should be noted that these principles can be very easily tested a posteriori by integrating $\overline{\kappa^{\mathrm{bb}}}$ and $\overline{\kappa^{\mathrm{bf}}}$ over the entire spectrum. The idea was initiated by Sampson [29]. Starting from the one-electron sum rule:

$$\sum_{n'\ell'}f_{n\ell,n'\ell'}+\int_{I_{n\ell}}^{\infty}\frac{df_{n\ell,E_{\ell'}}}{dE}\,dE=1,$$

and after some algebraic manipulations, he found:

$$\int_0^\infty[\overline{\kappa^{\mathrm{bf}}}(u)+(1-e^{-u})\overline{\kappa^{\mathrm{bb}}}(u)]du=\frac{C_\kappa}{A}\frac{(Z-\overline{Z})}{k_BT}. \tag{44}$$

u stands for $h\nu/k_BT$. Bound-bound emission, represented by $(1-e^{-u})$, is essential to obtain the former closed expression. Consequently, a dimensionless number can be defined by dividing the left term in Eq. (44) by the right term of the same equation. In practical applications, this ratio must be as close as possible to unity. Any deviation from one indicates either a lack of consistency between bound-bound and bound-free oscillator strengths or a violation of sum rules.

IV. RESULTS

The first example is a LTE aluminum plasma ($T=40$ eV, $\rho=1.35\times10^{-2}$ g/cm^3). We compare our calculation (Fig. 1) with an experimental transmission spectrum in

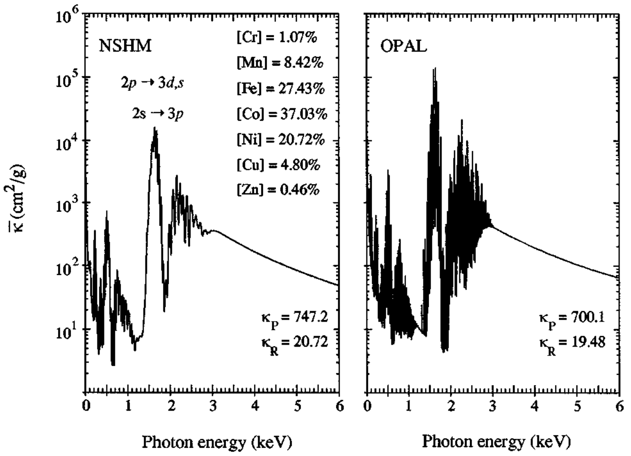

FIG. 2. Photoabsorption spectra of a LTE germanium plasma ($T = 300$ eV, $\rho = 10^{-2}$ g/cm^3): NSHM and OPAL (this latter has been drawn by using data from Ref. [32]). κ_R and κ_P are, respectively, the Rosseland and Planck opacities expressed in cm^2/g.

the energy range of $1s \rightarrow 2p$ transitions (Fig. 4 of Ref. [30]). The energy resolution is equal to 0.7 eV. Our aim is not to perform an accurate spectroscopic interpretation but to illustrate our method in a simple situation. It is clearly shown that each integer charge stage contribution (in full line), introduced by perturbation with respect to the average-atom data (in dashed line), appears on the spectrum. Three ion stages dominate: [N]-, [C]-, and [B]-like ions. Our estimation of the ion fractions is given on Fig. 1. The results are quite similar to those published by Kilcrease *et al.* [30]. Due to the modeling of density effects using the degeneracy-reduction model proposed by Zimermann and More [13] (the two parameters a_{ZM} and b_{ZM} being, respectively, equal to 3 and 1), and the fixed set of screening constants, the ionization of the plasma given by the NSHM is a little bit stronger [4]: [C]-like ions dominate in both cases but the relative weights of the neighbor ions ([N]- and [B]-like) are different, hence the difference concerning the asymmetry of the distributions between the two models. The table of screening constants explains the slight shift in energy close to 0.3% for the main charge stage too.

In Fig. 2, two spectra are shown for a LTE germanium plasma ($T = 300$ eV, $\rho = 10^{-2}$ g/cm^3). The NSHM calculation with the splitting in integer charge stages is compared to the OPAL [31,32] spectrum. Concerning our model, the contribution of the various ion species are predicted (the ion fractions are on Fig. 2). NSHM is weaker than OPAL between 0 and 1 keV. The reason lies in the ionization pressure treatment introduced by Zimmerman and More [13]. The orbital degeneracy reduction, which can reach several orders of magnitude, tends to cut the bound-free spectrum. This effect is mainly noticeable at low energies due to essentially the high n orbitals. This phenomenon is not systematic because, for light elements, the statistical broadening of radiative transitions may mask it. The Rosseland opacity (κ_R) and the Planck opacity (κ_P) are also given on Fig. 2. The NSHM value (20.72 cm^2/g) is very close to the OPAL one (19.48 cm^2/g). Since only the region around four times the temperature (1200 eV here) will contribute to κ_R, this example is a clear illustration of the importance of using both the description of atomic structure as good as we can imagine (here ℓ splitting for the NSHM) and the statistical treatment of radiative transitions. Moreover, we stress on using a procedure that goes beyond the independent-particle approximation. This phenomenon is illustrated on Fig. 3. The integrands of Rosseland (χ_R) and Planck (χ_P) opacities [4] have been added to the spectral opacity [(Eq. 23)]

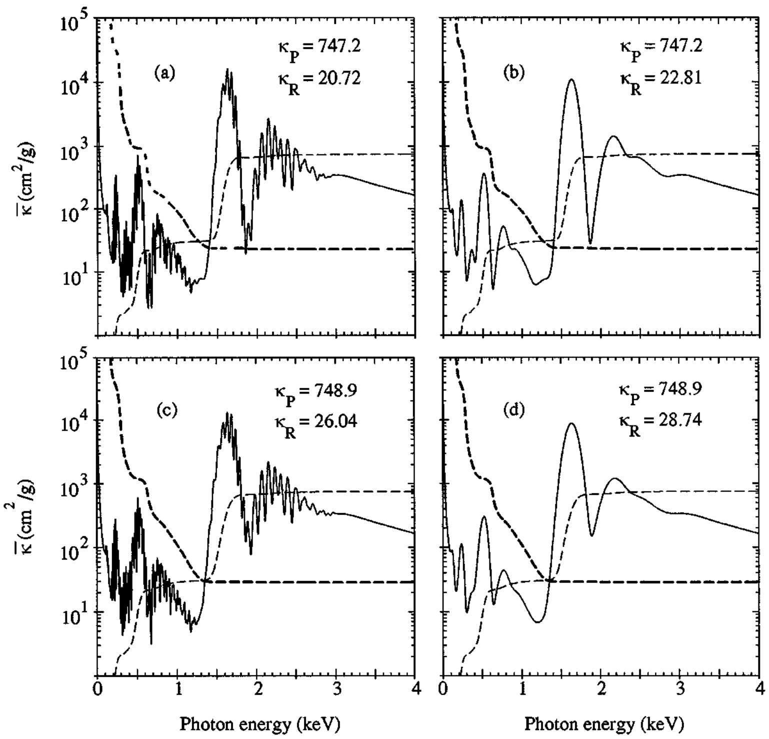

FIG. 3. Photoabsorption spectra of a LTE germanium plasma ($T = 300$ eV, $\rho = 10^{-2}$ g/cm^3) calculated with the NSHM: (a) splitting in integer charge stages with correlations, (b) average atom only with correlations, (c) splitting in integer charge stages without correlations, and (d) average atom only without correlations. Rosseland opacity (κ_R) and Planck opacity (κ_P) are in cm^2/g. The integrand of κ_R(κ_P) is in bold (normal) dashed line.

$$[\chi_R(h\nu)]^{-1} = \int_0^{h\nu/k_BT} du[\overline{\kappa(u)}]^{-1}\,\frac{15}{4\pi^4}\,\frac{u^4 e^{-u}}{(1-e^{-u})^2}$$

$$\chi_P(h\nu) = \int_0^{h\nu/k_BT} du[\overline{\kappa(u)} - \overline{\kappa^{\text{scat}}}(u)]\,\frac{15}{\pi^4}\,\frac{u^3}{e^u-1}, \quad (45)$$

with $\chi_{\rm R}(\infty)=\kappa_{\rm R}$ and $\chi_{\rm P}(\infty)=\kappa_P$. As in Eq. (44), the variable u stands for the photon energy divided by k_BT. The electrostatic interaction induce correlations [implicitly present in the matrix ω in Eq. (19)] which decrease the width of each Gaussian shapes of lines [here $2s\rightarrow 3p$, $2p\rightarrow 3s$, and $2p\rightarrow 3d$ transitions on Fig. 3(a) and Fig. 3(b)]. Neglecting them here would have decreased the well near 1200 eV, and consequently increased the value of $\kappa_{\rm R}$ [Fig. 3(c) and Fig. 3(b)]. In this example, $\kappa_{\rm P}$ appears to be independent of the correlations and the splitting in integer charge stages because, in this case, the key parameter is the line intensity whose calculation stays unmodified. By contrast, the most detailed treatment [Fig. 2(a) or Fig. 3(a)] is the one that gives the value of opacity coefficient closest to OPAL. From Fig. 3(d) to Fig. 3(a), the relative deviation with respect to OPAL Rosseland opacity falls from 48% to 34%, 17%, and 6% successively. This is only due to the slight differences which take place in the vicinity of the crossing between $\chi_{\rm R}$ and $\chi_{\rm P}$ on Fig. 3. In this example, the most important effect is the role played by correlations between bound electrons.

V. CONCLUSION

A method, based on the screened-hydrogenic average-atom model and on the classical theory of fluctuations, is presented in order to rapidly estimate LTE spectral opacities. Each average-atom line is replaced by a Gaussian shape which takes into account the contribution of the most probable configurations around the average-atom configuration. Photoabsorption spectra obtained are intermediate between a crude average-atom spectrum and a DCA treatment. The splitting in integer ion stages can be included. This method is not restricted to a description of the atomic structure through the screened hydrogenic model but can be extended to any average-atom formalism too.

Comparisons of our results to more detailed calculations and experimental spectra show the need of a joint use of a description of the atomic structure of the average atom as detailed as possible and a statistical treatment of the lines without performing an explicit detailed configuration accounting, which would be too time consuming in such a situation. The role of correlations between bound electrons is emphasized. From the photoabsorption spectra encountered, both the Rosseland mean opacity and the detailed charge stage accounting are well estimated. The next step is to extend the formalism to study the spectral properties of non-LTE plasmas.

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