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EQUATION OF STATE OF PARTIALLY-IONIZED PLASMAS IN THE PHYSICAL PICTURE

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RESUMEN. La ecuación de estado que utiliza el programa de opacidades OPAL, se basa en una expansión de actividad de muchos cuerpos de la función de partición gran canónica. Se presenta una descripción general del método. Este enfoque toma en cuenta, desde el principio, la interacción culómbica básica entre los electrones y los núcleos en el sistema. A consecuencia, no existe la necesidad de factorizar la energía libre, hacer afirmaciones sobre el efecto del medio ambiente del plasma sobre los estados ligados o introducir algún mecanismo para truncar la función de partición interna; tal como ocurre en los métodos donde se minimiza la energía libre.

ABSTRACT. The equation of state used by the OPAL opacity code is based on a many-body activity expansion of the grand canonical partition function. Herein we give an overview of the method. This approach considers, from the outset, the basic Coulomb interaction between the electrons and nuclei in the system. Consequently, there is no need to factorize the free energy, make assertions about the effect of the plasma environment on bound states, or invoke a mechanism for truncating the internal partition function; as in free energy minimization methods.

Key words: EQUATION OF STATE – PLASMAS

I. INTRODUCTION

In recent years the terms "chemical picture" and "physical picture" have become popular designations for approaches to calculate the equation of state of partially-ionized plasmas. The chemical picture refers to a free energy minimization approach. All current approaches of this type are based on the assumption that the Helmholtz free energy is separable into a series of uncoupled terms. In order to proceed in this way, it is necessary to assert what the effect of the plasma environment is on the bound states. Descriptions of recent work in the chemical picture are given by Däppen, Anderson, and Mihalas(1987), Hummer and Mihalas (1988), and Saumon and Chabrier (1991).

The physical picture refers to approaches based on many-body activity (fugacity) expansions of the grand canonical partition function (Ebeling, Kraeft, and Kremp, 1977; Kraeft, Kremp, Ebeling and Ropke, 1986; Rogers 1981); thus avoiding the need to compartmentalize the Helmholtz free energy. Since this approach deals at the outset with the pure Coulomb interaction between the electrons and nuclei of the system, there is no need to assert anything concerning the effect of plasma screening on the bound states. In addition, the heavily studied problem of the" divergence of the atomic partition function" never arises. As will be described, the bound state contribution to the partition function can be separated into a quantum part and a classical part. The quantum part is often referred to as the "Planck-Larkin Partition function" and it is automatically convergent. The classical part is not convergent, but it has divergences similar to continuum states. When all these divergences are added together using a systematic diagrammatic approach, a series of convergent, density dependent, terms is obtained. The leading term is just the familiar Debye-Hückel Coulomb correction.

Coulomb systems always display collective motion and do not approach a binary collision limit as the density is decreased. Nevertheless, an activity expansion exists for plasmas and it can be obtained from a diagrammatic resummation of the cluster coefficients. Our method takes advantage of the fact that the collective motion is highly classical. We first work out a global solution to the many-body problem using classical theory and in the final step replace classical expressions with their quantum mechanical analoques. This limits the theory to regions where the ratio of the de Broglie wavelength to the plasma screening length is less than unity. A condition well satisfied by most stellar plasmas. For dense cold objects, it is possible to use pseudopotentials to treat the region where this length ratio is greater than unity (Rogers, 1984).

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II. PLASMA DENSITY EXPANSIONS

As already mentioned, our first goal is to obtain a global classical many-body activity expansion. To do this it is convenient to start from the canonical ensemble and develop a systematic density expansion of the Mayer S function (Mayer, 1950), given by

$$S = -\sum_{\underline{j}=2}^{\infty} B_{\underline{j}} \frac{\rho^{\underline{j}}}{\underline{j}-1} \tag{1}$$

where the bar indicates multi-component structure, ρ is the density, and the $B_{\underline{j}}$ are virial coefficients. The function S is just the negative excess Helmholtz free energy, so that

$$(F - F_0)/V\,kT = -S \tag{2}$$

$$\frac{P}{kT} = \sum_{\nu} \rho_\nu + S - \sum_{\nu} \rho_\nu \frac{\partial S}{\partial \rho_\nu} \tag{3}$$

where ν is the species type.

Mayer (1950) was the first to show that the sum over the most divergent diagrams in the expansion of each virial coefficient, Bj, in powers of the potential (i.e. the so-called ring diagrams) yields the Debye-Hückel free energy. Abe (1959) showed how to systematically collect higher order diagrams to obtain an expansion which closely resembles the virial expansion for the Debye potential,

$$V_{\alpha\beta} = -Z_\alpha Z_\beta e^2 \frac{e^{-r/\lambda_D}}{r} , \tag{4}$$

where Z_α and Z_β are the ionic charge of particles α and β and λ_D is the Debye length. The analogy is not complete since the Abe functions are related to the B_j according to (for one component)

$$S_j(\lambda_D) = \rho^j[-B_j(\lambda_D) + \phi_j(\lambda_D)] , \tag{5}$$

where the ϕ_j are parts missing from the B_j because they were used to create the screening in lower order terms. The Abe expansion of S for a multi-component system explicitly displaying the components of $\underline{j}$ takes the form (Rogers, 1981; Rogers and DeWitt, 1973)

$$S = S_{\text{ring}} + \sum_{\alpha\beta} S_{\alpha\beta} + \sum_{\alpha\beta\gamma} S_{\alpha\beta\gamma} + \ldots \tag{6}$$

where α, β, γ, etc., range over all species.

$$S_{\text{ring}} = -F_{DH}/(VkT) = 1/12\,\pi\lambda_D^3 , \tag{7}$$

$$S_{\alpha\beta} = \rho_\alpha\rho_\beta[-B_{\alpha\beta}(T, \lambda_D) + \phi_{\alpha\beta}] , \tag{8}$$

and

$$\phi_{\alpha\beta} = 2\pi \int_0^\infty r^2\, dr \left(\beta V_{\alpha\beta} - \frac{(\beta V_{\alpha\beta})^2}{2} \right) . \tag{9}$$

Expressions for higher S_j can be found in the cited literature. In the following discussion it will be convenient to define

$$s_{\alpha\beta\gamma\ldots} \equiv \frac{S_{\alpha\beta\gamma\ldots}}{\rho_\alpha\rho_\beta\rho_\gamma\cdots} \qquad (10)$$

The Abe functions expand away from the weak coupling (low density) limit, while many interesting applications, especially for fully ionized plasmas, involve very strong coupling. Heavily studied in this regard are the one-component plasma (OCP) consisting of classical ions in a uniform neutralizing background of degenerate electrons and the screened OCP in which the electrons are allowed to respond to the heavy ions. The coupling in these cases can be characterized by the parameter Γ, given by

$$\Gamma = \frac{Z^2e^2}{kTa} \qquad (11)$$

where a is the ion sphere radius. When $\Gamma > 1$ it would be very difficult to systematically calculate terms in the Abe series to achieve convergence. However, it has been observed that to a good approximation the higher S_j can be systematically generated by operating on $S_{\alpha\beta}$ (Rogers, 1981).

III. PLASMA ACTIVITY EXPANSIONS

Section II gave a brief description of how to treat fully ionized plasmas in the range of weak to strong ion coupling provided the electron-ion coupling is not too strong; i.e. for conditions typical of most stars. Strong electron-ion coupling, such as occurs in white dwarf interiors, can be treated through the use of pseudopotentials (Rogers,1984; 1985). Classical Coulomb divergences are thus eliminated through many-body diagrammatic resummation. The next step is to introduce the formation of composite particles (bound states) into the formalism. This is best treated by switching from the canonical ensemble to the grand canonical ensemble and developing an activity expansion. For a one component system the pressure in the activity series can be expressed in terms of the S function through a sequence of differential operations (Rogers and DeWitt 1973)

$$\frac{P}{kT} = z + S + \sum_{m=2}^{\infty} \frac{z}{m!}\left(\frac{\partial}{\partial z}z\right)^{m-2}\left(\frac{\partial S}{\partial z}\right)^{m} \qquad (12)$$

where z is the activity given by

$$z = (2s+1)\,\lambda^{-3}e^{\mu/kT} \;, \qquad (13)$$

λ is the de Broglie wavelength and μ is the chemical potential. Equation (13) is subject to the constraint

$$\rho = z + \sum_{m=1}^{\infty} \frac{z}{m!}\left(\frac{\partial}{\partial z}z\right)^{m-1}\left(\frac{\partial S}{\partial z}\right)^{m} , \qquad (14)$$

where the Mayer S function in terms of the density defined by Eq. (1) is replaced by

$$S = -\sum_{j=2}^{\infty} \frac{B_j\, z^j}{j-1} \qquad (15)$$

which in the grand canonical ensemble is not simply the non-ideal free energy. Equations (1) and (15) differ only in that ρ is replaced by z. For plasmas an Abe type activity expansion similar to Eq. (6) also results from Eq. (15). Generalizations of Eq. (11) to several components is given in Rogers (1974). Equation (11) is obviously very complicated compared to the canonical ensemble expression for the pressure given by Eq.(3). Several questions arise: 1) Are Eq. (3) and Eqs. (12-15) equivalent ? If so, 2) why use the much more complicated version given by Eqs. (12-15).

A very simple example can answer the first question. Compare the solution of Eq. (3) to that of Eqs. (12-15) for the Debye approximation (Rogers and DeWitt, 1973). The result is that the pressure from the canonical ensemble and the grand canonical ensemble are in agreement everywhere in the fluid phase, but nowhere else (see Fig. 2 of Rogers and DeWitt,1973). Thus, either ensemble can be used for treating reacting plasmas.

The answer to the second question is two-fold. On the one hand it can be shown that the activity expansion is the natural expansion to use to account for reactions. On the other hand the Coulomb divergences present in the activity series are far more complicated than those that appear in the density series. Fortunately, however, a method for eliminating the divergences in S(ρ) was already given in Sec. II. Using this same approach to remove the divergences in S(z) appearing in Eqs. (12-15) provides an immediate solution to this problem. The main complication after this step concerns the fact that S is defined in terms of virial coefficients in the case of short-ranged interactions and by the Abe nodal functions in the case of long-ranged interactions; whereas the activity expansion works in terms of cluster coefficients that have direct physical meaning. That is, the b_j represent the total effect of turning on j particle interactions after sequentially turning on all possible interactions involving fewer particles; whereas, the virial coefficients possess no similar physical property.

It has been shown how to regroup systematically the terms in Eq. (12) such that a generalized cluster expansion is obtained (Rogers, 1974). The resulting expansion is generalized in the sense that the usual cluster expansion is obtained for short ranged interactions while temperature and activity dependent coefficients involving the Abe nodal functions, S_j, are obtained for long-range interactions. To illustrate the procedure consider the first few terms for a one-component system, described by Eq. (15)

$$\frac{P}{kT} = z + S + \frac{z}{2}\left(\frac{\partial S}{\partial z}\right)^2 + \frac{z}{3!}\frac{\partial}{\partial z}z\left(\frac{\partial S}{\partial z}\right)^3 + \ldots$$

$$= z + S_{ring} + S_2 + S_3 + S_4 \ldots + \frac{z}{2}\left(\frac{\partial S_{ring}}{\partial z} + \frac{\partial S_2}{\partial z} + \frac{\partial S_3}{\partial z} + \ldots\right)^2$$

$$+ \frac{z}{3!}\frac{\partial}{\partial z}z\left(\frac{\partial S_{ring}}{\partial z} + \frac{\partial}{\partial z}S_2 + \ldots\right)^3 \ldots \tag{16}$$

Now if we collect terms such that the occurrence of each Sj is considered to increase the order by the amount j - 1, we obtain

$$C_2 \equiv S_2 \tag{17}$$

$$C_3 \equiv S_3 + \frac{z}{2}\left(\frac{\partial S_3}{\partial z}\right)^2 \tag{18}$$

$$C_4 \equiv S_4 + z\left(\frac{\partial S_2}{\partial z}\right)\left(\frac{\partial S_3}{\partial z}\right) + \frac{z}{3!}\frac{\partial}{\partial z}z\left(\frac{\partial S_2}{\partial z}\right)^3 \tag{19}$$

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The sum of the indexes j - 1 in Eq. (17) is of course just unity. In Eq. (18) the sum in each term is equal to 2, etc. (Rogers 1974). As already mentioned the S_j for short ranged potentials are given directly from the definition (see Eq. 7) and it is easy to verify that

$$C_j = z^j b_j \ , \tag{20}$$

i.e., the C_j offer an alternative route to those generally presented in text books for generating the bj in terms of the B_j. For a Coulomb potential, however, the ratio C_j/z^j, which is normally only a function of temperature, depends on both temperature and activity through the Abe nodal functions, s_j. For short-ranged potentials the C_j given by Eq. (20) produce the usual result for the pressure,

$$\frac{P}{kT} = z + \sum_{j=2}^{\infty} C_j = z + \sum_{j=2}^{\infty} z^j b_j \ . \tag{21}$$

However, due to the activity dependence for long-ranged potentials the pressure equation takes a much more complicated form. The first terms for a two-component plasma of electrons and ions of type α, is given by

$$\frac{P}{kT} = z_e + z_\alpha + \chi_R + \sum_{j=2}^{\infty} C_{\underline{j}} + z_e \frac{\partial \chi_R}{\partial z_e} \frac{\partial C_{\underline{j}}}{\partial z_e} + z_\alpha \frac{\partial \chi_R}{\partial z_\alpha} \frac{\partial C_{\underline{j}}}{\partial z_\alpha} + \ldots \tag{22}$$

where to lowest order $\chi_R = S_{ring}$ and in general

$$\chi_R = \frac{P(S)}{kT} \bigg|_{S=S_R} - z_e - z_\alpha \ , \tag{23}$$

i.e., a multi-component generalization of Eq. (11) in which S is everywhere replaced with Sring, and the $C_{\underline{j}}$ are a multi-component generalization of Eqs. (17-19). A more complete version of Eq. (22) is given in Rogers and DeWitt (1973).

The complete multi-component version of Eq. (22) gives a classical activity expression for the pressure that is formally valid for all plasma couplings. However, it cannot avoid the collapse due to electron-ion interactions. To avoid this problem requires the introduction of quantum mechanics. This is mainly a few particle phenomena which has little effect on the collective motion when $\bar{\lambda} < \lambda_z$, where λ_z is the grand-canonical counterpart to the Debye length with ρ replaced by z. Consequently for most applications it is sufficient to simply replace the classical cluster coefficients for the screened potential appearing in the C_j with their quantum mechanical counterparts involving the appropriate traces over the few particle Hamiltonian operator. A quantum mechanical treatment that accounts for quantum effects on collective motion has been given by DeWitt (1966).

As a simple example of the proposed approximation consider the classical version of the electron-ion cluster coefficient, $C_{e\alpha}$, arising in $C_{\underline{2}}$, where

$$C_{\underline{2}} \equiv C_{ee} + 2C_{e\alpha} + C_{\alpha\alpha} \ . \tag{24}$$

From Eq. (17) we have $C_{e\alpha} = S_{e\alpha}$, so that, with β = e Eq. (8) gives a classical result for $C_{e\alpha}$. We now replace $b_{e\alpha} \equiv - B_{e\alpha}$ with

$$b_{e\alpha} = 4\pi\lambda_{e\alpha}^3 \, \mathrm{Tr}(e^{-\beta H_2} - e^{-\beta H_0}) \ , \tag{25}$$

but leave $\phi_{e\alpha}$ completely classical. The two particle trace in Eq. (25) is over a Debye-like potential in which the screening length is given by λ_z. Quantum corrections to $\phi_{e\alpha}$ are given by DeWitt (1966). The first order correction in powers of $\bar{\lambda}/\lambda_z$ is recovered by the described procedure (Rogers, 1979). The coefficient $b_{e\alpha}$ gives the correction to thermodynamic quantities due to the redistribution of states resulting from switching on two-body interactions, relative to that already included in the ideal gas distribution. No states are created in this process but some states may enter the negative energy domain. Even so $b_{e\alpha}$ is a continuous function of interaction strength (Ebeling, et al. 1977). Replacements similar to Eq. (25) are carried out for all the b_j occurring in higher C_j. Consequently Eq. (22) is a continuous function of temperature and activity (density) and does not suffer from the discontinuous behavior present in some versions of the chemical picture. It is important that this property be preserved in the subsequent analysis. Also since the $b_j(\lambda_z)$ have no bound states when the screening length λ_z is less than some critical value (0.84 a0 for H), pressure ionization is naturally included in Eq. (22).

Uhlenbeck and Beth (1936) long ago showed that $b_{e\alpha}$ can be evaluated in terms of bound states and scattering phase shifts according to

$$b_{e\alpha} = b^{b}_{e\alpha} + b^{s}_{e\alpha} \tag{26}$$

$$b^{b}_{e\alpha} = \sqrt{2}\,\lambda^{3}_{e\alpha} \sum_{n\ell} (2\ell + 1)\, e^{-\beta E_{n\ell}} \tag{27}$$

$$b^{s}_{e\alpha} = \frac{\sqrt{2}}{\pi}\,\lambda^{3}_{e\alpha} \sum_{\ell} (2\ell + 1) \int_{0}^{\infty} dp\, \frac{d\delta_{\ell}(p)}{dp}\, e^{-\beta p^{2}/2\mu_{e\alpha}} \tag{28}$$

where $\delta_\ell(p)$ is the phase shift for the lth partial wave, p is the relative momentum and $\mu_{e\alpha}$ is the reduced mass. A connection of Eq. (26) with the high temperature expansion for a Coulomb potential can readily be established. Integrate Eq. (28) by parts and use the Levinson theorem (Levinson, 1949) result that the scattering phase shift at zero energy is equal to $n\pi$, where n is the number of bound states. This gives

$$b^{s}_{e\alpha} = \frac{\sqrt{2}\,\beta}{\pi\mu_{ea}}\,\lambda^{3}_{e\alpha} \sum_{n\ell} (2\ell + 1) \int_{0}^{\infty} dp\, p\, \delta_{\ell}\, e^{-\beta\, p^{2}/2\mu_{e\alpha}} - n\pi \tag{29}$$

The last term in Eq. (29) is equal and opposite to the first term in the high temperature expression of Eq. (27). Higher order Levinson type theorems exist (Bolle, 1989; Pisani and McKellar 1989) that allow an additional integration by parts so that the second term in the high temperature expansion of Eq. (27) is also cancelled, i.e. after this analysis the two terms that cause the internal partition function to diverge at high T are found to be analytically missing from $b_{e\alpha}$. These terms are classical and their contribution to the pressure was already included in the ideal gas term. A detailed description of this point has been given in the WKB approximation (Rogers 1977; 1979). Similar cancellations were also shown to occur in the higher b_j. Note that the b_j are still all divergent, but the types of divergences occurring in the so called internal partition function are fictitious and do not occur in the complete result. It should also be noted that part of the confusion results from labeling the sum over states in $b^{b}_{e\alpha}$ as a partition function. The relevant physical quantity that corrects thermodynamic functions is the full $b_{e\alpha}$.

The form $b^{b}_{e\alpha}$ that results after the analytic compensation with the continuum is

$$b^{b}_{e\alpha} = \sqrt{2}\,\lambda^{3}_{e\alpha} \sum_{n\ell} (2\ell + 1)(e^{\beta E_{n\ell}} - 1 + \beta E_{n\ell}) \tag{30}$$

This is known as the Planck-Larkin partition function (Larkin, 1960). For short range forces no problem arises in splitting the cluster coefficient so that one can work directly from the Boltzmann factor to define composite particle activities. For a potential such as the Debye potential the number of bound states can be large and also the number varies with density in principle requiring the introduction of a large set of new activity variables with accompanying interaction potentials and Abe functions. However, use of Planck-Larkin weight factors to define composite particle activities effectively cuts the sum off when the binding energy is less than kT, so that generally only a few new activity variables are required. Everything else is simply treated as part of a redefined continuum. The occupation numbers are thus effective occupation numbers and not the actual occupation numbers, which explains the earlier remark. If the total occupation of a state is required, as for example in opacity calculations, it can be obtained from a complimentary calculation after the equation of state is obtained (Rogers, 1986).

Two additional steps are required before the Coulomb cluster expansion can be applied to partially ionized dense plasmas. The first is to introduce an augmented set of activity variables (Rogers, 1974) to account for reactions taking place in the plasma. The second is to account for the fact that in multiply ionized plasmas the heavy ions can be strongly coupled while the electrons are only moderately coupled to ions.

After the first step a multi-component version of Eq. (22) is obtained in which composite particles whose binding energy is > kT act analytically exactly like fundamental particles (see Eq. (42) of Rogers, 1974). As the density is changed, such that the binding energy becomes less than kT, states smoothly switch over to being weak and are treated along with the continuum states. An important result of the analysis is that strong states, having binding energy > kT, are unscreened by the plasma. The screening that was present in Eq. (22) has been used to create the new activity variables. The total number of bound states is still, however, determined by the Debye-like potential. The best way to handle the states having binding energy less than kT seems to be a procedure where these levels are also unscreened but their occupation numbers are greatly diminished due to interaction with neighbors. The occupation numbers are effectively zero for bound states not allowed by the screened potential (Rogers, 1986; 1990).

IV. DISCUSSION

The purpose of this paper has been to give a somewhat cursory description of the physical picture equation of state method used to provide occupation numbers for the OPAL opacity code. The highlights of this approach are that: 1) The divergence of the atomic partition function is completely avoided. 2) No assertion regarding the effect of plasma screening on bound states is needed. 3) A systematic set of corrections of increasingly higher order are available to treat very dense plasmas. A detailed account of this work can be obtained in the cited literature.

Even though the method bears little similarity to the chemical picture methods used by Mihalas, Hummer, and Däppen (MHD) (described elsewhere this volume), the agreement between the two methods is nearly exact at densities typical of stellar envelopes (Däppen, Lebreton, and Rogers, 1990; Däppen, Keady, and Rogers, 1991). At higher densities significant differences start to appear (Däppen this volume). It seems to us that the physical picture is more reliable under these conditions, since the MHD approach includes only the lowest order Coulomb interaction corrections, i.e., the Debye Hückel term.

One concern with the plasma activity expansion method is can one be sure it actually converges. There are no accurate experiments for real plasmas with which to compare. However, computer simulations for the classical OCP do exist. In this case both the plasma density expansion and the activity expansion converge quite nicely to the "exact" simulation result (Rogers and DeWitt, 1973; Rogers, 1981). Since the quantum effects in real plasmas occur at short distances, somewhat similar convergence properties should be expected.

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