PHYSICAL REVIEW E **79**, 016410 (2009)

Integrability criterion for lowering of ionization potentials and formulation of the solution of the inverse problem of constructing consistent thermodynamic functions of nonideal plasmas

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(Received 14 October 2008; published 26 January 2009)

Within the chemical picture, it is shown that self-consistent Coulomb nonideality corrections that satisfy Maxwell's thermodynamic identities can be constructed from formulas for lowering of ionization potentials, obtained from plasma electrostatic microfields or derived in *ad hoc* or empirical fashion, provided that a necessary integrability criterion is satisfied. The solution of such an inverse problem is formulated and introduced in terms of a simple integral that gives the correction to Helmholtz free energy function. The required integrability criterion is derived and applied to investigate the thermodynamic consistency of some models in the literature. Maintaining the same functional dependence on species densities as in the original models, a routine to fix thermodynamic inconsistencies found in some of these models is introduced. The advantages and usefulness of such a reverse scheme are discussed.

DOI: 10.1103/PhysRevE.79.016410 PACS number(s): 52.25.Kn, 52.27.Gr, 51.30.+i

I. INTRODUCTION

The use of precise and consistent equations of state and transport, and optical and thermodynamic properties is of utmost importance in the construction of stellar atmosphere and interior models. Accurate evaluation of these properties is also crucial in many applications involving high energy density plasmas such as controlled nuclear fusions, modern electrothermal launch technologies, and interaction of lasers and shock waves with matter. As it is commonly known, the quantitative investigation of these properties necessitates an accurate description of the plasma composition and species densities.

Within the chemical picture, the customary approach to the determination of species densities (ionized and excited), equation-of-state, and thermodynamic functions of plasma systems involves the construction and minimization of the Helmholtz free energy function [1–3]. Electrostatic interactions among charged particles and other possible coupling mechanisms are usually incorporated in a correction term, the so-called *excess free energy* ΔF^{int}, to be added to the ideal free energy function. This approach has the great advantage that the free energy minimization technique automatically generates thermodynamically consistent properties. Free energy minimization can also lead to a system of minimization equations having the form of the well-known Saha equation with lowered ionization energies [4–7]. The lowering of ionization energy for a *ζ-fold* ion in the plasma system can be written as

$$\Delta I_{\zeta} = -\left(\frac{\partial}{\partial N_e} - \frac{\partial}{\partial N_{\zeta}} + \frac{\partial}{\partial N_{\zeta+1}}\right)\Delta F^{int}, \qquad (1)$$

where N_e, N_{ζ}, and $N_{\zeta+1}$ are, respectively, the numbers of free electrons, *ζ-fold*, and $(\zeta+1)$-*fold* ionized species. It is worth noting that the lowering of ionization potentials given by Eq. (1) is the thermodynamic or composition lowering of ionization potentials to be incorporated in the generalized Saha equations [4]. This is different from the spectroscopic continuum lowering, that is, dissolution of emission or absorption lines. This latter is due to the microfields and related random shifts of energy levels, which occur for involved quantum states at much lower density than the true pressure ionization [8–11].

Considering the constraints of electroneutrality and conservation of nuclei, one can determine the detailed plasma composition either by optimization algorithms of the free energy function or by solving the set of coupled nonideal and nonlinear Saha equations [6,7]. Based on different physical arguments, different models for the excess free energy ΔF^{int} are derived and used in the literature (see, for example, [1–3]). Generally, ΔF^{int} can be expressed as the sum of a Coulomb part, ΔF^{Coub}, that describes electric interaction of the charged particles and a non-Coulomb part, $\Delta F^{non\text{-}Coub}$, which describes the interactions of neutral species with neutral and charged particles in the system; that is, $(\Delta F^{int} = \Delta F^{Coub} + \Delta F^{non\text{-}Coub})$.

An alternative approach to the determination of the plasma composition is based on the fact that in a nonideal plasma environment, the ionization energy is lowered due to the presence of the electrostatic microfields superimposed on the Coulomb electric field of an atomic nucleus. Hence one can derive this lowering of ionization energies from these electrostatic microfields [4,12–15] or even in an *ad hoc* or empirical fashion. Upon incorporating these lowering of ionization energies, the resulting corrected Saha equations can be used in conjunction with the aforementioned constraints to determine the detailed plasma composition. An important criticism to the latter approach was raised by Sweeney [16] who pointed out that the incorporation of the lowering of ionization potentials (pressure ionization term) in the Saha equation violates Maxwell's thermodynamic identities if corresponding changes are not made to the expressions for other thermodynamic functions. Negative values of the adiabatic gradient in the degenerate dwarf models of Böhm [17] and Straka [18] were explained in terms of this thermodynamic inconsistency.

It has to be noted that Sweeney did not provide the solution for how to reform thermodynamic functions in compliance with the corrected Saha equation in order to satisfy Maxwell's identities and the abstraction of the solution of this inverse problem is still unknown. It may also be useful to emphasize here that an inconsistent set of thermodynamic functions is not the sole reason for obtaining negative values of the adiabatic gradient. It is also possible to obtain such negative values of the adiabatic gradient from a consistent set of thermodynamic functions if the model used is inaccurate or used out of its range of applicability. In these cases, nonphysical properties such as negative pressure may also be obtained.

The objective of this work is to show how to solve the backward problem, to set the approach to clear Sweeney's concern, and to point out the necessary conditions required for a reachable solution with application to some models in the literature.

II. INTEGRABILITY CONDITION AND THE BACKWARD SCHEME FOR THE DERIVATION OF CONSISTENT THERMODYNAMIC FUNCTIONS

Starting from Eq. (1), which gives the relation between the depression of ionization potentials and the excess free energy, and rearranging the terms, one can obtain a recurrence relation in the form

$$\frac{\partial \Delta F^{int}}{\partial N_\zeta} = \frac{\partial \Delta F^{int}}{\partial N_{\zeta-1}} - \Delta I_{\zeta-1} - \frac{\partial \Delta F^{int}}{\partial N_e}, \quad \zeta = 1,2,\ldots,\zeta_{max}, \tag{2}$$

where ζ_{max} is the maximum possible ionization state of the atoms or ions under consideration. Restricting our discussion here to the Coulomb part of the excess free energy (function of charged particles' densities), successive use of the recurrence relation (2) leads to

$$\frac{\partial \Delta F^{Coub}}{\partial N_\zeta} = -\sum_{m=1}^{\zeta} \Delta I_{m-1} - \zeta \frac{\partial \Delta F^{Coub}}{\partial N_e}, \quad \zeta = 1,2,\ldots,\zeta_{max}. \tag{3}$$

In addition, the constraint of electroneutrality can be used to express the differential of the excess Coulomb free energy as

$$d\Delta F^{Coub} = \sum_{\zeta=1}^{\zeta_{max}} \left(\frac{\partial \Delta F^{Coub}}{\partial N_\zeta} + \zeta \frac{\partial \Delta F^{Coub}}{\partial N_e} \right) dN_\zeta. \tag{4}$$

Upon substitution from Eq. (3) into Eq. (4), one gets

$$d\Delta F^{Coub} = -\sum_{\zeta=1}^{\zeta_{max}} \left(\sum_{m=1}^{\zeta} \Delta I_{m-1} \right) dN_\zeta. \tag{5}$$

Equation (5) indicates that ΔF^{Coub} is effectively a function of the ions' densities with

$$\frac{\partial \Delta F^{Coub}}{\partial N_\zeta} = -\sum_{m=1}^{\zeta} \Delta I_{m-1}. \tag{6}$$

In view of the fact that ΔF^{Coub} must be a single-valued function of the equilibrium state of the assembly, $d\Delta F^{Coub}$ must be a complete, *exact*, differential, which requires the models of lowering of ionization energies to satisfy the following *integrability* or *self-consistency* condition:

$$\frac{\partial\left(-\sum_{m=1}^{\zeta} \Delta I_{m-1}\right)}{\partial N_z} = \frac{\partial\left(-\sum_{m=1}^{z} \Delta I_{m-1}\right)}{\partial N_\zeta},$$

$$z \neq \zeta, \quad z = 1,2,\ldots,\zeta_{max}, \quad \text{and} \quad \zeta = 1,2,\ldots,\zeta_{max}. \tag{7}$$

If the condition (7) is satisfied, one can integrate Eq. (5) to obtain the excess Coulomb free energy ΔF^{Coub}. During the integration of equations such as Eq. (5), it is convenient to increase the densities of all ions in the same ratio [19]. Denoting by λ the fraction of the final densities, which the ions have at any stage of integration, we then have

$$\Delta F^{Coub} = -N_H \sum_{\zeta=1}^{\zeta_{max}} \alpha_\zeta \int_0^1 \sum_{m=1}^{\zeta} \Delta I_{m-1}(\lambda) d\lambda, \tag{8}$$

where N_H is the total number of heavy particles and $\alpha_r = N_r / N_H$. Equation (8) can even be integrated numerically for cases in which analytical integration of $(\Sigma_{m=1}^{\zeta} \Delta I_{m-1}(\lambda))$ is not easily obtainable.

At this stage one can derive the Coulomb excess free energy from Eq. (8) and use it to derive the corrections to different thermodynamic properties. The derivation of Coulomb nonideality corrections to different thermodynamic functions from ΔF^{Coub} [as given by Eq. (8)] assures thermodynamic consistency among the calculated species densities and thermodynamic properties. It has to be noted that although the integration in Eq. (8) can be evaluated analytically for some cases giving rise to exact closed-form expressions for the corrections to thermodynamic functions, in several other cases numerical evaluation of Eq. (8) may become unavoidable. In all cases, the corrections to thermodynamic functions can be derived from the standard thermodynamic relations and they depend on the derivatives of the excess free energy with respect to the independent state variables, namely, volume V and temperature T.

III. VALUE OF THE SOLUTION OF THE INVERSE PROBLEM

Given the depression of ionization energies, the detailed composition of a nonideal plasma can be easily determined by solving the set of nonideal Saha equations subjected to the constraints of electroneutrality and conservation of nuclei. This allows investigating and clearing difficulties typically encountered in the well-known ionization models [20] with relative simplicity. Moreover, the ease of determining the detailed population densities of a nonideal plasma enables the calculation of the transport properties of such nonideal plasma systems without any prior knowledge of the free energy function. In principle, this is quite valuable as the transport properties of nonideal plasmas are easily and accurately measurable, in contrast with the set of thermodynamic properties, and this provides a reliable means of judging the accuracy of modeling the nonideal effects.

IV. INCONSISTENCIES IN SOME MODELS IN THE LITERATURE AND A RECOMMENDED ROUTINE TO RECOVER CONSISTENCY

Apart from their level of accuracy, most of the *ad hoc* formulas for depression of ionization energies, in addition to those derived from the plasma electrostatic microfield, suffer from inherent thermodynamic inconsistencies, which can be easily recognized by applying the criterion in Eq. (7). It is noteworthy that Potekhin [15] indicated that the occupation probabilities based on the plasma microfield distribution are in fact the optical or spectroscopic ones, and that their implication in thermodynamics leads to physically unrealistic equations of state.

Roughly speaking, the lowering of ionization energy of the mth ion can be expressed *in many* cases in the form

$$\Delta I_{m-1} = \sum_i C_i f_i(m) g_i(N_{r's}), \tag{9}$$

where C_i is a constant, $f_i(m)$ is a weighting function of the ion state m, and $g_i(N_{r's})$ is a function of the population densities of plasma species. The term $(-\Sigma_{m=1}^{\zeta}\Delta I_{m-1})$ found in Eq. (7) can therefore be written as

$$\left(-\sum_{m=1}^{\zeta}\Delta I_{m-1}\right) = -\sum_i C_i g_i(N_{r's})\sum_{m=1}^{\zeta} f_i(m), \tag{10}$$

with the result that the symmetry or consistency condition (7) implies that

$$\frac{\partial g_i(N_{r's})}{\partial N_z} = c\chi(N_{r's})\sum_{m=1}^{z} f_i(m). \tag{11}$$

Changing the form of the weighting function $f_i(m)$ to satisfy the requirement (11) fixes the inconsistencies in different formulas of lowering of ionization energies found in the literature. Equation (11) simply indicates that $f_i(m)$ is not independent from $g_i(N_{r's})$. In the following illustrative examples, we investigate and show the inconsistency of some models in the literature and provide optional reforms to recover thermodynamic consistencies as guided by Eq. (11). It has to be remembered that these optional reforms aim only at fixing the inconsistencies in these models with no claim regarding improving accuracy, even if the latter comes sometimes as a by-product of these reforms.

A. Unsöld's model

Unsöld [12] considered the influence of the next-neighbor's microfield on the potential distribution in the environment of the test nucleus and derived the following expression for the lowering of ionization energies:

$$\Delta I_{m-1} = C\underbrace{(m)^{2/3}}_{f(m)}\underbrace{(n_e)^{1/3}}_{g(N_{r's})}, \quad m = 1,2,\ldots,\zeta_{max}, \tag{12}$$

where $n_e = N_e/V = (\Sigma_{r=1}^{\zeta_{max}} rN_r)/V$ is the number density of free electrons and the constant C is given in the SI system of units by $C = 1.1136\times 10^{-27}$ J m.

It is straightforward to show the inconsistency of Unsöld's formula by applying the criterion in Eq. (7). To fix such an inconsistency while keeping the same functional dependence on the population densities, one needs to change $f(m)$ to satisfy Eq. (11). The left-hand side of Eq. (11) gives $(1/3V^{1/3})zN_e^{-2/3}$, which means that $z = \Sigma_{m=1}^{z} f(m)$ or, equivalently, that $f(m)$ must be *unity* instead of $m^{2/3}$ in the original model. This can be confirmed and also replicated using the above result, namely, $z = \Sigma_{m=1}^{z} f(m)$, and substituting into Eq. (8) to find the excess free energy as follows:

$$\Delta F^{Coub} = -CN_H n_e^{1/3}\sum_{\zeta=1}^{\zeta_{max}} \alpha_\zeta \zeta \int_0^1 \lambda^{1/3} d\lambda = -\frac{3}{4}CVn_e^{4/3}. \tag{13}$$

Now, one can proceed using Eq. (1) to find the lowering of ionization energies as follows:

$$\Delta I_\zeta = Cn_e^{1/3}, \tag{14}$$

which gives the same lowering of ionization energy for all ions as shown above. This finding is different from the original Unsöld's model in which the lowering of ionization energies to different ionization states is weighted by the ionization state of the ion to the power 2/3. For completeness, we give here the Coulomb corrections to pressure and internal energy derived from ΔF^{Coub} in Eq. (13) and standard thermodynamic relations.

$$\Delta P^{Coub} = -\frac{1}{4}Cn_e^{4/3}, \tag{15}$$

and

$$\frac{\Delta U^{Coub}}{V} = -\frac{3}{4}Cn_e^{4/3}. \tag{16}$$

We are not aware of expressions available in the literature for ΔF^{Coub}, ΔP^{Coub}, and ΔU^{Coub} in the original Unsöld's model in order to carry out a quantitative comparison with the expressions in Eqs. (13), (15), and (16).

B. Anisimov-Petrov

Anisimov and Petrov [15] obtained analytical expressions for the ionization potentials of neutral atoms and ions in the screened Coulomb potential of a nonideal plasma. According to the Anisimov and Petrov model and using the same notation as in [15], the lowering of ionization potential of an electron in the (n,l) state is expressed (in atomic units) as

$$\Delta I_{n,l} = (I_{n,l}^0 - I_{n,l}) = f_1(n,l)\frac{1}{\lambda_D} - f_2(n,l)\frac{1}{\lambda_D^2} + f_3(n,l)\frac{1}{\lambda_D^3}, \tag{17}$$

where

$$f_1(n,l) = \frac{1}{\sqrt{2}}\left(n - \frac{l}{n}(l-1) + l\right)\sqrt{I_{n,l}^0}, \tag{18}$$

$$f_2(n,l) = \frac{1}{2}\frac{1}{n^2}\left[\left(\frac{n^2 - l(l-1)}{2}\right)^2 + nl[n^2 - l(l-1)]\right], \tag{19}$$

$$f_3(n,l) = \frac{1}{8\sqrt{2}}\frac{l}{n^2}[n^2 - l(l-1)]^2\sqrt{\frac{1}{I^0_{n,l}}}, \tag{20}$$

and

$$\lambda_D = \sqrt{\frac{TV}{4\pi\Sigma_{r=1}^{\zeta_{max}} r(1+r)N_r}}. \tag{21}$$

For a specific chemical element, the ionization state $(m-1)$ of an ion determines the number of bound electrons and the quantum numbers (n,l) for the outermost electron. Accordingly, one can write

$$\Delta I_{n,l} = \Delta I_{m-1} = C_1 f_1(m)\underbrace{\frac{1}{\lambda_D}}_{g_1(N_{r'}s)} - C_2 f_2(m)\underbrace{\frac{1}{\lambda_D^2}}_{g_2(N_{r'}s)} + C_3 f_3(m)\underbrace{\frac{1}{\lambda_D^3}}_{g_3(N_{r'}s)}, \tag{22}$$

where C_1, C_2, and C_3 are numerical dimensionless constants. The functions $f_1(m)$, $f_2(m)$, and $f_3(m)$ may not be continuous; in most cases, they are piecewise continuous or tabulated functions.

Now, applying the self-consistency criterion Eq. (7) to the lowering of ionization energies given above, one gets

$$\begin{aligned}\frac{\partial}{\partial N_z}\left(-\sum_{m=1}^{\zeta}\Delta I_{m-1}\right) &= \left[-\sum_{n.l\equiv m=1}^{\zeta} f_1(n,l)\right]\frac{\partial\lambda_D^{-1}}{\partial N_z} - \left[-\sum_{n.l\equiv m=1}^{\zeta} f_2(n,l)\right]\frac{\partial\lambda_D^{-2}}{\partial N_z} + \left[-\sum_{n.l\equiv m=1}^{\zeta} f_3(n,l)\right]\frac{\partial\lambda_D^{-3}}{\partial N_z}\\ &= \left[-\sum_{n.l\equiv m=1}^{\zeta} f_1(n,l)\right]z(1+z)\frac{2\pi}{TV}\lambda_D - \left[-\sum_{n.l\equiv m=1}^{\zeta} f_2(n,l)\right]z(1+z)\frac{4\pi}{TV} + \left[-\sum_{n.l\equiv m=1}^{\zeta} f_3(n,l)\right]z(1+z)\left(\frac{6\pi}{TV}\right)\lambda_D^{-1}.\end{aligned} \tag{23}$$

The fact that the factor $\zeta(1+\zeta)$ cannot be factored out from each of the terms in the square brackets means that the expression is not symmetric in both z and ζ, and accordingly, it does not satisfy the integrability criterion. In order to fix this inconsistency, one can follow the same procedure as above where we assign

$$\sum_{m=1}^{\zeta} f_1(m) = \zeta(\zeta+1),$$

$$\sum_{m=1}^{\zeta} f_2(m) = \zeta(\zeta+1),$$

$$\sum_{m=1}^{\zeta} f_2(m) = \zeta(\zeta+1), \tag{24}$$

which gives

$$f_1(m) = 2m, \quad m = 1,2,\ldots,\zeta,$$

$$f_2(m) = 2m, \quad m = 1,2,\ldots,\zeta,$$

$$f_3(m) = 2m, \quad m = 1,2,\ldots,\zeta, \tag{25}$$

with the result that

$$\Delta I_{m-1} = 2C_1 m\frac{1}{\lambda_D} - 2C_2 m\frac{1}{\lambda_D^2} + 2C_3 m\frac{1}{\lambda_D^3}. \tag{26}$$

Following the same routine as above, one can substitute $\Sigma^{z}_{\substack{m=1\\ i=1,2,3}} f_i(m) = z(1+z)$ into Eq. (8) and perform the integration to get the free energy function as follows:

$$\begin{aligned}\Delta F^{Coub} &= -N_H\sum_{\zeta=1}^{\zeta_{max}}\alpha_\zeta\int_0^1\sum_{m=1}^{\zeta}\Delta I_{m-1}(\lambda)d\lambda = -N_H^{3/2}C_1\sum_{\zeta=1}^{\zeta_{max}}\alpha_\zeta\left[\frac{\zeta(1+\zeta)\sqrt{4\pi}}{\sqrt{TV}}\left(\sum_{r=1}^{\zeta_{max}} r(1+r)\alpha_r\right)^{1/2}\right]\int_0^1\lambda^{1/2}d\lambda\\ &+ N_H^2 C_2\sum_{\zeta=1}^{\zeta_{max}}\alpha_\varsigma\left[\frac{\zeta(1+\zeta)4\pi}{TV}\left(\sum_{r=1}^{\zeta_{max}} r(1+r)\alpha_r\right)\right]\int_0^{1^1}\lambda d\lambda - N_H^{5/2}C_3\sum_{\zeta=1}^{\zeta_{max}}\alpha_\varsigma\\ &\times\left[\frac{\zeta(1+\zeta)(4\pi)^{3/2}}{(TV)^{3/2}}\left(\sum_{r=1}^{\zeta_{max}} r(1+r)\alpha_r\right)^{3/2}\right]\int_0^{1^1}\lambda^{3/2}d\lambda = -\frac{C_1 TV}{6\pi\lambda_D^3} + \frac{C_2 TV}{8\pi\lambda_D^4} - \frac{C_3 TV}{10\pi\lambda_D^5},\end{aligned} \tag{27}$$

which gives, according to Eq. (1), the following expression for the depression of ionization energies:

$$\Delta I_{m-1} = 2C_1 m \frac{1}{\lambda_D} - 2C_2 m \frac{1}{\lambda_D^2} + 2C_3 m \frac{1}{\lambda_D^3}. \qquad (28)$$

Equation (28) is in complete agreement with our previous findings in Eq. (26). It is interesting to note that the above expressions (27) and (28) reduce to Debye-like formulas at weak nonideality where λ_D is large. In fact, the equations reduce exactly to the Debye model at weak nonideality for ($l=0$) if the effective charge Z^* in [15] is taken to be equal to the ionic charge.

V. CONCLUSIONS

It has been shown that self-consistent Coulomb nonideality corrections that satisfy Maxwell's thermodynamic identities can be constructed from formulas of lowering of ionization potentials derived in an *ad hoc* fashion or from plasma electrostatic microfields provided that a necessary consistency criterion is satisfied. The criterion of self-consistency of formulas of lowering of ionization potentials, the *integrability condition*, is derived and applied to illustratively investigate the consistency of a set of models in the literature. Maintaining the same dependence on the population densities as in the original models, a routine to fix inconsistencies of such models is introduced. An "inverse method" for deriving a consistent set of Coulomb corrections to thermodynamic functions is also introduced and cast in the form of a simple integral that gives the correction of the Helmholtz free energy function from the measured or modeled lowering of ionization potentials. This solution of the inverse problem apparently removes one of the main shortcomings of average ion models where it now provides a means of constructing consistent thermodynamic functions either analytically or numerically.

ACKNOWLEDGMENTS

Improvements suggested by Professor A. Abada from UAEU and by Professor M. Bourham from NCSU are highly appreciated.

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