Superconfiguration accounting approach versus average-atom model in local-thermodynamic-equilibrium highly ionized plasmas

G. Faussurier

Commissariat à l'Energie Atomique, 91680 Bruyères-le-Châtel, Boîte Postale 12, France

Statistical methods of describing and simulating complex ionized plasmas requires the development of reliable and computationally tractable models. In that spirit, we propose the screened-hydrogenic average atom, augmented with corrections resulting from fluctuations of the occupation probabilities around the mean-field equilibrium, as an approximation to calculate the grand potential and related statistical properties. Our main objective is to check the validity of this approach by comparing its predictions with those given by the superconfiguration accounting method. The latter is well-suited to this purpose. In effect, this method makes it possible to go beyond the mean-field model by using nonperturbative, analytic, and systematic techniques. Besides, it allows us to establish the relationship between the detailed configuration accounting and the average-atom methods. To our knowledge, this is the first time that the superconfiguration description has been used in this context. Finally, this study is also the occasion for presenting a powerful technique from analytic number theory to calculate superconfiguration averaged quantities. [S1063-651X(99)04106-9]

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I. INTRODUCTION

The properties of hot dense matter are important in astrophysics and in laboratory-plasma physics where equations of state, photoabsorption, and transport coefficients are required to perform accurate numerical simulations [1]. Their calculation depends on the electronic structure of the atoms constituting the plasma, regardless of thermodynamic conditions. For plasmas in local thermodynamic equilibrium (LTE), the only thermodynamic state considered in this paper, methods of varying degrees of complexity have been used to extend pioneering works based on the Thomas-Fermi approach [2–8] and the screened-hydrogenic average-atom model [9]. This goal has been achieved by using two kinds of models: the average-atom model (AAM) [10–16] and the density-functional theory (DFT) [17–22]. In the AAM, electrons are assumed to occupy single-particle levels according to Fermi statistics. They are moving in an average effective potential which is consistent with the single-particle wave functions. In the DFT, electron density has the dominant role. The grand potential at finite temperature of a fermion system embedded in an external potential is a unique functional of the electron density. Since the exact expression of this functional is unknown, one must resort to additional assumptions concerning electron density, kinetic energy, and exchange-correlation effects, which lead to the local-density-functional approximation. The resulting tractable set of wave equations, which must be solved self-consistently to determine the electron density, is referred to generically as the Kohn and Sham equations. For an atomic system at finite temperature, the profound similarity between the Kohn and Sham equations and the average-atom equations can be emphasized by expressing both models in terms of functional integrals [23]. This extends the formulation of the screened-hydrogenic AAM, which has been shown to stand on the saddle-point evaluation of an integral representation of the partition function [24,25]. The AAM and the DFT are de-duced by (i) finding a specific functional-integral representation of the grand-canonical partition function of the system of interest and (ii) expanding the functional integral by means of the saddle-point method. As far as the DFT is concerned, it has permitted us to find an exact expression of the exchange-correlation term to the grand potential. From our point of view, the formulation of the AAM and the DFT in the same theoretical framework is one of the most interesting and fruitful features of the functional-integral method. Indeed, it is worth mentioning that the evaluation of a specific integral representation (with or without path integral) of a partition function delivers mainly mean-field results for the many-particle systems. Consequently, in spite of their usefulness, the accuracy of DFT and AAM is not better understood than that of screened-hydrogenic AAM.

In this paper, the mean-field results are revisited and compared to calculations done in the framework of the super configuration accounting (SCA) approach [26]. Restricting oneself to the screened-hydrogenic AAM for the sake of simplicity [27], one shows that the AAM accuracy becomes open to constructive criticism and basic notions deduced from it can be examined. The SCA method has its origin in the supertransition array (STA) model [28–32]. In recent years, the STA method has extensively been used to interpret bound-bound and bound-free spectra of LTE plasmas. To summarize, the entire spectrum is divided into STA's i.e., between pairs of superconfigurations where each superconfiguration is a particular set of near-lying configurations. Each STA spectrum is represented by a Gaussian constructed from array moments—total intensity, average energy, and variance—that are analytically calculated. The fine details of the spectrum are gradually evidenced by a convergence procedure obtained by splitting each STA into a number of smaller STA's until the desired spectral resolution is reached. By doing so, the brute-force summation over the individual lines one by one is avoided. Needless to say, an enormous number of configurations are needed to characterize a plasma at equilibrium and a detailed account method

(or DCA for detailed configuration accounting) is still today computationally impractical. In fact, the essential reason is that it would consume an outrageous amount of computer time. The central achievement of STA theory is precisely a way to overcome this difficulty to some extent. Since the AAM can be proven to originate from the saddle-point evaluation of an integral representation of the grand-canonical partition function Z_G [25], and since the SCA evaluation of Z_G converges to a complete DCA evaluation (starting from the AAM for instance), it is tempting to compare both methods. In summary, SCA offers the opportunity to go beyond the given limit of a nonintegrable mean-field model by using nonperturbative, analytic methods. Moreover, SCA is intended to bridge the gap between an intractable discrete description of matter, the DCA method, and a questionable continuous one, the AAM. Furthermore, a technique, known as the circle method in analytic number theory [33], is utilized in the SCA approach, to lighten and improve the calculation of the statistical sums of interest.

The paper is organized as follows. The formulation of the screened-hydrogenic AAM within the framework of the integral representation of a partition function is reproduced in Sec. II, along with the required background and notations. In Sec. III, the SCA method is considered: useful formulas are derived to obtain analytic expressions for the plasma statistical averages, such as, e.g., atomic-shell mean occupancies, ionization-distribution parameters (mean, variance, skewness, and kurtosis), or integer ion-stage fractions. Section IV is devoted to numerical applications and Sec. V summarizes results.

II. SCREENED-HYDROGENIC AVERAGE-ATOM MODEL

Different methods exist to study the statistical properties of highly charged LTE one-component ion plasmas at given temperature T and mass density ρ. The screened-hydrogenic atom model has the benefits of being easily usable, reasonably accurate, and fast enough to be implemented into an atomic-physics package of a hydrodynamic code. Moreover, it is well-defined and thermodynamically consistent [25]. The grand-canonical partition function Z_G of bound electrons is the starting point of all relevant developments

$$Z_G = e^{-\beta\Omega} = \sum_C \mathcal{D}_C e^{-\beta[E_C - \mu N_C]}. \quad (2.1)$$

Ω, E_C, N_C, and $\mathcal{D}_C$ are the grand potential, the energy, the total electron number, and the statistical weight of an electronic configuration C, respectively. Introducing the shell occupation number (P_i) and the shell degeneracies (D_i), $N_C = \sum_{i=1}^{K_{max}} P_i$ and $\mathcal{D}_C = \Pi_{i=1}^{K_{max}} \binom{D_i}{P_i}$; $\binom{D_i}{P_i}$ is the standard binomial coefficient: $\binom{D_i}{P_i} = D_i!/[P_i!(D_i-P_i)!]$. The shell index i depends on the shell quantum numbers: $i = n$ or $n\ell$, where n and ℓ are principal and orbital quantum numbers, respectively. μ is the chemical potential and β the inverse temperature ($\beta = 1/k_B T$, k_B is the Boltzmann constant), whereas the sum Σ_C covers the set of all configurations constructed from the finite number K_{max} of bound shells. So Σ_C denotes $\Sigma_{P_1=0}^{D_1} \cdots \Sigma_{P_i=0}^{D_i} \cdots \Sigma_{P_{K_{max}}=0}^{D_{K_{max}}}$. The chemical potential μ is cal-

culated by imposing the average neutrality of the ion cell. Z, $(\overline{P_i})$, $\overline{Z^*}$, and $F_\alpha(\eta)$ are, successively, the ion change number, the shell mean occupancies, the average ionization, and the Fermi-Dirac function $[F_\alpha(\eta) = \int_0^\infty dx\, x^\alpha/(1+e^{x-\eta})]$; μ obeys the equations ($\eta = \beta\mu$)

$$\overline{N} + \overline{Z^*} = Z, \quad \sum_{i=1}^{K_{max}} \overline{P_i} = \overline{N} = -\left(\frac{\partial\Omega}{\partial\mu}\right)_{\rho,T},$$

$$\overline{Z^*} = 4\pi \frac{A}{\rho\mathcal{N}} \left(\frac{2m}{\beta h^2}\right)^{3/2} F_{1/2}(\eta). \quad (2.2)$$

A is the molar mass of the element, $\mathcal{N}$ the Avogadro number, m the electron mass, and h the Planck constant. The thermodynamic limit is assumed, hence the use of the mass density ρ instead of the volume V of the system. For completeness, we recall that the electron density N_e, the atomic particle density N_a, and the ion-sphere radius R_0 satisfy the relations $(4/3)\pi R_0^3 N_a = 1$, $N_a = \rho\mathcal{N}/A$, and $\overline{Z^*} = N_e/N_a$. Throughout this paper, the shell degeneracies are assumed to be integer, so that no pressure-ionization phenomenon is taken into account by reducing them [14]; the thermodynamic variables, kept constant when partial derivatives are performed, will not be mentioned each time. Finally, (P_i) is used subsequently to depict a configuration C, which justifies the notation $E[(P_i)] = E_C$. For example [27], within the framework of the Mayer's model (in atomic units),

$$E[(P_i)] = \sum_{i=1}^{K_{max}} P_i\left(E_i - \frac{V_{ii}}{2}\right) + \frac{1}{2}\sum_{i,j=1}^{K_{max}} P_i P_j V_{ij}, \quad (2.3)$$

where $E_i = -Z^2/(2n_i^2)$ and $V_{ij} = (Z\sigma_{ij})/n_i^2$. The screening constants (σ_{ij}) are configuration-independent. By contrast, in the screened-hydrogenic model (SHM),

$$E[(P_i)] = -\sum_{i=1}^{K_{max}} \frac{Z_i^2}{2n_i^2} P_i,$$

$$Z_i = Z + \alpha_i - \sum_{j=1}^{K_{max}} \sigma_{ij} P_j, \quad (2.4)$$

where $Z_i = Z + \alpha_i - \Sigma_{j=1}^{K_{max}} \sigma_{ij} P_j$. (σ_{ij}) is a set of screening parameters independent of the electronic configuration and (α_i) are SHM-specific constants.

The usual and proper way to analyze the thermodynamic properties of equilibrium systems is to resort to a partition function (here Z_G). Z_G is of fundamental importance to make apparent the thermodynamic consistency of the formalism and to calculate the statistical average $\overline{O}$ of any physical quantity O which depends explicitly on the electronic configuration

$$\overline{O} = \frac{1}{Z_G} \sum_C \mathcal{D}_C O_C e^{-\beta[E_C - \mu N_C]}. \quad (2.5)$$

Unfortunately, the exact value of Z_G is unknown in the majority of cases and a brute-force computation of the discrete sum Σ_C is difficult to achieve due to the large number of configurations. Furthermore, a closed form is rarely possible

to write down when E_C is a nonlinear function of (P_i). This nonlinearity reflects the many-body effects and explains why the standard textbook factorization of Z_G, which is well-suited for ideal Fermi gas, does not directly apply here. A solution is to find an integral representation of Z_G. In short, Σ_C is replaced by an integral at the expense of introducing auxiliary variables. Its factorization thus becomes possible, Z_G can be evaluated by using the saddle-point technique, and one finds that the saddle point is identical to the AAM.

At this stage, it is worthwhile noting that the integral representation of Z_G is not unique. As a consequence, it is clear that the AAM and the corrections to the mean-field equations are not independent of the approximation retained to calculate a particular integral. This aspect will be illustrated by choosing, first, a universal representation and, then, another one which depends on E_C.

For the sake of simplicity and generality, we can take the forthcoming integral representation which holds for any expression of E_C. Only the main results are given in the plain text. Algebraic intermediate calculations are detailed in Appendix A.

Starting from Eq. (2.1), Z_G can be written as follows [25,34]:

$$Z_G = \int [dU] e^{-\beta S(U)},$$

$$[dU] = \frac{d^{K_{max}} x \, d^{K_{max}} \omega}{(2\pi)^{K_{max}}},$$

$$U_j = x_j, \quad U_{j+K_{max}} = \omega_j, \quad j = 1, \ldots, K_{max}, \tag{2.6}$$

$$S(U) = E[(x_i)] - \sum_{j=1}^{K_{max}} i\omega_j x_j / \beta - D_j \ln[1 + e^{-i\omega_j + \eta}]/\beta.$$

Since we are dealing with the partition function of a system at thermodynamic equilibrium, the saddle-point method can be used to estimate Z_G in Eq. (2.6). After a few manipulations, one finds that the coupled nonlinear Fermi-Dirac equations

$$P_j^0 = D_j f_j^0, \quad e_j^0 = \left.\frac{\partial E}{\partial P_j}\right|_{(P_i^0)} - \mu, \quad f_j^0 = 1/(1 + e^{\beta e_j^0}), \tag{2.7}$$

which define the fractional occupations (P_i^0) of the bound orbitals of the screened-hydrogenic average-atom model, are identical to the saddle-point equation

$$\left.\frac{\partial S}{\partial U_j}\right|_{(U_i^0)} = 0. \tag{2.8}$$

The second-order Taylor expansion terms [15] have to be calculated to incorporate the average-atom model with corrections resulting from fluctuations of the occupation probabilities around the mean-field description of statistical equilibrium (or FAA for fluctuations around average atom). They can be expressed in terms of the average-atom populations (P_i^0) only. The first corrections to the average-atom model

are then estimated without handling complicated perturbation strategy. Using the grand potential defined in Eq. (2.1), the final result simply reads

$$\Omega \approx \Omega^{eff} = \Omega^0 + \frac{\text{Tr}[\ln(\Delta S^0)]}{2\beta},$$

$$\Omega^0 = E[(P_i^0)] - \mu \sum_{i=1}^{K_{max}} P_i^0 + \frac{1}{\beta} \sum_{i=1}^{K_{max}} D_i(f_i^0 \ln f_i^0 + g_i^0 \ln g_i^0), \tag{2.9}$$

$$(\Delta S^0)_{ij} = \delta_{ij} + \beta V_{ij}^0 \Lambda_i^0,$$

where [Eq. (2.7)]

$$g_i^0 = 1 - f_i^0, \quad \Lambda_i^0 = D_i f_i^0 g_i^0, \quad V_{ij}^0 = \left.\frac{\partial^2 E}{\partial P_i \partial P_j}\right|_{(P_k^0)}. \tag{2.10}$$

Equation (2.9) requires some explanation. The effective grand potential Ω^{eff} gives an approximate expression for the true grand potential Ω. Ω^0 is the usual expression obtained for an ideal Fermi gas. The second term represents the first correction to Ω^0 due to mutual electrostatic interactions, symbolized here by (V_{ij}^0). The saddle-point method allows for the definition of an average atom, whose shell populations satisfy Fermi-Dirac equations (2.7). Interactions seem to have disappeared and the original many-particle problem is finally reduced to a one-body problem. This fact is well-known [11,15,35] and very powerful for practical reasons. Yet, one must be careful not to pursue the analogy with the ideal Fermi gas too far, because the average atom is not constituted of noninteracting electrons. Interactions are still present through the self-consistency of Eq. (2.7), since the one-electron energies (ε_i^0) $(\varepsilon_i^0 = \partial E/\partial P_i|_{(P_j^0)})$ incorporate a nonlinear (P_i^0) dependence. Moreover, there is the danger of misinterpreting quantities such as (ε_i^0) or (P_i^0). They have no other physical meaning than defining a mean field, or effective field, from which Z_G can be estimated. P_i^0 is not equal to the mean occupation $\bar{P}_i = -\partial\Omega/\partial\mu_i|_{\mu_i=\mu}$. This remark applies to $E^0 = E[(P_i^0)]$ as well: $E^0 \neq \bar{E} = [\partial(\beta\Omega)/\partial\beta] + \mu\bar{N}$. Therefore, great care is required when using average-atom quantities in place of strict average-thermodynamic quantities.

As mentioned above, the notion of AAM depends on the approximation strategy to calculate Z_G. The integral representation is not unique and many AAM's can be defined [15,23]. As an illustration, in the framework of Mayer's model, Z_G can be written as [24,25] $Z_G = \langle Z_G^{ind}[(x_i)]\rangle_{(x_i)}$, where

$$\langle\{\cdots\}\rangle_{(x_i)}$$

$$= \int d^{K_{max}} x\{\cdots\} e^{-(1/2)x^T \beta V x} \Big/ \int d^{K_{max}} x \, e^{-(1/2)x^T \beta V x},$$

$$Z_G^{ind}[(x_i)] = \prod_{j=1}^{K_{max}} (1 + e^{-\beta e_j})^{D_j},$$

$$e_j = E_j - V_{jj}/2 - \mu + i \sum_k V_{jk} x_k. \qquad (2.11)$$

Z_G can be interpreted as follows: $Z_G^{\text{ind}}[(x_i)]$ is the partition function of a noninteracting-electron gas in an external field (x_i) that has to be averaged over its Gaussian distribution. Surprisingly, both Eq. (2.9) and Eq. (2.10) are recovered by applying the saddle-point technique to this specific expression. One can easily find counterexamples [36]. Of course, if the exact expression of a given multidimensional integral were known, and if the complete saddle-point expansion around the average-atom solution could be done, the important physical question regarding the validity of this expansion could be answered. Indeed, the choice of performing a saddle-point expansion is closely connected with this lack of any explicit small perturbation parameter. The recurrent and problematic accuracy of such an expansion does not preclude the use of the saddle-point method. Intuitively, one expects this technique to bring accurate low-order approximations when thermal equilibrium is very stable around the mean-field description of statistical equilibrium. A similar situation typically occurs in hot dense plasma physics where many-electron ions are considered: the AAM is recognized to be well-matched, evidencing that the saddle point has very large second derivatives along the direction of steepest descent. In the absence of a formal expansion parameter, one must be guided by the physics of the problem and choose a formulation which includes the relevant physical contributions [15]. Like the saddle-point method, the mean-field notion itself is subject to severe limitations requiring additional clarification.

The AAM does not stem exclusively from the saddle-point method. Indeed, one can throw new light on this model by formulating it in the framework of a variational principle [37–41]. Let us imagine that an integral representation of Z_G [Eq. (2.1)] has been found,

$$Z_G = \int [dx] e^{-\beta S(x)}, \qquad (2.12)$$

where $[dx]$ is an integration measure and S a function that depends explicitly on the dummy variable x. Suppose we have another "S," say S_0, that is easier to work with. Then, Eq. (2.12) may be written as

$$Z_G = e^{-\beta \Omega_0} \langle e^{-\beta(S-S_0)} \rangle_{S_0},$$

$$e^{-\beta \Omega_0} = \int [dx] e^{-\beta S_0(x)}, \qquad (2.13)$$

$$\langle \{\cdots\} \rangle_{S_0} = e^{\beta \Omega_0} \int [dx] \{\cdots\} e^{-\beta S_0(x)}.$$

Now, suppose that S and S_0 are real, the inequality

$$\langle e^{-f} \rangle \geq e^{-\langle f \rangle} \qquad (2.14)$$

may be used to get

$$\Omega \leq \Omega_0 + \langle S - S_0 \rangle_{S_0}. \qquad (2.15)$$

In general, S_0 is chosen to be close to the problem and sufficiently simple to make possible the $\langle S - S_0 \rangle_{S_0}$ calculation. S_0 depends on several parameters that are adjusted to minimize the right-hand side of Eq. (2.15). The geometrical interpretation of Eq. (2.14) comes from the convexity of the exponential function and is invoked as the Peierls-Jensen [37] or Gibbs-Bogoliubov [42] inequality.

As an illustration, Eq. (2.15) is applied to Mayer's model. Let us choose the partition function of an ideal Fermi gas, where the one-electron energies (ε_i) are variational quantities

$$Z_{G_0} = \sum_{(P_k)} \left[\prod_k \binom{D_k}{P_k} e^{-\beta(\varepsilon_k - \mu) P_k} \right]. \qquad (2.16)$$

Using Eq. (2.15), it is then a simple task to find the optimized (ε_i) and define an associated AAM. Equation (2.7) is still valid by changing $\varepsilon_j^0 = \partial E / \partial P_j |_{(P_i^0)}$ into

$$\varepsilon_j^0 = E_k + \sum_{k'} P_{k'}^0 V_{kk'} \left(1 - \frac{\delta_{kk'}}{D_k} \right). \qquad (2.17)$$

In spite of the apparent similarity, both AAM (2.7) and (2.17) are in essence different: this fact is corroborated by the various expressions of one-electron energies. The variational AAM can be considered the best fit for the thermodynamic potential Ω. One cannot infer, however, that this solution is best fitted to quantities other than Ω, such as the evaluation of Eq. (2.5). This consideration applies to the SHM too: one finds that the one-electron energies match neither Eq. (2.7) nor the rather intuitive quantity

$$\varepsilon_i^0 = \frac{\partial E^{\text{eff}}}{\partial P_i} \bigg|_{(P_i^0)}, \qquad (2.18)$$

where $E^{\text{eff}}[(P_k)] = -\Sigma_k (\tilde{Z}_k^2 / 2n_k^2) P_k$ and $\tilde{Z}_k = Z - \Sigma_{k'} \sigma_{kk'} P_{k'} (1 - \delta_{kk'}/D_k)$. Finally, first corrections to the variational AAM cannot be implemented easily. This is the main drawback of this formalism because one has to change S_0 in order to improve the calculation of Ω in Eq. (2.15). This makes it difficult to build a systematic variational approach that could lead to a convergent perturbation expansion for the grand potential [43].

In summary, the AAM can be viewed using two strategies in order to evaluate the grand-canonical partition function Z_G (2.1): a saddle-point method or a variational principle. Yet, for mathematical convenience and central processing unit (CPU) considerations, the domain of validity of the AAM remains questionable, as well as the opportunity to go beyond this mean-field approach (the independent-electron description augmented with second-order corrections associated with fluctuations of occupation probabilities around the average mean-field equilibrium). These considerations led us to adopt an alternative approach using the SCA. This method makes possible the calculation of Z_G; the SCA is an analytic technique, which inherently converges to the solution without any recourse to stochastic method [15]. Consequently, the SCA provides a powerful and systematic tool for getting answers to certain classes of otherwise unsolvable many-

particle problems, such as those involving the screened-hydrogenic LTE average-atom model.

III. SUPERCONFIGURATION ACCOUNTING

Let us introduce the required theoretical background. The leading notations, commonly used by Bar-Shalom *et al.* [26,28] or Blenski *et al.* [44–46], have been used whenever possible. A supershell σ is a set of ordinary atomic subshells $s \in \sigma$. A superconfiguration (SC) Ξ of a Q electron ion, defined by its supershell occupation numbers Q_σ, is a group of ordinary configurations C symbolically written as the product over supershells:

$$\Xi = \prod_\sigma \sigma^{Q_\sigma}, \quad \sum_\sigma Q_\sigma = Q. \quad (3.1)$$

In other words, the SC is constructed by simply dispatching the Q_σ electrons occupying supershell σ among the subshells in all possible ways subject to the constraint $\{\Sigma_{s \in \sigma} P_s = Q_\sigma\}$: $\sigma^{Q_\sigma} = \Sigma_{\Upsilon_\sigma} \Pi_s s^{P_s}$. Υ_σ means $\{\Sigma_{s \in \sigma} P_s = Q_\sigma\}$. One should mention that each partition of Q is an ordinary configuration C: $C = \Pi_s s^{P_s} \equiv \Pi_\sigma \Pi_{s \in \sigma} s^{P_s}$. The main role is transferred from subshells s to supershells σ, in the same way the concept of SC supersedes the trivial notion of configuration. This fact can be exploited to rewrite Eq. (2.1) in terms of SC only: $Z_G = \Sigma_\Xi U_\Xi$, $U_\Xi = \Sigma_{C \in \Xi} U_C$. $U_C = \mathcal{D}_C e^{-\beta[E_C - \mu Q]}$ and U_Ξ are, respectively, the partition functions of configuration N_C of SC Ξ. Note that the total number of electron N_C of configuration C has been replaced by Q, since $N_C = Q$ by definition. The SC notion clearly bridges a gap between the integer-charge stage Q and the configuration C partitions: $Z_G = \Sigma_Q U_Q$, $U_Q = \Sigma_{C \in Q} U_C = \Sigma_{\Xi \in Q} U_\Xi$, where U_Q is the partition function of ions with Q electrons.

As first pointed out by Bar-Shalom *et al.* [28], a SC contains ordinary configurations lying sufficiently near in energy by construction. As a result, we can take advantage of the dramatic simplification of U_Q occurring in the noninteracting limit, where E_C is linear with respect to (P_i). Consequently,

$$U_\Xi \approx e^{-\beta \Delta E_\Xi} \sum_{C \in \Xi} \prod_s \binom{D_s}{P_s} X_s^{P_s}, \quad (3.2)$$

where

$$X_s = e^{-\beta(\varepsilon_s^\Xi - \mu)}, \quad \varepsilon_s^\Xi = \left.\frac{\partial E}{\partial P_s}\right|_{(P_r^\Xi)} \quad (3.3)$$

and

$$\Delta E_\Xi = E[(P_s^\Xi)] - P^T \varepsilon^\Xi. \quad (3.4)$$

Equation (3.2) can be more compactly written by introducing the partition function $U_{Q_\sigma}(g)$ of a supershell σ,

$$U_\Xi \approx e^{-\beta \Delta E_\Xi} \prod_\sigma U_{Q_\sigma}(g), \quad U_{Q_\sigma}(g) = \sum_{\Upsilon_\sigma} \binom{D_s}{P_s} X_s^{P_s}, \quad (3.5)$$

where (g) stands for the set of shell degeneracies (D_s). From here on, this notation is generalized to $(g^{rs\cdots}) = (D_i - \delta_{ir} - \delta_{is} - \cdots)$. The only approximation lies in the Taylor expansion of E_C truncated after the linear terms. This procedure is known to be open to criticism when average-atom atomic data are used as reference. Yet, it becomes less and less questionable as the SC partitioning of the configuration space reaches DCA. In practice, the main drawback of this method is that it takes into account only configurations whose contribution is estimated to be the most significant *a priori*. SCA provides a test of this approximation, since it can easily include all contributions and contains a systematic convergence procedure in its roots. Here, this formalism is applied to calculate standard-textbook thermodynamic quantities such as average and variance of ionization and ion populations. The results can thus be compared to AAM results, as well as to indirect computations starting with the grand potential Ω.

In quantum field theory, it is well known that the connected Green functions are generated by the logarithm of the partition function in the presence of a source term [15]. A similar phenomenon occurs here with Ω. Indeed, Eq. (2.5) can be rewritten as follows: $Z_O = e^{-\beta \Omega_O} = \Sigma_C \mathcal{D}_C e^{-\beta[E_C - \mu N_C + \lambda O_C]}$ and $\bar{O} = \partial \Omega_O / \partial \lambda|_0$. The centered moment $(O - \bar{O})^n$ of order n can be obtained by iterating the derivation with respect to λ. As an example, for fixed ρ, β, and μ, we have the identity [47,48] [Eq. (2.2)]

$$\Omega(\mu + \lambda) = \Omega(\mu) - (1/\beta) \sum_{k=1}^\infty \frac{(\lambda\beta)^k}{k!} \langle N^k \rangle_c, \quad (3.6)$$

where $\langle N^k \rangle_c = -\partial^k \Omega / \partial \lambda^k|_0 / \beta^{k-1} = -\partial^k \Omega / \partial \mu^k|_\mu / \beta^{k-1}$ is the kth cumulant and is related to the moments $\overline{N^m}$ with $m \leq k$. For instance, $\langle N^1 \rangle_c = Z - \bar{Z}^*$, $\langle N^2 \rangle_c = \sigma_{Z*}^2$, $\langle N^3 \rangle_c = -(Z^* - \overline{Z^*})^3$, and $\langle N^4 \rangle_c = (Z^* - \overline{Z^*})^4 - 3\sigma_{Z*}^4$. Generally, $\langle N^k \rangle_c$ is not equal to the kth centered moment $\overline{(N - \bar{N})^k}$. $\langle N^1 \rangle_c$ is the expectation $\bar{N}$ which, according to Eq. (2.2), is related to the average ionization, and $\langle N^2 \rangle_c$ is the variance of ionization. When normalized to the standard deviation of ionization σ_{Z*}, the quantities $\sigma_{Z*} = -\langle N^3 \rangle_c / \sigma_{Z*}^3$ and $\kappa_{Z*} = \langle N^4 \rangle_c / \sigma_{Z*}^4$ denote the skewness and the kurtosis (or flatness), respectively [49]. A characteristic feature of the normal (or Gaussian) distribution is that cumulants higher than the third are zero. Thus, $\langle N^k \rangle_c$, with $3 \leq k$, gives a measure of any deviation from the normal distribution. The kurtosis is the most common indicator of this trend. With respect to the normal distribution, flat curves have a negative kurtosis and sharp curves a positive one. These distributions are termed leptokurtic and platykurtic, respectively. Cumulants beyond the kurtosis are rarely considered for practical reasons. A similar strategy is adopted in this paper: only the skewness and the kurtosis are of great interest in terms of enhancing any deviation of the ionization distribution with respect to the normal distribution.

Let us consider the one-parameter family of probability density $(I_\alpha = e^{-|x|^\alpha})$, where $\alpha > 0$. Since the mean value is zero, the centered moments are identical to the moments. It is then a straightforward calculation to show that the vari-
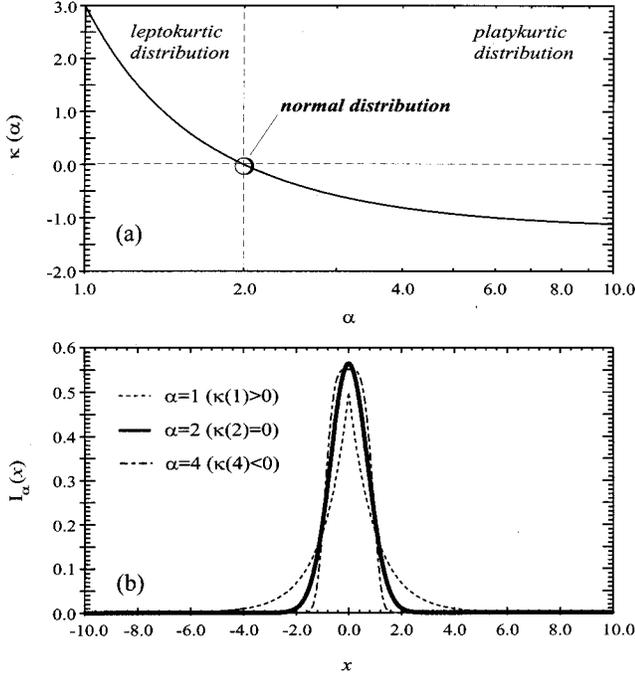
FIG. 1. (a) Behavior of the kurtosis $\kappa(\alpha)$ of the distribution $I_\alpha(x) = \alpha/[2\Gamma(1/\alpha)]e^{-|x|^\alpha}$ (normalized to unity) as a function of α. (b) Plots of a leptokurtic ($\alpha=1$), normal (or Gaussian, $\alpha=2$), and platykurtic ($\alpha=4$) distributions.

ance $\sigma^2(\alpha)$ and the kurtosis $\kappa(\alpha)$ are given by $\sigma^2(\alpha) = \Gamma(3/\alpha)/\Gamma(1/\alpha)$ and $\kappa(\alpha) = \Gamma(5/\alpha)\Gamma(1/\alpha)/\Gamma^2(3/\alpha) - 3$, where $\Gamma(z) = \int_0^\infty du\, u^{z-1}e^{-u}$. One can check the equalities $\kappa(2)=0$ and $d\kappa/d\alpha(2) = -1$; so $\kappa(2+\varepsilon) \underset{\varepsilon\to 0}{\approx} -\varepsilon$ and the sign of $\kappa(\alpha)$ changes towards $\alpha=2$ (see Fig. 1).

Any cumulant may be calculated in the SCA language by using an operator technique [26]. Yet, the computation of the kth centered moments of ionization rapidly becomes painstaking with increasing k, like the successive derivations of the effective grand potential Ω^{eff} in Eq. (2.9) with respect to the chemical potential μ. This is especially true when one is compelled to replace, for numerical reasons, the electron counting by the hole counting in the statistical sums involving supershells with a large number of bound electrons [44]. We propose to calculate such superconfiguration-averaged quantities with a technique widely used in analytic number theory. This formalism is based on the notion of integral representation in the complex plane and is entirely equivalent to the aforementioned operator technique. However, the physical significance of the relevant quantities we are dealing with are often clearer with this new viewpoint. Somehow, this reminds us of the situation of the path integral versus the more conventional operator formalism in quantum field theory. We can see how this method works by computing the following statistical sum that appears again and again in the SCA approach:

$$U_Q(g) = \sum_Y \binom{D_s}{P_s} X_s^{P_s}, \qquad (3.7)$$

where Y stands for $\Sigma_s P_s = Q$. Algebraic analysis is simplified by introducing the Kronecker-symbol integral represen-

tation into the summation, leading to $U_Q(g) = (1/2i\pi)\oint(dz/z^{Q+1})\Pi_s(1+zX_s)^{D_s}$. $\oint$ denotes an integration in the complex plane around a circle centered at $z=0$. This expression is the starting point to calculate various averages, such as powers of shell occupation number in the hole or particle language [26,44–46], that are needed to get the ionization-distribution moments.

First, let us prove Eqs. (42) and (43) of Ref. [28]:

$$U_Q(g) = \sum_{n=1}^{Q} \chi_n U_{Q-n}(g) \Big/ Q, \quad \chi_n = -\sum_s D_s(-X_s)^n, \qquad (3.8)$$

with $U_0(g) = 1$. Such identities are readily obtained by applying the Cauchy formula to $U_Q(g)$, since

$$U_Q(g) = (1/Q!)\frac{\partial^Q}{\partial z^Q}\left[\prod_s (1+zX_s)^{D_s}\right]\Big|_0. \qquad (3.9)$$

A similar recursion formula can be found—in conjunction with the notion of a generating function—in the single-particle ideal-gas model [28] and in the computation of the partition number of an integer [see Eq. (B19) and Appendix B for more details]. Indeed, $U_Q(g)$ and χ_n are generated by $F(z)$ and $G(z)$, respectively:

$$\sum_{Q=0}^{\infty} U_Q(g)z^Q = \prod_s (1+zX_s)^{D_s} \equiv s(z) = F(z) \qquad (3.10)$$

and

$$\sum_{n=0}^{\infty} \chi_n z^n = -\sum_s D_s \Big/ (1+zX_s) = G(z). \qquad (3.11)$$

For $Q > 0$,

$$U_Q(g) = \oint \frac{dz}{2i\pi} \frac{s(z)}{z^{Q+1}}, \qquad (3.12)$$

and, by performing an integration by parts,

$$U_Q(g) = \frac{1}{Q} \oint \frac{dz}{2i\pi} \frac{1}{z^{Q+1}} \left(\frac{z}{s(z)}\frac{ds(z)}{dz}\right)s(z). \qquad (3.13)$$

But

$$\frac{z}{s(z)}\frac{ds(z)}{dz} = \sum_s D_s - \sum_s D_s \Big/ (1+zX_s) \qquad (3.14)$$

and

$$\frac{z}{s(z)}\frac{ds(z)}{dz} = \widetilde{G}(z) \equiv \sum_{n=1}^{\infty} \chi_n z^n; \qquad (3.15)$$

consequently,

$$U_Q(g) = \frac{1}{Q} \oint \frac{dz}{2i\pi} \frac{1}{z^{Q+1}} F(z)\widetilde{G}(z) = \frac{\widetilde{a}_Q}{Q}, \qquad (3.16)$$

where

$$\tilde{a}_Q = \sum_{n=1}^{Q} \chi_n U_{Q-n}(g) \tag{3.17}$$

with

$$F(z)\tilde{G}(z) = \sum_{Q=1}^{\infty} \tilde{a}_Q z^Q. \tag{3.18}$$

In the same spirit, the relationship between $U_Q(g)$ and $U_Q(g^r)$, namely

$$U_Q(g) = U_Q(g^r) + X_r U_{Q-1}(g^r) \tag{3.19}$$

[Eq. (45) of Ref. [26]], simply comes from the following identity:

$$U_Q(g) = (1/2i\pi) \oint (dz/z^{Q+1})(1+zX_r)$$
$$\times \prod_s (1+zX_s)^{D_s - \delta_{rs}}. \tag{3.20}$$

It is then straightforward to infer the expressions of $U_Q(g^{rs\cdots})$ [26]. Finally, a simple factorization inside the integral representation of a statistical sum leads from the electron counting (no star) to the hole counting (with star):

$$U_Q(g) = \left(\prod_s X_s^{D_s} \right) U_{Q*}(g),$$
$$U_{Q*}(g) = (1/2i\pi) \oint (dz/z^{Q*+1}) \prod_s (1+z\tilde{X}_s)^{D_s}, \tag{3.21}$$

where $Q^* = G_s - Q$, $G_s = \Sigma_s D_s$, and $\tilde{X}_s = 1/X_s$ [Eq. (5) of Ref. [44]]. The integral representation is very useful because the average of a polynomial in the shell-occupation numbers is thus obtained by simply deriving under the integral symbol $\oint$ with respect to the term X_i of interest, which is formally equivalent to using a chemical potential μ_i for each subshell i. In the case where many subshells are involved, one must be careful when some of them belong to the same supershell. In summary, any standard-textbook formula of interest, which is valid for noninteracting Fermi gas, can be applied to calculate various averages, such as powers of shell occupation number, in the hole or the particle language [26,44–46].

As a result, we find the following explicit formulas for the average ionization and the variance of ionization coming from the averages involving $(\overline{P_i})$ and $(\overline{P_iP_j})$:

$$\overline{Z^*} = Z - \sum_{i=1}^{K_{\max}} \overline{P_i}, \quad \sigma_{Z*}^2 = \sum_{i,j=1}^{K_{\max}} \overline{P_iP_j} - \overline{P_i}\,\overline{P_j}, \tag{3.22}$$

where

$$\overline{P_i} = D_i \left(1 - \frac{1}{Z_G} \sum_{\Xi} U_{\Xi} \frac{U_{Q_{\sigma_i}}(g^i)}{U_{Q_{\sigma_i}}(g)} \right). \tag{3.23}$$

If the subshells i and j do not belong to the same supershell $(\sigma_i \neq \sigma_j)$, then

$$\overline{P_iP_j} = (D_iD_j/Z_G) \left[\sum_{\Xi} U_{\Xi} \left(1 - \frac{U_{Q_{\sigma_i}}(g^i)}{U_{Q_{\sigma_i}}(g)} \right) \right.$$
$$\left. \times \left(1 - \frac{U_{Q_{\sigma_j}}(g^j)}{U_{Q_{\sigma_j}}(g)} \right) \right]. \tag{3.24}$$

Conversely $(\sigma_i = \sigma_j = \sigma)$,

$$\overline{P_iP_j} = (D_iD_j/Z_G) \left[\sum_{\Xi} U_{\Xi} \left(1 - \frac{U_{Q_{\sigma}}(g^i)}{U_{Q_{\sigma}}(g)} - \frac{U_{Q_{\sigma}}(g^j)}{U_{Q_{\sigma}}(g)} \right. \right.$$
$$\left. \left. + \frac{U_{Q_{\sigma}}(g^{ij})}{U_{Q_{\sigma}}(g)} \right) \right] \tag{3.25}$$

if $i \neq j$ and

$$\overline{P_i^2} = (D_i^2/Z_G) \left[\sum_{\Xi} U_{\Xi} \left(1 - (2-1/D_i) \frac{U_{Q_{\sigma}}(g^i)}{U_{Q_{\sigma}}(g)} \right. \right.$$
$$\left. \left. + (1-1/D_i) \frac{U_{Q_{\sigma}}(g^{ii})}{U_{Q_{\sigma}}(g)} \right) \right] \tag{3.26}$$

otherwise. In order to go rapidly from the electron to hole language, the modified statistical sums of a supershell, such as $U_{Q_{\sigma}}(g^i)$ or $U_{Q_{\sigma}}(g^{ij})$, are normalized by the unaltered $U_{Q_{\sigma}}(g)$.

The fraction $\mathcal{F}_Q$ of ion with Q electrons, or charge stage $(Z-Q)$, is then easily computed since $\mathcal{F}_Q = U_Q/Z_G$. The SCA method gives $\mathcal{F}_Q = \Sigma_{\Xi \in Q} U_{\Xi}/Z_G$, whereas within the framework of the AAM $\mathcal{F}_Q \approx e^{-(Q-\bar{N})^2/(2\sigma_{Z*}^2)}/\Sigma_{Q'} e^{-(Q'-\bar{N})^2/(2\sigma_{Z*}^2)}$. Of course, the skewness s_{Z*} and the kurtosis κ_{Z*}, estimated within the same theoretical model, can be used to improve this guess and go beyond the Gaussian assumption. The SCA method can provide an indication concerning the statistical weight $\mathcal{F}_C$ of any particular configuration C. If C belongs to the superconfiguration Ξ, $\mathcal{F}_C \approx \Pi_s \binom{D_s}{P_s} X_s^{P_k}/\Pi_{\sigma} U_{Q_{\sigma}}(g)$ [Eq. (3.5)]. If no selected superconfiguration contains C, one can infer that $\mathcal{F}_C$ is negligible.

IV. NUMERICAL APPLICATIONS

As an illustration, we begin by comparing the average ionization and the ionization variance values obtained from different methods [Eq. (3.22)]. The first is well known and consists in using the AAM only, with or without FAA corrective terms [Eq. (2.7)]. The second one is an explicit calculation of $\overline{Z^*}$ and σ_{Z*}^2 with the SCA technique. All the results are drawn in Fig. 2. The SHM [27] has been employed with the finite-temperature convention (2.18). We restrict ourselves to the nonrelativistic regime; moreover, plasmas effects on the electron structure are neglected. Calculations have been made with $n\ell$ subshells ranging from $1s$ to $5g$. A LTE germanium plasma ($\rho = 0.053\,07\,\text{g cm}^{-3}$) has been considered, since a series of experiments were carried out on this element [50] to explore Ge photoabsorption properties at temperatures where the M
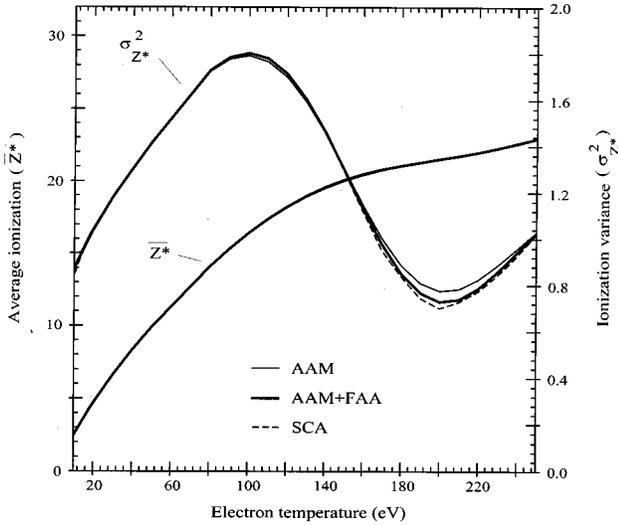
FIG. 2. Average ionization and ionization variance of a LTE germanium plasma ($\rho = 0.053\,07\,\text{g cm}^{-3}$) calculated by using an average-atom model—AAM, an average-atom model and FAA correction—AAM+FAA, and a direct SCA computation—SCA.

FIG. 3. Relative errors of the M-shell occupation-numbers, with respect to the reference SCA values of a LTE germanium plasma ($\rho = 0.053\,07\,\text{g cm}^{-3}$). Two average-atom model calculations are considered: with (AAM+FAA) or without (AAM) FAA correction.

shell is almost filled. The temperature domain ranges from 10 to 250 eV, in order to sweep the conditions where this shell progressively empties with increasing temperature. Surprisingly, the agreement upon $\overline{Z^*}$ is good, even when the M shell is almost filled or empty. Conversely, things change a little bit for $\sigma^2_{Z^*}$. The main point is the close agreement between the mean-field method with FAA correction and the SCA. As far as the bare AAM is concerned, the situation progressively deteriorates when the M shell becomes filled (near 20 eV) or empty (around 200 eV): the AAM tends then to overestimate the fluctuations around $\overline{Z^*}$. The adequacy gets better at higher temperature due to the progressive emptiness of the L shell. We have performed similar calculations with the grand potential. The comparisons show less of an influence of the FAA correction to match with the SCA computation, which is intended to be considered as the reference. In other words, the simple AAM calculations give very good values for the grand potential and the average ionization; a reasonably good estimation of the variance of ionization is found too, especially where the model is not guaranteed to yield accurate results, i.e., when a shell is completely empty or full.

Same conclusions can be drawn as far as the shell-occupation numbers are considered. For clarity and for the aforementioned reasons, only the relative errors for M-shell occupation numbers are presented in Fig. 3. The SCA computations serve as a reference; the FAA inclusion constitutes again the key parameter to be discussed and significant effects can be noted. Clearly, the mismatch between a simple AAM and a SCA calculation is moderate. In this example, a maximum amount of 10% is reached for the $3d$ subshell. As expected, this occurs when the M shell is empty, or, in other words, when the occupation numbers become quite small. The FAA correction is efficient everywhere: as a result, the maximum relative error does not exceed 3% for the chosen range of electron temperatures.

Finally, let us comment on Eq. (3.6). This formula has
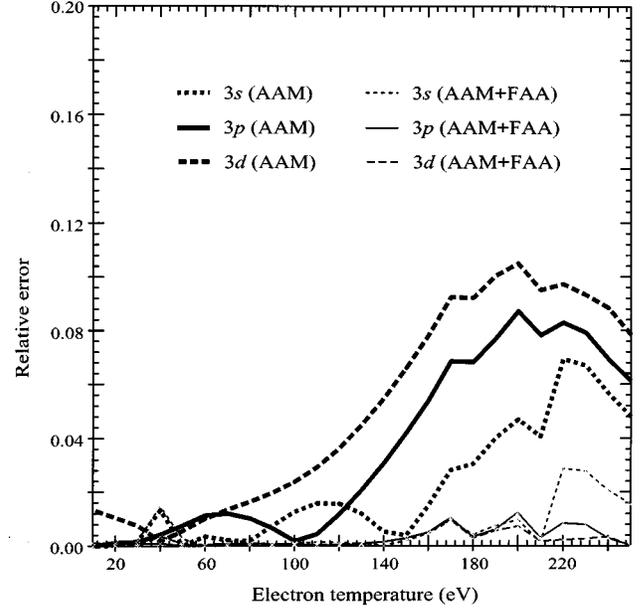
been used to check direct SCA calculations. As for ionization, λ is allowed to vary in a small range centered on zero. A Chebyshev approximation of $\Omega(\mu + \lambda)$ has been constructed for $\lambda \in [-0.05\mu, 0.05\mu]$, with a moderately large number of polynomials (here 32). A power of 2 is preferentially chosen in order to use a fast cosine transform for calculating the collocation-point coefficients of the Chebyshev approximation [51]. The precision encountered for $\Omega(\mu)$, $\partial\Omega/\partial\mu$, and $\partial^2\Omega/\partial\mu^2$ was quite impressive. This well-known property of the Chebyshev approximating polynomial [52,53] is used to estimate higher derivatives $\partial^k\Omega/\partial\mu^k$. By doing so, higher centered moments of ionization (or cumulants) can be obtained by alleviating direct calculations, which generally become more and more tedious with increasing k. This is a convenient way to get around this difficulty and to tackle $(O - \overline{O})^n$, especially when $O[(P_i)]$ is a nonpolynomial function of (P_i).

As an illustration (Fig. 4), the skewness (s_{Z^*}) and the kurtosis (κ_{Z^*}) of the ionization distribution have been computed by using the Chebyshev approximating-polynomial technique and by keeping the same thermodynamic conditions for the germanium plasma of interest. The corresponding third ($\mu^3_{Z^*}$) and fourth ($\mu^4_{Z^*}$) centered moments have been added too. As expected, $\mu^4_{Z^*}$ is minimum when the M shell is closed or empty and is maximum when it is half-populated (near 100 eV). In this region, many ions of different charged stage contribute to the partition function and the ionization distribution is relatively symmetric: $\mu^3_{Z^*}$ is thus relatively small. Yet, when we approach the emptiness of the M shell from below in temperature, $\mu^3_{Z^*}$ decreases down to a minimum and then increases with a change of sign. When $\mu^3_{Z^*}$ is positive, this indicate that we are above the M-shell emptiness in temperature, or equivalently below the closure
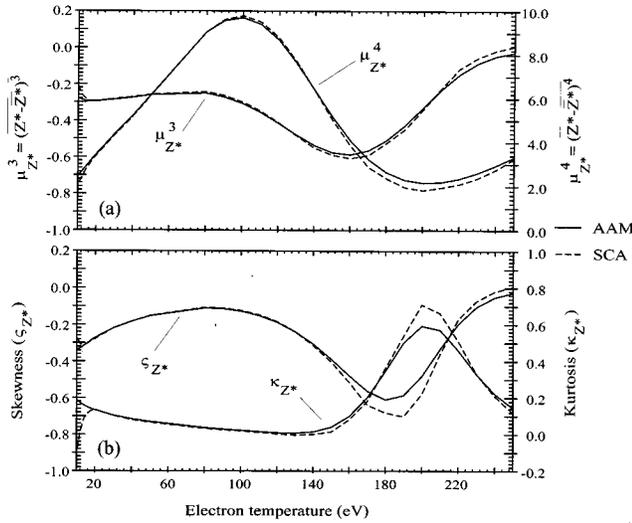
FIG. 4. Third (μ_{Z*}^3) and fourth centered moments (μ_{Z*}^4), skewness (s_{Z*}), and kurtosis (κ_{Z*}) of the ionization distribution of a LTE germanium plasma ($\rho = 0.053\,07\,\text{g cm}^{-3}$) as function of temperature. All quantities are found by deriving the grand potential Ω with respect to the chemical potential μ. The Chebyshev approximating-polynomial technique [51] is used for SCA calculations—SCA. By contrast, explicit derivation of Ω^0 in Eq. (2.9) are performed as far as average-atom data are concerned—AAM [25,41] (Appendix A).

of the L shell: μ_{Z*}^3 begins to decrease and changes sign when, as above, the dominant principal shell (here L-shell) is half-populated. Differences between AAM and SCA are quite moderate. Let us now give an insight into the skewness and kurtosis curves. At first glance, the discrepancies between AAM and SCA keep increasing with the order of the cumulant, especially into the considered region where a dominant principal shell is closed or empty. First of all, except in this region, the ionization distribution presents a high degree of normal-distribution character. Obviously, around 200 eV, the peakedness of the ionization distribution is fairly pronounced (κ_{Z*} is positive) and its asymmetry is changing: s_{Z*} is negative below 200 eV and positive above. This fact is well-known and is due to the large ionization-potential gap between [Mg]- and [Na]-like ions and [Ne]- and [F]-like ions. As an illustration, we have plotted in Fig. 5 the ionization distribution calculated with the SCA method for two temperatures: 160 and 260 eV. Clearly, the ionization-distribution skewness at 160 eV is negative because ions with ionization degrees higher than the neonlike ionization stage ([F]-like ions, [O]-like ions, . . .) are playing a minor role due to the aforementioned ionization-potential gap. On the contrary, the ionization-distribution skewness at 260 eV is positive due, now, to the dominant statistical weights of these ions.

V. CONCLUSION

In this paper, the screened-hydrogenic average-atom model has been compared to the systematic, analytic, and nonperturbative superconfiguration accounting method. First, a powerful method has been presented for calculating superconfiguration-averaged quantities. It has been proven to
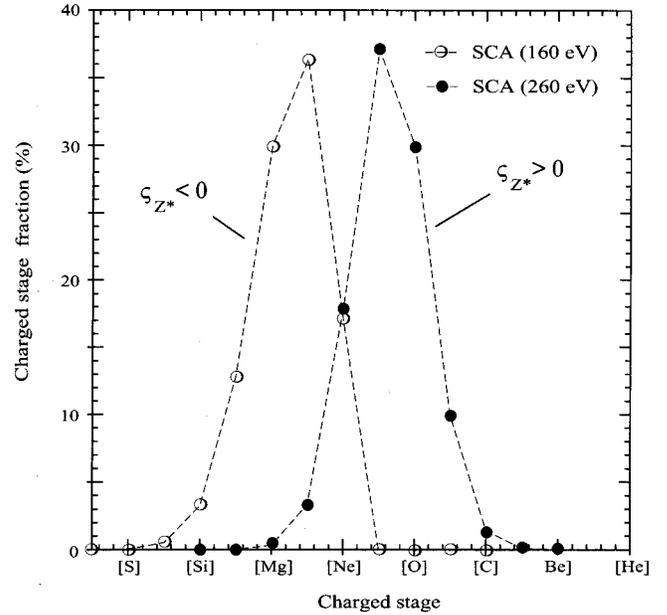
FIG. 5. Charged-stage distribution of LTE germanium plasma ($\rho = 0.053\,07\,\text{g cm}^{-3}$) at two electron temperatures: 160 and 260 eV obtained with the SCA method. For instance, [Ne] denotes the neonlike ion stage. The skewness (s_{Z*}) at 160 and 260 eV is negative and positive, respectively.

be related to the notion of a partition used in analytic number theory. This new viewpoint extends the original operator technique and almost offers a clearer insight into the physical significance of the quantities being dealt with. Second, though the superconfiguration accounting approach is unrelated to the saddle-point method, it has been shown that both techniques yield similar results for the grand potential, the average ionization, and the variance of ionization. It has been shown that higher-order centered moments of the ionization distribution can be calculated within the framework of the average-atom model. The robustness of the average-atom model keeps constant, except, perhaps, towards a principal-shell closure (or emptiness), in which case mean-field results deteriorate progressively with increasing order of the centered moment. To sum up, the average-atom model calculations remain competitive with respect to the superconfiguration accounting results in a widespread range of temperatures and densities for the considered matter model.

The LTE case has been criticized in the present document. For future works, the first step consists of extending the superconfiguration formalism to tackle non-LTE plasmas without reference to the ionization temperature notion [54–58]. Then, it would offer the possibility to study the worth of the screened-hydrogenic average-atom model, in such a thermodynamic situation [59,60], as well as Busquet's model. Second, the important question of density effects within the superconfiguration formalism might be addressed in the context of a thorough and rigorous statistical treatment of ions in LTE or non-LTE plasmas.

APPENDIX A

Equation (2.6) is found from Eq. (2.1) by introducing auxiliary variables (x_i) and by using the Fourier integral representation of the Dirac distribution [34]:

$$Z_G = \int \frac{d^{K_{\max}}x\, d^{K_{\max}}\omega}{(2\pi)^{K_{\max}}} e^{-\beta E[(x_k)] + i\omega^T x} \prod_{k=1}^{K_{\max}} [1 + e^{-i\omega_k + \eta}]^{D_k}. \tag{A1}$$

Equation (2.6) naturally comes from straightforward elementary algebra. ω^T is the line vector transposed from the $K_{\max}$-dimensional column vector ω whose components are the dummy variables (ω_i). Equation (2.6) is valid for any expression of the configuration energy E_C. Let us calculate $\partial S/\partial U_i|_{(U_j)}$ and $\partial^2 S/\partial U_i \partial U_j|_{(U_k)}$, respectively. The former quantity leads to the AAM (2.7) equations and the latter to the FAA correction (2.9). To this end, the original variables (x_i) and (ω_i) are preferred to the compact notation (U_i), and one finds that

$$\frac{\partial S}{\partial x_j} = \frac{\partial E}{\partial x_j} - i\omega_j/\beta,$$

$$\frac{\partial S}{\partial \omega_j} = -ix_j/\beta + iD_j/\{\beta[1 + \exp(i\omega_j - \eta)]\}, \tag{A2}$$

$$\frac{\partial^2 S}{\partial x_j \partial x_k} = \frac{\partial^2 E}{\partial x_j \partial x_k} = V_{jk}, \qquad \frac{\partial^2 S}{\partial x_j \partial \omega_k} = -i\delta_{jk}/\beta,$$

$$\frac{\partial^2 S}{\partial \omega_j \partial \omega_k} \tag{A3}$$

$$= \delta_{jk}D_j/\{\beta[1 + \exp(i\omega_j - \eta)][1 + \exp-(i\omega_j - \eta)]\}.$$

δ_{jk} is the Kronecker symbol. Equation (2.7) is deduced from the stationary condition $\partial S/\partial x_j = \partial S/\partial \omega_j = 0$. Consequently, it is easy to establish Eq. (2.9) by following the successive steps [Eq. (2.10)]

$$Z_G \approx e^{-\beta S[(U_i^0)]} \int \frac{d^{K_{\max}}x\, d^{K_{\max}}\omega}{(2\pi)^{K_{\max}}}$$
$$\times e^{-(1/2)\Sigma_{j,k}(x_j \beta V_{jk}^0 x_k + \omega_j \Lambda_j^0 \delta_{jk}\omega_k - 2ix_j \delta_{jk}\omega_k)}, \tag{A4}$$

$$Z_G \approx \frac{e^{-\beta S[(U_i^0)]}}{\left(\prod_{j=1}^{K_{\max}} 2\pi\Lambda_j^0\right)^{1/2}} \int d^{K_{\max}}x\, e^{-(1/2)\Sigma_{j,k}x_j(\beta V_{jk}^0 + \delta_{jk}/\Lambda_j^0)x_k}, \tag{A5}$$

$$Z_G \approx \frac{e^{-\beta S[(U_i^0)]}}{\sqrt{\det(\Delta S^0)}}, \tag{A6}$$

through which formula $1/\sqrt{\det(A)} = \exp[-\frac{1}{2}\operatorname{Tr}\ln(A)]$ and the well-known Gaussian identity

$$\sqrt{[(2\pi)^{K_{\max}}/\det(A)]}e^{(1/2)b^T A^{-1}b} = \int d^{K_{\max}}x\, e^{-(1/2)x^T Ax - b^T x}$$

have been employed [15,37]. b is a $K_{\max}$-dimensional line vector and A a $K_{\max} \times K_{\max}$-dimensional definite positive matrix. It is instructive to compare these results with the continuous version of Eq. (2.1),

$$Z_G \approx e^{-\beta\Omega^0} \int d^{K_{\max}}\Delta P\, e^{-(1/2)\Delta P^T A \Delta P},$$

$$A_{ij} = \beta V_{ij}^0 + \delta_{ij}/\Lambda_i^0, \tag{A7}$$

found by replacing the original discrete summation with a $K_{\max}$-dimensional integral, using the Stirling formula to approximate the binomial coefficients, and by developing the action around its minimum up to second order [25,61,62]. Then,

$$\Omega \approx \Omega^0 + \frac{\operatorname{Tr}\ln(A)}{2\beta} \neq \Omega^0 + \frac{\operatorname{Tr}\ln(\Delta S^0)}{2\beta}. \tag{A8}$$

The difference matters in the calculation of the thermodynamical potential but also in quantities reached by deriving Ω with respect to relevant parameters (β or μ), because (Λ_i^0) are not constant. They depend on the thermodynamical conditions through (P_i^0). In summary, great care is required when using such developments. One really needs another viewpoint to grasp their meaning and to compare to. This is precisely the role assigned to the SCA technique.

Since Ω^{eff} depends on μ and β, it is possible to reach any kth derivative with respect to both thermodynamical variables $[(\partial^k \Omega/\partial \mu^k)_{\rho,\beta}$ or $(\partial^k \Omega/\partial \beta^k)_{\rho,\mu}]$. The key points are $\Sigma_{l=1}^{K_{\max}} \Delta S_{kl}^0 \partial P_l^0/\partial \mu = \beta\Lambda_k^0$ and $\Sigma_{l=1}^{K_{\max}} \Delta S_{kl}^0 \partial P_l^0/\partial \beta = -\Lambda_k^0 e_k^0$ [Eqs. (2.9) and (2.10)] [25,41]. This allows us to solve the apparent paradox of computing a kth centered moment of ionization from the average-atom populations (P_i^0) only [34]. At first sight, (P_i^0) is naively understood to give only an approximate value for $\overline{Z^*}$. Yet, the self-consistency of the average-atom equations, that is to say the dependence of the one-electron parameters (ε_i^0) on (P_i^0), leads to a nontrivial dependence of (P_i^0) (and hence of Ω^{eff}) on the thermodynamical parameters β and μ.

Although well-adapted to get the cumulants of the ionization distribution, the quantity Ω is not efficient enough to study the properties of the energy distribution. It is therefore better to consider the quantity βF, where F is the free energy ($F = \Omega + \mu\overline{N}$). More precisely, any kth cumulant of the energy distribution can be found from $-\partial^k(\beta F)/\partial\beta^k$.

Conversely, the electron pressure P can be estimated without any derivative with respect to density since $P = -\Omega^{\text{tot}}N_a$, or equivalently, $P = -\Omega^{\text{tot}}\rho\mathcal{N}/A$. Here, Ω^{tot} is the sum of two terms: Ω and the free-electron component Ω^{free} [61] $\{\Omega^{\text{free}} = -2\overline{Z^*}F_{3/2}(\eta)/[3\beta F_{1/2}(\eta)]\}$.

APPENDIX B

The integral representation of the Kronecker symbol δ_{ij} (or the circle method [33]) is well-suited to standard combinatorial issues with constraints. For instance, it can be used to count the number N_{conf^N} of N-electron configurations C_N constructed from $K_{\max}$ shells with degeneracies (D_k). By definition, N_{conf^N} is equal to

$$N_{\mathrm{conf}^N} = \sum_{C_N} 1 = \sum_C \delta_{0\Upsilon}, \qquad (B1)$$

where Υ denotes $\sum_{k=1}^{K_{\max}} P_k - N$. An unrestricted summation is provided by using the forthcoming integral representation of the Kronecker symbol:

$$\delta_{0N} = \frac{1}{2i\pi} \int_{-i\pi+\alpha_0}^{i\pi+\alpha_0} dt \, e^{tN}, \qquad (B2)$$

where N and α_0 are integer and real, respectively. A closed form for N_{conf^N} can then be derived:

$$N_{\mathrm{conf}^N} = \int_{-i\pi+\alpha_0}^{i\pi+\alpha_0} \frac{dt}{2i\pi} e^{tN} \prod_{k=1}^{K_{\max}} \frac{1 - e^{-t(D_k+1)}}{1 - e^{-t}} \qquad (B3)$$

or

$$N_{\mathrm{conf}^N} = \frac{1}{2i\pi} \oint \frac{dz}{z^{N+1}} \prod_{k=1}^{K_{\max}} \frac{1 - z^{(D_k+1)}}{1 - z}. \qquad (B4)$$

$\oint$ denotes an integration in the complex plane around a circle of radius $e^{-\alpha_0} (z = e^{-t})$ centered in zero. The last expression is just the Cauchy formula $N_{\mathrm{conf}^N} = (1/N!)(d^N/dz^N)[\Pi_{k=1}^{K_{\max}} \times (1 - z^{(D_k+1)})/(1-z)|_0]$.

As an example, with $n\ell$ subshells from $1s$ to $5g$, when $N=7$ we can construct 101 126 configurations, when $N=13$, 1.12×10^7 configurations, when $N=26$, 2.96×10^9 configurations, and finally, when $N=79$, 1.05×10^{10} configurations. It gives a simple illustration of the impressive numbers of configurations typically encountered when a brute-force summation of a partition function is performed.

The total number N_{tot} of all possible configurations C_N, where $N \in [0, N_T]$, and the total number $N_{\mathrm{tot}}^{k_i - k_f}$ of one-electron transitions can be found in the same spirit:

$$N_{\mathrm{tot}} = \sum_{N=0}^{N_T} N_{\mathrm{conf}^N}$$

$$= \int_{-i\pi+\alpha_0}^{i\pi+\alpha_0} \frac{dt}{2i\pi} \frac{1 - e^{t(N_T+1)}}{1 - e^t} \prod_{k=1}^{K_{\max}} \frac{1 - e^{-t(D_k+1)}}{1 - e^{-t}}. \qquad (B5)$$

For a transition $k_i \rightarrow k_f$, both shells k_i and k_f are discarded when the former is empty or the latter is full:

$$N_{\mathrm{tot}}^{k_i \rightarrow k_f} = \int_{-i\pi+\alpha_0}^{i\pi+\alpha_0} \frac{dt}{2i\pi} \frac{1 - e^{t(N_T+1)}}{1 - e^t}$$

$$\times \prod_{k=1}^{K_{\max}} \frac{1 - e^{-t(D_k + 1 - \delta_{kk_i} - \delta_{kk_f})}}{1 - e^{-t}}. \qquad (B6)$$

A numerical evaluation of these integrals is to be performed with caution. This originates from the oscillatory character of the arguments: in practice the results appear to depend on α_0 due to numerical uncertainties. Mathematically, it should not be the case. This freedom with respect to α_0 can be used to evaluate the aforementioned integrals with the saddle-point method. Since all integrals are of the same type, $\int_{-i\pi+\alpha_0}^{i\pi+\alpha_0} (dt/2i\pi) e^{f(t)}$, the optimum value $\tilde{\alpha}_0$ of α_0 to choose is the associated saddle point [40] $(df/dt|_{\tilde{\alpha}_0} = 0)$. At this occasion, an approximate value of this type of integral can be deduced: $\int_{-i\pi+\alpha_0}^{i\pi+\alpha_0} (dt/2i\pi) e^{f(t)} \approx e^{f(\tilde{\alpha}_0)} / \sqrt{2\pi(d^2 f/dt^2)|_{\tilde{\alpha}_0}}$.

Such tricks are clearly powerful but there are situations for which direct computations ought to be preferred. We have in mind numbers $S_m(Q)$ (originally called $N_k^{(m)}$ by Oreg et al. [26]),

$$S_m(Q) = \sum_{n_{m-1}=0}^{Q} \sum_{n_{m-2}=0}^{n_{m-1}} \cdots \sum_{n_1=0}^{n_2} 1, \qquad (B7)$$

where $Q \geq 0$ and $m \geq 2$. These numbers were computed and tabulated using Bernoulli functions. Yet, simple algebra shows that

$$S_m(Q) = \prod_{k=1}^{m-1} \frac{Q+k}{k} = \binom{Q+m-1}{m-1}. \qquad (B8)$$

This relation is proven by induction on m, whereby Q is held fixed. The result for $m=2$ is trivial since $S_2(Q) = \sum_{n_1=0}^{Q} 1 = \binom{Q+1}{1}$. By noting that $(m>2)$,

$$S_m(Q) = \sum_{n_{m-1}=0}^{Q} S_{m-1}(n_{m-1}), \qquad (B9)$$

we have

$$S_m(Q) = \sum_{n_{m-1}=0}^{Q} \binom{n_{m-1}+m-2}{m-2}. \qquad (B10)$$

The identity

$$\sum_{n=0}^{Q} \binom{n+p}{p} = \binom{Q+p+1}{p+1} \qquad (B11)$$

is then used to get Eq. (B8), which ends the demonstration by induction.

Identity (B11) can be shown as follows [63]. Let us note that

$$\sum_{n=0}^{Q} (1+x)^{p+n} = \cdots + x^p \sum_{n=0}^{Q} \binom{n+p}{p} + \cdots. \qquad (B12)$$

Since for $x \neq 0$

$$\sum_{n=0}^{Q} (1+x)^{p+n} = \frac{(1+x)^{Q+p+1} - (1+x)^p}{x}, \qquad (B13)$$

the coefficient of x^p originates from expansion of $(1+x)^{Q+p+1}$ only, which yields Eq. (B11).

$S_m(Q)$ numbers are much more than a mathematical curiosity. The original expression can be slightly modify to obtain the following formula:

$$p(n) = \sum_{q_n \geq 0} \sum_{q_{n-1} \geq q_n} \cdots \sum_{q_2 \geq q_3} \sum_{q_1 \geq q_2} \delta_{0\gamma}, \qquad (B14)$$

where $p(n)$ and γ denote the number of partitions of n and $n - \Sigma_{i=1}^{n} q_i$, respectively. In other words, $p(n)$ is equal to the number of ways a positive integer n can be represented as a sum of positive integers without regard to order and with no restrictions [33,64,65]. As an example, $p(5) = 7$ because the partitions of 5 are 5, $4+1$, $3+2$, $3+1+1$, $2+2+1$, $2+1+1+1$, and $1+1+1+1+1$. It may appear tempting to insert the integral representation of the Kronecker symbol to get a tractable formula for $p(n)$. However, the fact that q_k takes its values into the set $\{q_{k-1}, q_{k-1}+1, \ldots, n-1, n\}$ prevents any factorization, and consequently, any closed expression of practical interest for $p(n)$.

Indeed, the generating function of $p(n)$ is known [33] to be the infinite product $\Pi_{k=1}^{\infty}(1-z^k)^{-1}$. With the convention $p(0) = 1$, we thus have

$$\sum_{n=0}^{\infty} p(n)z^n = \prod_{n=1}^{\infty} (1-z^n)^{-1}, \qquad \text{(B15)}$$

where $p(n) = 1/(2i\pi)\oint(dz/z^{n+1})\Pi_{k=1}^{n}(1-z^k)^{-1}$. The radius of the integration circle should be chosen lower to unity ($\alpha_0 > 0$). This way of thinking can be extended further by considering also $d(n)$ and $\sigma(n)$, which are the number of divisors and the sum of the divisors of n, respectively:

$$\sum_{n=1}^{\infty} d(n)z^n = \sum_{n=1}^{\infty} z^n/(1-z^n), \qquad \text{(B16)}$$

$$\sum_{n=1}^{\infty} \sigma(n)z^n = \sum_{n=1}^{\infty} nz^n/(1-z^n). \qquad \text{(B17)}$$

Similar integrations in the complex plane allow one to calculate $d(n)$ and $\sigma(n)$. But a much more powerful method can be built. First, let us introduce $s(z) = \Pi_{n=1}^{\infty}(1-z^n)$, thus $\Sigma_{n=1}^{\infty}\sigma(n)z^n = -[z/s(z)]ds(z)/dz$. By multiplying both sides by $s(z)$ and identifying term by term the coefficients of the null polynomial $s(z)\Sigma_{n=1}^{\infty}\sigma(n)z^n + z[ds(z)/dz]$, Euler found the recursion relation

$$\sigma(n) = \sigma(n-1) + \sigma(n-2) - \sigma(n-5) - \sigma(n-7)$$
$$+ \sigma(n-12) + \sigma(n-15) - \sigma(n-22) - \sigma(n-26)$$
$$+ \cdots, \qquad \text{(B18)}$$

where the sum is limited to positive arguments with the convention $\sigma(0) = n$. The integers differ by the numbers 1,3,2,5,3,7,4,9,5,11,6, ... The polynomial $s(z)$ and the generating functions of $p(n)$ and $\sigma(n)$ lead [65] to a recursion formula for $p(n)$:

$$p(n) = \frac{1}{n}\sum_{k=1}^{n} \sigma(k)p(n-k). \qquad \text{(B19)}$$

This equation is obtained as follows. Let us define $F(z)$ and $G(z)$ the generating functions of $p(n)$ and $\sigma(n)$: $\Sigma_{n=0}^{\infty}p(n)z^n = 1/s(z) = F(z)$ and $\Sigma_{n=1}^{\infty}\sigma(n)z^n = -[z/s(z)]ds(z)/dz = G(z)$. By integrating by parts,
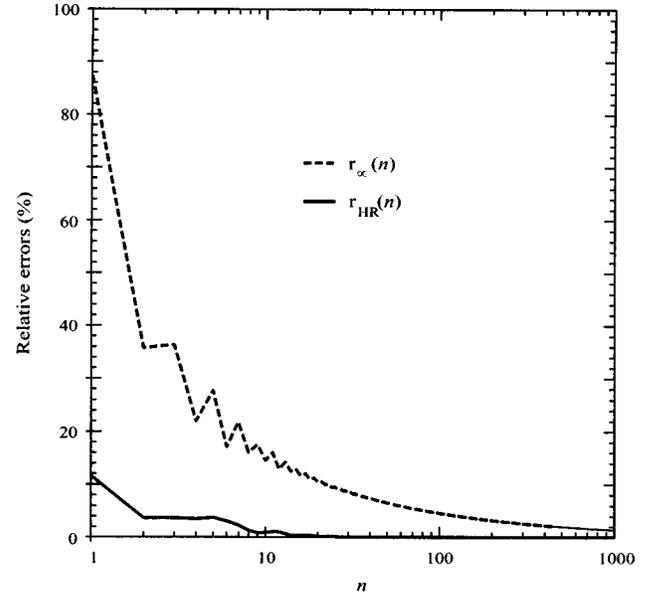
FIG. 6. Relative errors $r_{\infty}(n) = |1 - p_{\infty}(n)/p(n)|$ and $r_{HR}(n) = |1 - p_{HR}(n)/p(n)|$. $p(n)$ is the number of partitions of n. $p_{\infty}(n)$ and $p_{HR}(n)$ are two asymptotic analytic expressions of $p(n)$.

$p(n) = (1/n)\oint(dz/2i\pi)(1/z^{n+1})F(z)G(z)$. Or, $F(z)G(z) = \Sigma_{n=0}^{\infty}a_n z^n$, with $a_0 = 1$ and $a_n = \Sigma_{k=1}^{n}\sigma(k)p(n-k)$. Hence, $p(n) = a_n/n$.

The partitions $p(n)$ are thus exactly obtained within n steps. The CPU time is drastically reduced and no more integration in the complex plane is required. Here, $p(n)$ is calculated in the same way the partition function is computed in the STA and SCA models because the recursion formulas are analogous to the recursion formulas (42), (43), and (45) of Ref. [28]. $p(n)$ and $\sigma(n)$ play the role of U_Q and χ_n, respectively [see Eq. (3.8)]. Finally, note that one can go further by eliminating $\sigma(n)$ to find a closed recursion formula for $p(n)$, namely,

$$p(n) = \sum_{k \geqslant 1} (-1)^{k-1}\left[p\left(n - \frac{k(3k-1)}{2}\right) + p\left(n - \frac{k(3k+1)}{2}\right)\right]$$

with the convention $p(m) = 0$ for $m < 0$.

As an illustration, we have drawn in Fig. 6 the relative errors $r_{\infty}(n) = |1 - p_{\infty}(n)/p(n)|$ and $r_{HR}(n) = |1 - p_{HR}(n)/p(n)|$ as a function of n, for $n \in \{1, \ldots, 1000\}$. $p_{\infty}(n)$ and $p_{HR}(n)$ are both asymptotic approximations of $p(n)$, especially valid for large values of n:

$$p_{\infty}(n) = e^{\pi(2n/3)^{1/2}}/(4n3^{1/2})$$

$$p(n) \underset{n-\infty}{\approx} p_{HR}(n)$$

$$= \frac{d}{dn}[e^{\pi(2/3)^{1/2}(n-1/24)^{1/2}}/(n-1/24)^{1/2}]/(2\pi2^{1/2}).$$

$$\text{(B20)}$$

The last approximation (established by Hardy and Ramanujan [48,64–66]) is more precise than p_∞, which appears as a limit case [67]. In Fig. 6, we can see that the convergence towards zero of $r_\infty(n)$ is slow [$r_\infty(1000) \approx 2\%$] and rather noisy below 20. Conversely, the convergence of $r_\infty(n)$ is smoother and very rapid. It could be interesting to look for a similar approximation for the superconfiguration averages, like the statistical sum $U_Q(g)$ in Eq. (3.8) to avoid the sums with alternate sign. Unfortunately, we fail to propose such an approximation, if it really exists.

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