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A simple formulation and solution strategy of the Saha equation for ideal and nonideal plasmas

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Abstract. A simple formulation and solution strategy for the Saha equation is introduced. The formulation discriminates between the cases in which either the pressure or the number density of heavy particles is known. This discrimination allows the method to be generalized to include all problems of practical interest, as well as to clarify ambiguities found in other formulations in the literature. The present method overcomes restrictions imposed on other competitive techniques and takes into account all possible formulae for nonideality corrections. In most practical cases the solution of the nonlinear set of the Saha equations is reduced to the simple problem of solving a single transcendental equation.

Nomenclature

n_e	number density of free electrons
n_r	number density of all r-fold ionized atoms (e.g. $r = 0$ for neutral particles, $r = 1$ for one-fold ionized particle, etc)
U_r	partition function of r-fold ionized atoms
T	absolute temperature
I_r^{eff}	effective ionization energy for the ionization process $r \rightarrow (r + 1)$
ΔI_r	the lowering of ionization energy for the ionization process $r \rightarrow (r + 1)$ due to the presence of other particles (nonideal effects)
m_e	electron's rest mass
h	Planck's constant
K_B	Boltzmann's constant
Z	the highest-fold ionization to be reached in the plasma under consideration
n_H	number density of heavy particles (nuclei)
$\alpha_r = n_r/n_H$	proportion of the gas at ionization state r
$Z_{av} = \alpha_e = n_e/n_H$	average charge state of heavy particles
$Z_{eff} = (r + 1)$	the effective charge state of an atom (ion) disturbed by the nearest neighbouring particle
P	kinetic pressure
$P_e = n_e K_B T/P$	
$P_r = n_r K_B T/P$	
ΔP	decrease in pressure due to nonideal effects

1. Introduction

The quantitative investigation of plasma transport properties necessitates information on the plasma composition at fixed temperature and volume, with either a constant pressure or constant number density of heavy particles (nuclei). Particle densities of plasma components (charged particles as well as neutral particles) are required for the calculation of plasma transport properties such as electric conductivity, thermal conductivity, etc. The quantitative study of ionization equilibrium is also important in plasma spectroscopy, astroplasmas, and high energy density physics (controlled nuclear fusion, gas phase nuclear reactors, interaction of lasers and shock waves with matter, etc).

For plasmas in local thermodynamic equilibrium (LTE), the distribution of atoms and their ionization products (ions and electrons) obeys the well-known Saha equation [1]. Taking into account the lowering of ionization potentials due to nonideal effects (density effect or pressure ionization) [2], the Saha equation can be written as

$$\frac{n_{r+1}n_e}{n_r} = 2\frac{U_{r+1}}{U_r}\left[\frac{2\pi m_e K_B T}{h^2}\right]^{3/2} \exp\left(-\frac{I_r^{eff}}{K_B T}\right) \qquad r = 0, 1, \ldots, (Z-1) \tag{1}$$

where U_r is the temperature dependent partition function of r-fold ionized atoms and I_r^{eff} is the effective ionization energy for the ionization process $r \rightarrow (r + 1)$.

The system of Saha equations (1), supplemented by the condition of electro-neutrality,

$$\sum_{i=1}^{Z} i\, n_i = n_e \tag{2}$$

and requiring a constant number of heavy particles (conservation of nuclei in the ionization and recombination processes),

$$\sum_{r=0}^{Z} n_r = n_H = \text{constant} \tag{3}$$

is a closed system of nonlinear algebraic equations, the solution of which is required to determine the detailed plasma composition. Equations (1)–(3) can alternatively be written in terms of the proportions of the gas at the ionization state i, $\alpha_i = n_i/n_H$ and the average charge of heavy particles Z_{av}, or in terms of $P_e = n_e K_B T/P$ and $P_r = n_r K_B T/P$.

2. Current available methods

The solution of the set of nonlinear Saha equations has attracted the interest of many investigators. As mentioned by Trayner and Glowacki [3], 'Many software algorithms have been used over the years to solve this set of equations... The solution is nontrivial because of the nonlinearity and because of the appearance of all the α_i in all equations.' Rouse [4] introduced a solution technique that involved iteration with respect to the electron pressure or electron concentration $C = n_e/(n_H + n_e)$. The method assumes an equation-of-state for an ideal plasma and iterates over all the equations. Drellishak *et al* [5] derived a polynomial of the order $Z + 1$ in the electron number density, in addition to recurrence relations for the number densities of heavy particles of different ionization states. To obtain the polynomial form for the nonideal case, they assumed a formula for the lowering of ionization potential that does not depend on the electron number density. However, the method does not take into account the decrease in pressure due to high density and also assumes an equation-of-state for an ideal plasma. Kannappan and Bose [6] derived a transcendental equation in the electron mole fraction for a two temperature plasma, in addition to recurrence relations for the mole fraction of heavy particles of different ionization states. They also used the equation-of-state of an ideal plasma and a formula for the lowering of ionization energy that depends explicitly on the electron mole fraction. The method cannot be used for high density corrections of the type proposed by Griem [2] or Ebeling and Sandig [7]. Zel'dovich and Raizer [8], Kerely [9] and Sato [10] proposed different approximate methods for the solution of the Saha equation. Trayner and Glowacki [3] presented the most recent work in this aspect. They introduced a technique for the solution of the Saha equation which is similar to that by Rouse [4]. However, their work reported the numerical details and accuracy limitations of using such a formulation and method of solution.

3. Present approach

3.1. Ideal plasma

Before presenting the details of the present method, it is important to discriminate between two cases: 1) the case in which n_H is known; and 2) the case in which the pressure, P, is known. Both of these cases are of practical importance. Pressure is a measurable quantity and n_H can be calculated from the plasma mass density, which can also be measured in some applications as pointed out in [11, 12]. It is meaningless to consider the case where both n_H and P are known for ideal plasmas since for this case a pure analytical solution is possible, as will be shown.

For the case in which n_H is known, equations (1)–(3) are rewritten in terms of α_i and Z_{av}

$$\sum_{r=0}^{Z} \alpha_r = 1 \tag{4}$$

$$\sum_{i=1}^{Z} i\,\alpha_i = Z_{av} \tag{5}$$

$$\frac{\alpha_{r+1} Z_{av} n_H}{\alpha_r} = 2\frac{U_{r+1}}{U_r}\left[\frac{2\pi m_e K_B T}{h^2}\right]^{3/2} \exp\left(-\frac{I_r}{K_B T}\right) = f_{r+1} \qquad r = 0, 1, \ldots, (Z-1). \tag{6}$$

Equation (6) provides the recurrence relation:

$$\alpha_{r+1} = \frac{\alpha_r}{(Z_{av} n_H)} f_{r+1}. \tag{7}$$

Substituting (7) into (5), one gets the following relation for α_0 in terms of Z_{av}

$$\alpha_0 = Z_{av}\left(\sum_{i=1}^{Z} \frac{i \prod_{j=1}^{i} f_j}{(Z_{av} n_H)^i}\right)^{-1}. \tag{8}$$

Using this relation with the recurrence relation (equation (7)) and substituting in equation (4) one gets the transcendental equation in Z_{av}

$$1 - Z_{av}\left(\sum_{i=1}^{Z} \frac{i \prod_{j=1}^{i} f_j}{(Z_{av} n_H)^i}\right)^{-1}\left[1 + \sum_{i=1}^{Z} \frac{\prod_{j=1}^{i} f_j}{(Z_{av} n_H)^i}\right] = 0. \tag{9}$$

By solving equation (9) and substituting back into equation (8) and equation (7), each individual α_i, and therefore the composition of an ideal plasma, can be determined. Many software packages contain solvers for transcendental equations or algorithms for determining the zeros of a function. However, the solution of equation (9) is sufficiently simple—that is to say, to a reasonable number of ionization states, it can be solved even using a 'pocket' scientific calculator. Additionally, equation (9) permits the calculation of the average charge of heavy particles without iterating over the α_i equations. From the above formulation it is easy to show that, when both n_H and P are known, a purely analytic solution is possible through equations (7) and (8), where ideal plasmas are characterized by the simple equation-of-state, $P = n_H K_B T(1 + Z_{av})$ or $Z_{av} = (P/n_H K_B T) - 1$. In principle, equation (9) can be solved to any desired accuracy at the expense of the solution time. For an ideal plasma that is composed of more than one monatomic chemical species, the number of independent transcendental equations is equal to the number of chemical species.

For the case in which the pressure P is known, equation (9) can still be used by substituting $n_H = P/K_B T(1 + Z_{av})$.

However, it is useful to derive an equation similar to equation (9) in terms of the relative partial pressures of the individual components.

Multiplying equation (3) by $K_B T$ and dividing by the total pressure P yields

$$\sum_{r=0}^{Z} P_r = 1 - P_e. \tag{10}$$

Similarly, equations (2) and (3) can be written as

$$\sum_{i=1}^{Z} i\, P_i = P_e \tag{11}$$

$$\frac{P_{r+1}(P_e P)}{P_r} = 2\frac{U_{r+1}}{U_r}\left[\frac{2\pi m_e}{h^2}\right]^{3/2}(K_B T)^{5/2}\exp\left(-\frac{I_r}{K_B T}\right)$$
$$= \eta_{r+1} \qquad r = 0, 1, \ldots, (Z-1). \tag{12}$$

Equation (12) gives the following recurrence relation

$$P_{r+1} = \frac{P_r}{(P_e P)}\eta_{r+1}. \tag{13}$$

Upon substituting from equation (13) into equation (11) one gets

$$P_0 = P_e\left(\sum_{i=1}^{Z}\frac{i\prod_{j=1}^{i}\eta_j}{(P_e P)^i}\right)^{-1}. \tag{14}$$

Similar to the case of known n_H, if one substitutes equation (14) and the recurrence relation (equation (13)) into equation (10) one obtains the transcendental equation in P_e

$$(1-P_e) - P_e\left(\sum_{i=1}^{Z}\frac{i\prod_{j=1}^{i}\eta_j}{(P_e P)^i}\right)^{-1}\left[1+\sum_{i=1}^{Z}\frac{\prod_{j=1}^{i}\eta_j}{(P_e P)^i}\right] = 0. \tag{15}$$

Equation (15) is more convenient and can be easily modified to accommodate nonideal effects for the case of known pressure.

3.2. Nonideal plasmas

For nonideal plasmas, high density corrections to both the ionization energy and the kinetic pressure should be taken into account. Both the ionization energy and kinetic pressure decrease with high density and can generally be expressed as, $I_r^{eff} = I_r - \Delta I_r$ and $P = P_{ideal} - \Delta P$. These effects have been studied and described comprehensively in the literature [2, 13, 14] and there are many models to quantitatively represent them. It is not intended to study these effects here. However, it is important to note their impact on the present formulation and method of solution.

As long as ΔI_r and ΔP can be expressed explicitly in terms of Z_{av} and n_H (or P_e and P), the above method, for ideal plasmas, can be used to determine the nonideal plasma composition by replacing I_r by $I_r - \Delta I_r$ and modifying equation (15) to

$$(1-\Delta P - P_e) - P_e\left(\sum_{i=1}^{Z}\frac{i\prod_{j=1}^{i}\eta_j}{(P_e P)^i}\right)^{-1}\left[1+\sum_{i=1}^{Z}\frac{\prod_{j=1}^{i}\eta_j}{(P_e P)^i}\right] = 0 \tag{16}$$

where P in equation (16) is the measured or known plasma kinetic pressure. It should be noted that, for nonideal plasmas, P_e and P_r no longer represent the relative partial pressures but the ratio of the ideal pressure of each species to the total pressure. Equation (16) is important for the case of known pressure and physical models of ΔP, which have complicated expressions in n_H and Z_{av} such that n_H and/or $n_H + n_e$ cannot be expressed explicitly in terms of P.

It is not always possible to represent ΔI_r and ΔP in terms of Z_{av} and n_H (or P_e and P). The model proposed by Griem [2] is an example of such a case where ΔI_r and ΔP are expressed as

$$\Delta I_r = \frac{(r+1)e^2}{4\pi\varepsilon_0\lambda_D}$$
$$\Delta P = \frac{1}{6}\left(\frac{e^2}{4\pi\varepsilon_0\lambda_D}\right)(n_e + \sum_r r^2 n_r) = \frac{K_B T}{24\pi\lambda_D^3} \tag{17}$$

where

$$\lambda_D = [\varepsilon_0 K_B T/e^2(n_e + \sum_r r^2 n_r)]^{1/2}.$$

This model is based on the Debye theory and is valid for cases in which the inequality $\xi = n_e + \Sigma n_i/(8\pi\lambda_D^3)^{-1} \geq 1$ is satisfied. This model represents the case where ΔI_r and ΔP are functions of a common variable, λ_D, which cannot be expressed explicitly in terms of Z_{av} and n_H (or P_e and P). For this case the solution can also be obtained with relative simplicity using the following algorithm.

(1) Start with a guess for the value for λ_D. This can be done either by assigning a guess for λ_D directly or by assigning a guess for Z_{av} (or P_e), calculating α_r (or P_r) from the recurrence relations (7) and (8) (or (13) and (14)) using another model for ΔI_r that can be explicitly expressed in terms of n_H and Z_{av} (or P and P_e), and computing the guess for the common parameter, λ_D where $n_r = n_H\alpha_r$ (or $n_r = P_r P/K_B T$) and $n_e = n_H Z_{av}$ (or $n_e = P_e P/K_B T$).
(2) Calculate Z_{av} (or P_e) from equation (9) (or equation (16)) after replacing I_r by $I_r - \Delta I_r$.
(3) With the help of the recurrence relations, calculate a new value for λ_D as pointed out in step (1).
(4) If the calculated value for λ_D is different from the guess, use it as an updated guess for the next cycle or iteration.
(5) Repeat until the difference between the calculated value for λ_D and the guess satisfies the desired accuracy for λ_D.

A more detailed discussion concerning the initial guess and convergence rates is provided below following the third sample problem.

The most complicated case occurs if ΔI_r and ΔP are not functions of a common variable and cannot be expressed in terms of Z_{av} and n_H (or P_e and P) at the same time. If n_H is the known quantity the above algorithm can still be used where, in general, ΔI_r can be used instead of λ_D. The iteration process in this case embodies the use of the nonideal version of equation (9) and the expression of ΔI_r. However, in the case of known pressure, the algorithm needs to be modified to include the expression for ΔP and it can be summarized as follows.

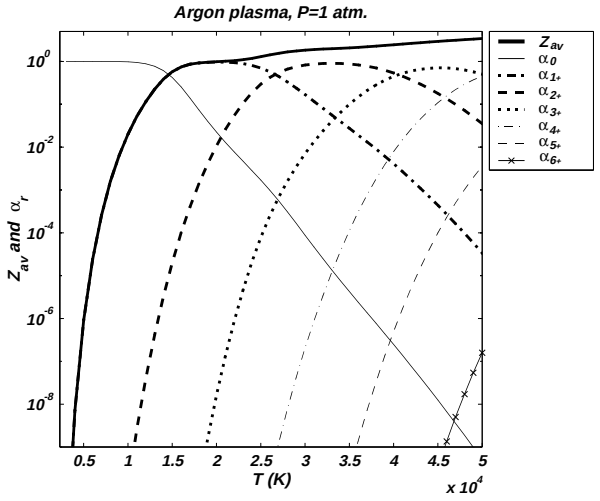


Figure 1. Composition of an ideal argon plasma at 1 atmosphere.

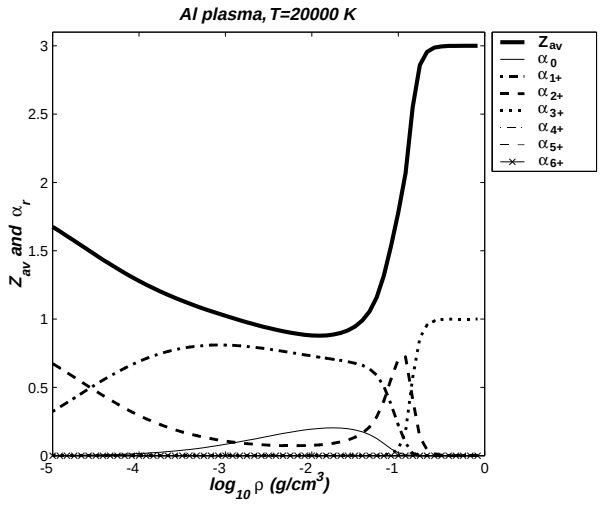
(1) Guess values for ΔI_r and ΔP. This can also be done by assigning guesses for ΔI_r and ΔP directly or by assigning a guess for Z_{av} (or P_e), then calculating α_r (or P_r) from the recurrence relations (7) and (8) (or (13) and (14)) which will be sufficient to compute the guesses for ΔI_r and ΔP for any proposed expressions.
(2) Calculate Z_{av} (or P_e) from equation (9) (or equation (16)) after replacing I_r by $I_r - \Delta I_r$.
(3) With the help of the recurrence relations calculate new values for ΔI_r and ΔP.
(4) If the calculated values for ΔI_r and ΔP are different from the guessed ones, use them to update the guess for the next cycle or iteration.
(5) Repeat until the difference between the calculated values for ΔI_r and ΔP and the guess satisfies the desired accuracy for each of them.

4. Sample problems

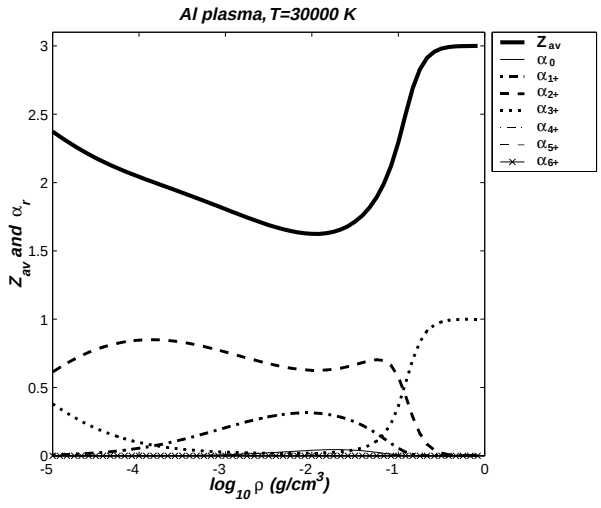
In these sample calculations the partition functions have been approximated to be the statistical weights of the ground states. The maximum allowed ionization state has been set to 6. Among the elements of the periodic table, argon and aluminium have been chosen to run the current sample problems. Necessary spectroscopic data, as well as the detailed plasma composition for these two elements, are available in the literature. Tables 1 and 2 show the unperturbed ionization energies and the statistical weights of the ground states for Ar and Al, respectively.

4.1. Ideal plasma

The present method has been used to calculate the detailed plasma composition for an ideal atmospheric argon plasma at different temperatures. Figure 1 shows the plasma composition for argon at atmospheric pressure and different temperatures. For the sake of comparison, the proportions shown are with respect to n_H and have been calculated for constant pressure by replacing n_H in equation (9) by $P/K_BT(1 + Z_{av})$. The results are in agreement with those presented in [3].



(a)



(b)

Figure 2. Composition of a dense nonideal Al plasma at (a) 20 000 K and (b) 30 000 K. Nonideality corrections described by equation (18).

4.2. Nonideal plasma with high density corrections expressible in Z_{av} and n_H (or P_e and P)

As pointed out above, for this case the problem reduces to the solution of a single transcendental equation. Detailed composition for a dense nonideal aluminium plasma at two different temperatures, 20 000 and 30 000 K, and a mass density range from 10^{-5} g cm^{-3} to near the critical density, has been computed and shown in figures 2(a) and (b), respectively. The lowering of ionization energy has been expressed as [14]

$$\Delta I_r = 6.96 \times 10^{-7} \sqrt[3]{n_e[\mathrm{cm}^{-3}]}\, Z_{eff}^{2/3}\,[\mathrm{eV}] \qquad (18)$$

where $Z_{eff} = (r + 1)$ is the effective charge state of the disturbed atom (ion). The average charge of heavy particles decreases as the density increases until the effect of lowering of the ionization potential manifests itself, and then Z_{av} starts to increase with the increase of mass density. This behaviour is in agreement with the results from other models and other methods of calculation [15].

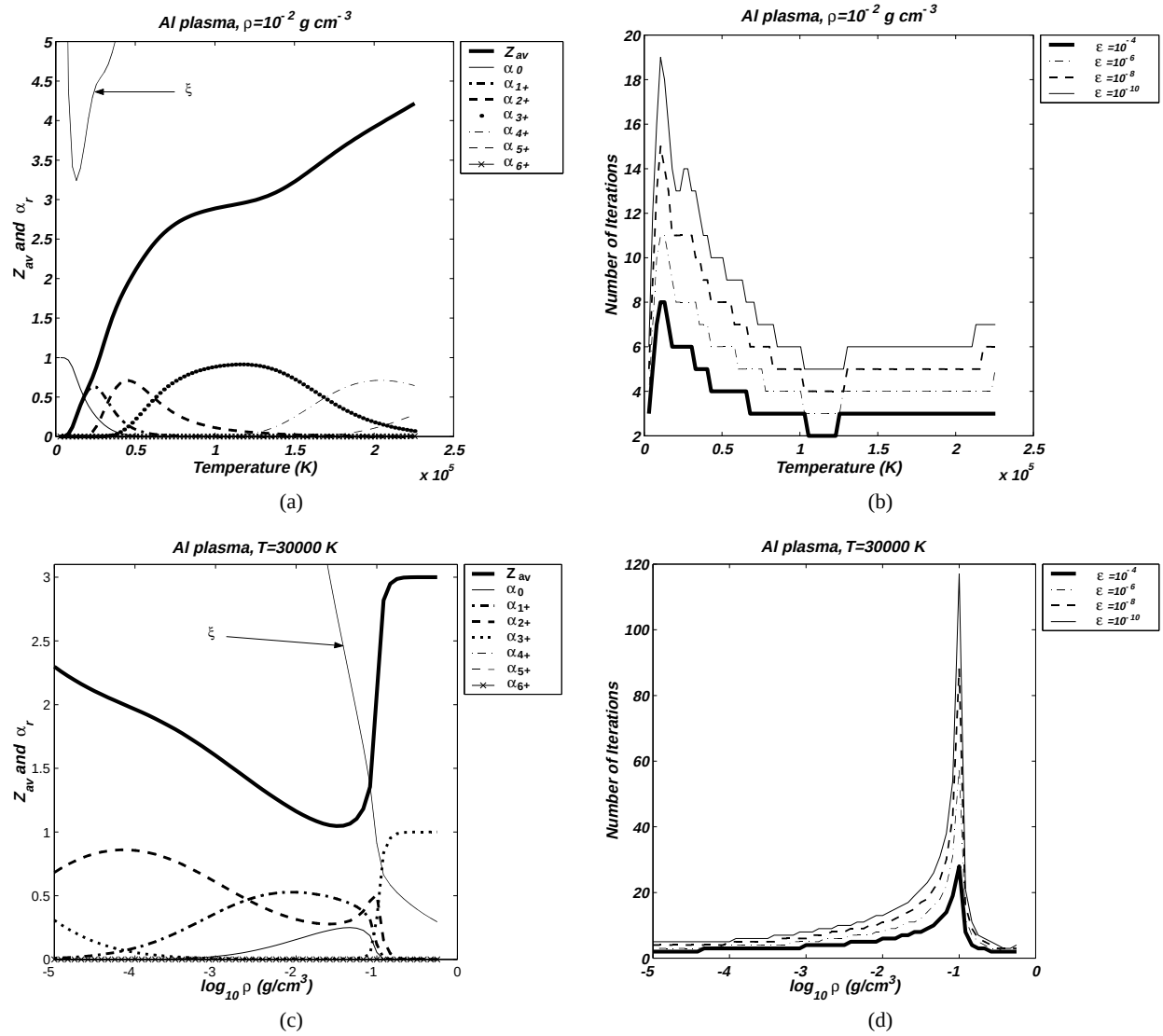


Figure 3. (a) Composition of Al plasma of mass density 0.01 g cm^{-3}. Nonideality corrections described by equation (17). (b) Number of iterations required for convergence for different values of the desired accuracy, related to the problem shown in figure 3(a). (c) Composition of Al plasma of $T = 30\,000$ K. Nonideality corrections described by equation (17). (d) Number of iterations required for convergence for different values of the desired accuracy, related to the problem shown in figure 3(c).

Table 1. Ionization potentials in eV and the statistical weights g_r of the ground states for argon [14].

g_0	E_0	g_0	E_1	g_0	E_2	g_0	E_3	g_0	E_4	g_0	E_5	g_0	E_6
1	15.755	6	27.62	9	40.90	4	59.79	9	75.0	6	91.3	1	124.0

Table 2. Ionization potentials in eV and the statistical weights g_r of the ground states for aluminium [14].

g_0	E_0	g_0	E_1	g_0	E_2	g_0	E_3	g_0	E_4	g_0	E_5	g_0	E_6
6	5.9844	1	18.823	2	28.44	1	119.96	6	153.77	9	190.42	4	241.93

4.3. Nonideal plasma with high density corrections expressible in terms of a common parameter

As examples for the case in which ΔI_r and ΔP cannot be expressed explicitly in terms of Z_{av} and n_H (or P_e and P) but can be expressed in terms of a common parameter such as λ_D, the plasma composition for Al plasma has been computed using the algorithm given above for two cases: i) for constant mass density, 10^{-2} g cm^{-3}, and a wide range of temperatures; ii) for constant temperature, 30 000 K, and mass density range from 10^{-5} g cm^{-3} to near the critical density. Iterative solutions are obtained using the aforementioned algorithm and the determined composition is shown in figures 3(a) and 3(c). Superimposed on these plots is the function $\xi = n_e + \sum n_i/(8\pi\lambda_D^3)^{-1}$ which represents the physical validity criterion of the model used for the nonideality corrections.

Regions of $\xi \succeq 1$ are the regions over which the model is valid. Of particular interest in such an iterative method is the number of iterations required for convergence, i.e. the convergence rate. The convergence rate is important in assessing the computational effort necessary to obtain the solution to a desired accuracy. Figures 3(b) and 3(d) show the convergence rates—number of iterations required to reach the desired accuracy tolerance $\left|(\lambda_D^{new} - \lambda_D^{old})/\lambda_D^{old}\right| \preceq \epsilon$—for different values of ϵ for each of the cases in figures 3(a) and 3(c), respectively. The initial guess for Z_{av} was obtained by solving equation (9) using nonideality corrections of the form given by equation (18). Values of such a variable initial guess are the solution for the second case in sample problem in section 4.2 and are shown in figure 2(b).

5. Convergence rate, sensitivity to initial guess, and validity of the physical model

For situations similar to those represented by the sample problems in sections 4.1 and 4.2, where the solution reduces to solving a single transcendental equation, there is little concern regarding initial guess or convergence rate. Algorithms that use a combination of bisection, secant, and inverse quadratic interpolation methods [16, 17] may be recommended as efficient for finding the zeros of a function. Such algorithms usually require an interval over which the function changes sign (or an initial estimate (guess) of the x-coordinate of a zero of the function). It might be worthwhile to state here that the confining interval between a small positive number close to zero and the maximum allowed ionization state (or an arbitrary estimate from this interval) can serve for this purpose.

For situations similar to that described in the sample problem in section 4.3, where the solution embodies iteration over a transcendental equation and an algebraic expression, it is important to study the impact of choosing the initial guess on the convergence rate. The initial guess may be taken as an arbitrary value for Z_{av} from the confining interval, or may be improved by using a state-dependent value. One way to generate such a state-dependent guess has been introduced in the sample problem in section 4.3 which requires the solution of an additional transcendental equation. To study the impact of choosing the initial guess on the convergence rate, the composition of aluminium plasma has been computed for a wide range of T and ρ using the variable (state-dependent) initial guess obtained by the solution of equation (9) with nonideality corrections described by equation (18). Surface plots of the initial guess and the average ionization state, as calculated using nonideality corrections described by equation (17), are shown in figures 4(a) and 4(b), respectively. As indicated in the figures, the behaviour is similar except in the region of strong nonideality. A surface plot of the convergence rate (number of iterations to attain convergence) is presented in figure 5(a). The number of iterations required for convergence is small for most of the ρ–T phase space except the region of high density and low temperature (strong nonideality) where the iteration count increases sharply. To determine whether the reduction in convergence rate (increase of number of iterations) in this region of the ρ–T phase space is due to computational

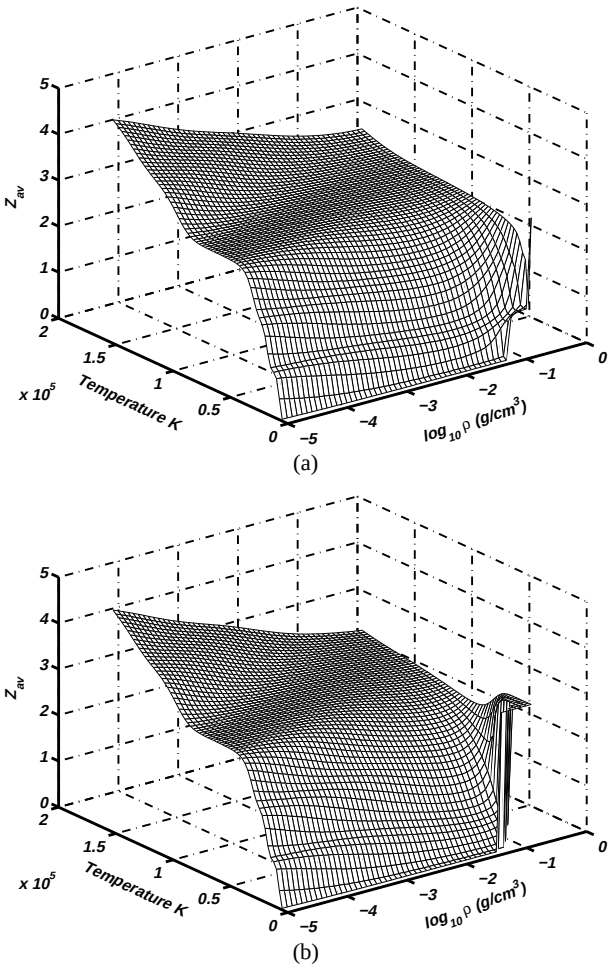
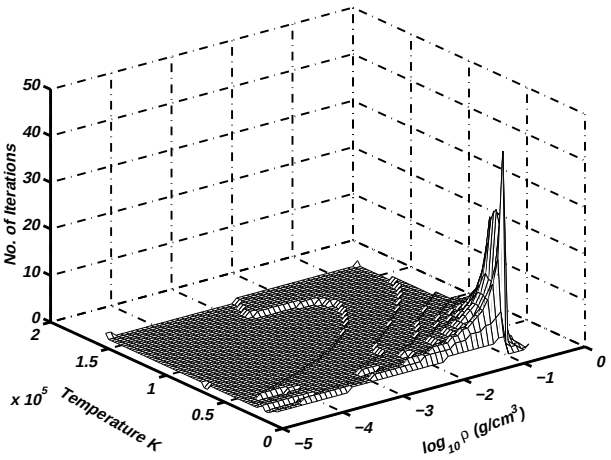
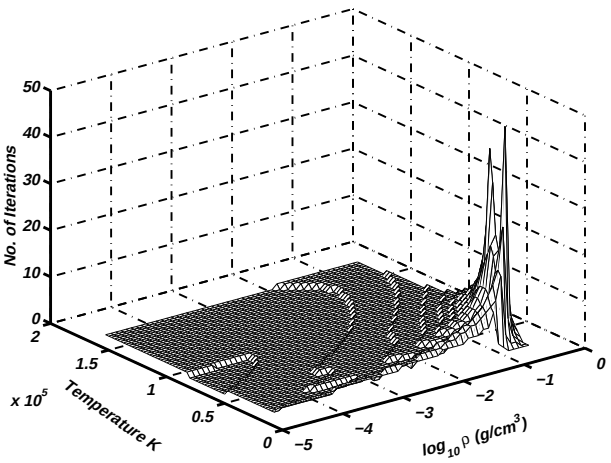


Figure 4. (a) A surface plot of the variable initial guess computed by the solution of equation (9) with nonideality corrections described by equation (18). (b) A surface plot of the average ionization state as calculated using Griem's model for the nonideality corrections.

reasons (initial guess sensitivity) or is a characteristic nature of the model used for nonideality corrections, an arbitrary constant (state-independent) initial guess ($Z_{av} = 0.5$) from the confining interval was used instead of the variable initial guess shown in figure 4(a). A surface plot of the number of iterations required for convergence has been constructed as shown in figure 5(b), where the behaviour and order of magnitude of the convergence rate is nearly the same as for the variable initial guess (figure 5(a)). This suggests that the proposed algorithm and computational scheme is insensitive to the initial guess. As a result, assuming a constant value for the initial guess may be more desirable, as it eliminates any computational work required to generate a state-dependent guess. Figure 6 shows a surface plot of the function ξ as well as the plane of $\xi = 1$. It is clear that the validity criterion $\xi \succeq 1$ is satisfied for regions of weak nonideality in the ρ–T phase space, but fails in the region of strong nonideality where the required number of iterations increases. Accordingly, the proposed algorithm and computational scheme is computationally efficient for all regions of phase space over which the physical model is valid.



(a)



(b)

Figure 5. Surface plots of the number of iterations required for convergence ($\epsilon = 10^{-4}$) using (a) the variable initial guess shown in figure 4(b), and (b) an arbitrary constant initial guess ($Z_{av} = 0.5$).

A physical model for high density corrections in which neither ΔI_r and ΔP can be expressed in terms of Z_{av} and n_H (or P_e and P) nor in terms of a common parameter is not available for the authors at the present time.

6. Discussion and conclusions

The most recent published technique for the solution of the Saha equation is that by Trayner and Glowacki [3], referred to here as TG. The method is nearly identical to that proposed by Rouse [4] and implicitly considers the ideal plasma case. In the TG formulation, the pressure appears explicitly in the Saha coefficients, while the ionization fractions are calculated with respect to n_H. This ambiguous formulation may suggest, at first glance, that both n_H and P are known. As has been seen, for an ideal plasma, an analytical solution is possible in such a case and no numerical techniques are required. Having P explicitly in the Saha coefficients suggests that the TG formulation is sufficient for the case of a known pressure. However, in such a case the calculation of particle densities—which is the goal of the solution of the Saha equation—necessitates the recovery of n_H from the

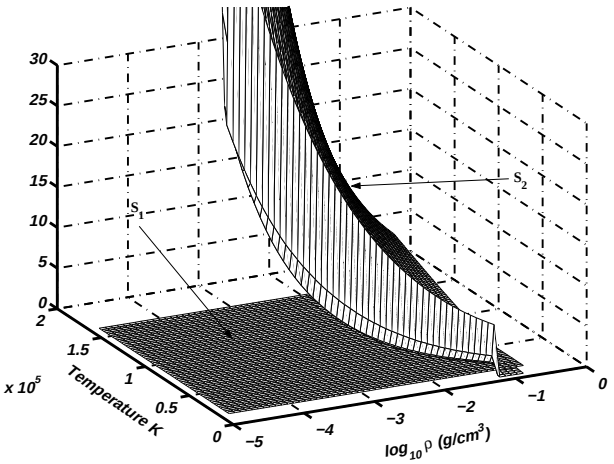


Figure 6. Validity criterion of the nonideality corrections described by equation (17): S_1, $\xi = 1$; S_2, $\xi(\rho, T)$. The model is valid for regions of $\xi \succeq 1$.

known pressure, which can be done through the calculated α_e or Z_{av} and restricted formulae for the equation-of-state. Needless to say this requires special attention be paid to the accuracy of the calculation of α_e or Z_{av}, which is not available in the TG method since the iteration process is proposed to be stopped according to the error (absolute, not relative) in α_i or lack of change [3]. The TG formulation and solution technique can be used in the case of known n_H only if P is expressed in terms of n_H and α_e. However the accuracy of the technique cannot be compared to that of the present formulation and method of solution. The TG technique experienced practical difficulties in getting the desired accuracy (which was in the order of 10^{-4}) for some cases [3]. These difficulties are not present in the method proposed here. For example, the sample problems in figures 1 and 2 have been solved to an accuracy of relative error tolerance equal to the floating-point relative accuracy (eps = 2.22×10^{-16}) in the MATLAB software package. The time frame for each was a few seconds, including the plotting of the calculated data and generating graphs using a SUN ULTRA10 workstation.

Compared to the formulation and methods of solution given by Drellishak *et al* [5] and Kannappan and Bose [6] the present formulation is as simple as theirs. However, it overcomes all of the restrictions imposed on their methods especially for the cases in which $n_H + n_e$ cannot be expressed explicitly as functions of the pressure. Clearly their work did not consider the case of known n_H (or mass density). In addition, these methods did not handle the case in which ΔI_r and ΔP are given by an expression such as that in equation (17), while the algorithm proposed here solves this problem efficiently with relative simplicity.

A simple algorithm has been also presented herein to solve the most general case in which ΔI_r and ΔP are not functions of a common variable.

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