Institute of Physics Publishing Journal of Physics: Conference Series **11** (2005) 124–130
doi:10.1088/1742-6596/11/1/012 Kinetic Theory of Nonideal Plasmas

Relaxation of reacting two-temperature plasmas

G K Grubert[1], M Schlanges[1], Th Bornath[2], and D O Gericke[1]

[1] Institut für Physik, E.-M.-Arndt-Universität, 17487 Greifswald, Germany
[2] Institut für Physik, Universität Rostock, 18051 Rostock, Germany

E-mail: `grubert@physik.uni-greifswald.de`

E-mail: `gericke@physik.uni-greifswald.de`

Abstract. We investigate the equilibration of nonideal plasmas from initial states where each species has already established a Maxwellian distribution, but the species temperatures and the chemical composition are not in equilibrium. On the basis of quantum kinetic equations, we derive hydrodynamic balance equations for the species densities and temperatures. The coupled density-temperature relaxation is then given in terms of the energy transfer between the subsystems and the population kinetics. We use the Landau-Spitzer approach for the energy transfer rates and a system of rate equations to describe the nonequilibrium plasma composition. Nonideality corrections are included in the rate coefficients and as potential energy contributions in the temperature equations on the simplest level of a Debye shift.

1. Introduction

To investigate the properties of dense plasmas experimentally, it is necessary to deposit a large amount of energy by means of lasers, ion beams, shock waves, or z-pinches into small targets. These techniques produce systems in extreme nonequilibrium states. Therefore, the relaxation towards the equilibrium can be of high importance for the interpretation of these experiments.

The equilibration of the different physical quantities occurs often on separated time scales: after a few femtoseconds, i.e. within the plasma creation, the electrons establish an equilibrium momentum distribution function. For the heavier atoms and ions, this process takes about one or two orders of magnitude longer. Due to the effective energy transfer between same mass particles, we can however assume that all heavy species have the same temperature after this time. Often the plasma is also created with a nonequilibrium charge states distribution which typically equilibrates on a picosecond time scale. A consistent description of the relaxation process requires then a solution of the coupled equations for the temperature equilibration and the population kinetics.

The density population [1–4] and the energy transfer rates [5–9] have been mostly studied separately. Based on a kinetic equation for reacting plasmas [10], Ohde *et al.* considered the coupled relaxation for a hydrogen plasma including first-order nonideality corrections [11]. In this contribution, we will follow this way and extend it to other elements. Since we often find a separation of time scales for the population kinetics and the temperature equilibration, we finally derive a scheme which considers the density population on a quasi-stationary level.

2. Kinetic and balance equations

The basis of our investigations are the kinetic equations for nonideal, partially ionized plasmas which were derived by Klimontovich and Kremp [10]. For the distributions of free carriers f_a, we have [12]

$$\left(\frac{\partial}{\partial t} + \nabla_{\mathbf{p}} E_a(\mathbf{p},\mathbf{R}t)\nabla_{\mathbf{R}} - \nabla_{\mathbf{R}} E_a(\mathbf{p},\mathbf{R}t)\nabla_{\mathbf{p}}\right) f_a(\mathbf{p},\mathbf{R}t) = \sum_b I_{ab}(\mathbf{p},\mathbf{R}t) + \sum_{bc} I_{abc}(\mathbf{p},\mathbf{R}t)\,. \tag{1}$$

The l.h.s. of this equation is the well-known drift term where we have incorporated quasi-particle energies E_a. The collision integrals on the r.h.s. describe all possible two- and three-particle collisions. The description of partially ionized plasmas is completed by a similar equation for the distribution of bound complexes [10].

From Eq. (1), we can derive hydrodynamic balance equations for the species densities and temperatures. Since elastic two-particle collisions do not change the plasma composition, the density of free carriers in homogeneous systems is determined by

$$\frac{\partial}{\partial t} n_a = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \sum_{bc} I_{abc}(\mathbf{p},t)\,. \tag{2}$$

The bound states density is then easily computed from the conservation of the total particle number. In a similar way, the temperature evolution can be obtained from Eq. (1) with a moment $p^2/2m_a$

$$\begin{aligned} \frac{\partial}{\partial t}\left\langle E_a^{\rm kin}\right\rangle &= \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \frac{p^2}{2m_a} \left\{\sum_b I_{ab}(\mathbf{p},t) + \sum_{bc} I_{abc}(\mathbf{p},t)\right\} \\ &= \sum_b Z_{ab} + \sum_{bc} Z_{a(bc)}^{\rm elastic} + \sum_{bc} Z_{a(bc)}^{\rm inelastic}\,. \end{aligned} \tag{3}$$

Here, the quantities Z_{ab} denote the energy transfer rate between the electron and ion subsystems due to binary collisions. The three-particle term was split in an elastic and an inelastic part. It turned out that the energy transfer rate due to elastic three-particle collisions is only important for weakly ionized plasmas. Therefore, it is omitted in the following calculations. The inelastic part contains the influence of ionization and recombination processes on the temperature of species 'a'.

3. Energy transfer rates

The energy transfer between the subsystems is one major input quantity for the coupled density-temperature relaxation. The binary collision contribution Z_{ab} is equivalent to the one calculated from the quantum Boltzmann equation[1]. For the energy transfer rates between nondegenerate electrons and an ion species, we obtain [8]

$$\begin{aligned} Z_{eb}^T &= -\sqrt{2\pi}\,\frac{8}{\pi}\, n_e n_b k_B\, \frac{\mu_{eb}}{m_e+m_b} \sqrt{\frac{m_e k_B T_b + m_b k_B T_e}{m_e m_b}} \\ &\times \frac{(T_e - T_b)}{(2m_e k_B T_e)^3} \int_0^\infty \mathrm{dp}\ \mathrm{p}^5\ \mathrm{Q}_{\rm eb}^{\rm T}(\mathrm{p})\ \exp\left(-\frac{\mathrm{p}^2}{2\mathrm{m_e k_B T_e}}\right)\,. \end{aligned} \tag{4}$$

[1] Since the scattering probability is given here by the T-matrix, this approach is further refered to as T-matrix approach.

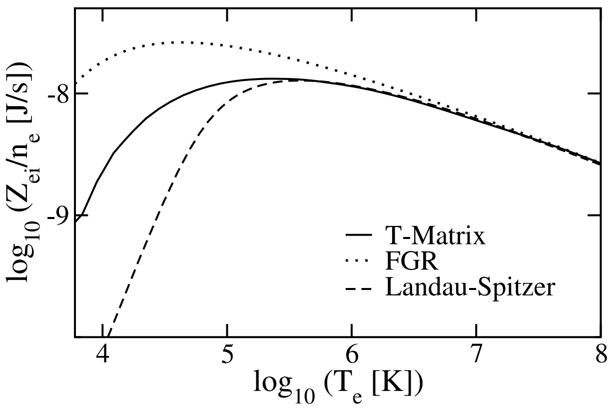

Figure 1. Comparison of the energy transfer rates in different approximation schemes. The system is an aluminum plasma with an ionization degree of three, an electron density of $n_e = 3 \times 10^{20}\,\mathrm{cm}^{-3}$, and an ion temperature of $T_i = 10^3\,\mathrm{K}$.

Here, the latin index 'b' denotes the ion species. The main input quantity is the transport cross section Q^T. It is calculated by a phase shift analysis that uses numerical solutions of a Schrödinger equation with a screened potential.

The calculation of the energy transfer rates using the T-matrix approach is numerically very extensive. Therefore, we also review the easy Landau-Spitzer (LS) result for the energy transfer due to classical binary collisions [5, 6]

$$Z_{eb}^{LS} = \frac{3}{2} n_e k_B \, \frac{T_b - T_e}{\tau_{eb}} \quad \text{with} \quad \tau_{\mathrm{eb}} = \frac{3 \mathrm{m_e m_b}}{8\sqrt{2\pi}\mathrm{n_b Z_b^2 e^4} \ln \Lambda} \left(\frac{\mathrm{k_B T_e}}{\mathrm{m_e}} + \frac{\mathrm{k_B T_b}}{\mathrm{m_b}} \right)^{3/2} . \tag{5}$$

Here, $\ln \Lambda$ denotes the Coulomb logarithm. To allow for strong electron-ion collisions, we use the form [9]

$$\ln \Lambda = \frac{1}{2} \ln \left(1 + \frac{r_0^2}{\varrho_\perp^2 + \lambda_{dB}^2} \right) , \tag{6}$$

where the upper cut-off parameter is given by the electron Debye length r_0. For the lower cut-off, we use a quadratic interpolation between the distance of closest approach $\varrho_\perp$ and the deBroglie wave length λ_{dB} [9].

The main short-coming of the approaches above for the energy transfer rates is the application of static screening. Therefore, collective excitations like plasma oscillations cannot be described. The easiest approach that considers such collective excitations is the Fermi-Golden-Rule (FGR) approach [7]. With response functions in random phase approximation, one obtains for a nondegenerate plasma [13]

$$\begin{aligned} Z_{eb}^{FGR} &= (T_e - T_b) \, \frac{8\sqrt{2\pi} n_e n_b Z_b^2 e^4}{2 m_e m_b} \left(\frac{m_e}{k_B T_e} \right)^{3/2} \\ &\quad \times \int_0^\infty \mathrm{dk} \, \frac{\mathrm{k}^3}{\left(\mathrm{k}^2 + \mathrm{r}_0^{-2}\right)^2} \, \exp\left(-\frac{1}{8} \mathrm{k}^2 \lambda_{\mathrm{dB}}^2 \right) . \end{aligned} \tag{7}$$

In Fig. 1, the energy transfer rates according to the approaches above are shown for an aluminum plasmas. For low electron temperatures, we find large differences. The FGR result is larger than the T-matrix data since the FGR corresponds to a Born approximation and, therefore, cannot describe strong electron-ion scattering. The LS approach on the other hand underestimates the energy transfer due to the classical treatment of the collisions. Nevertheless, all approaches agree for a wide range of high temperatures or weakly to moderately coupled systems. We, therefore, will use the easy LS formula in our further calculations.

4. Ionization kinetics & plasma composition

To describe the equilibration of the charge distribution, we use the following system of rate equations

$$\begin{aligned}\frac{\partial}{\partial t}n_0 &= n_e^2 n_1 \beta_0 - n_e n_0 \alpha_0 \\ \frac{\partial}{\partial t}n_1 &= n_e^2 n_2 \beta_1 - n_e n_1 \alpha_1 - n_e^2 n_1 \beta_0 + n_e n_0 \alpha_0 \\ &\vdots \\ \frac{\partial}{\partial t}n_{Z-1} &= n_e^2 n_Z \beta_{Z-1} - n_e n_{Z-1} \alpha_{Z-1} \\ &\quad - n_e^2 n_{Z-1} \beta_{Z-2} + n_e n_{Z-2} \alpha_{Z-2}\,. \end{aligned} \tag{8}$$

The quasi-neutrality results in a relation for the electron density

$$\frac{\partial}{\partial t}n_e = -\sum_{i=1}^{Z} W^{i\to i-1} \quad \text{with} \quad \mathrm{W^{i\to i-1}} = \sum_{\mathrm{k=0}}^{\mathrm{i-1}} \frac{\partial}{\partial \mathrm{t}} \mathrm{n_k}\,. \tag{9}$$

The rate coefficients α_i and β_i have to be determined from the quantum kinetic equation (1). We use the rate coefficients in the form [1]

$$\alpha_i = \alpha_i^{\mathrm{id}} \exp\left(-\beta[\Delta_{i+1} - \Delta_i + \Delta_e]\right) \qquad \text{and} \qquad \beta_{\mathrm{i}} = \beta_{\mathrm{i}}^{\mathrm{id}}\,. \tag{10}$$

The ideal part of the rate coefficients are calculated using the fit formula of Seaton [14]. Nonideality effects are included by quasi-particle shifts which are used in Debye approximation with an electron screening length, i.e.,

$$\Delta_a = -\frac{Z_a^2 e^2 \kappa}{2} \quad \text{and} \quad \kappa^2 = \frac{1}{\mathrm{r_0^2}} = \frac{4\pi \mathrm{n_e e^2}}{\mathrm{k_B T_e}}\,. \tag{11}$$

With this system of equations, the population kinetics towards equilibrium can be calculated. The thermodynamic equilibrium is described by a generalized Saha-equation

$$\frac{n_i}{n_{i+1}} = \frac{g_i}{g_{i+1}} \exp\left(\beta\left[\mu_e^{\mathrm{id}} + I_i^{\mathrm{eff}}\right]\right)\,. \tag{12}$$

Here, g_i are the statistical weights and $I_i^{\mathrm{eff}} = |E_i| + \Delta_{i+1} - \Delta_i + \Delta_e$ is the effective ionization energy of the bound state with a charge Z_i.

In Fig. 2, the evolution of the ionization degree is shown for a beryllium plasma. On a short time scale, one can observe a rapid decrease of the ionization degree: Be^{4+} recombines to Be^{3+}. Then lower charge states occur until the equilibrium composition is reached in about one picosecond. For comparison, the ionization degree that follows from ideal rate coefficients is shown. One clearly observes a lower ionization and a slightly longer relaxation in this case. The reason is that the nonideality reduces the effective ionization energy and bound states can therefore be ionized more easily.

5. Temperature relaxation in reacting plasmas

We start from the hydrodynamic balance equations (2) and (3) to derive explicit equations for the species temperatures. The evaluation of the collision integrals is done in a similar way as shown in Ref. [11]. Due to the known inefficiency, we also neglect ionization by ion collisions and ion assisted recombination.

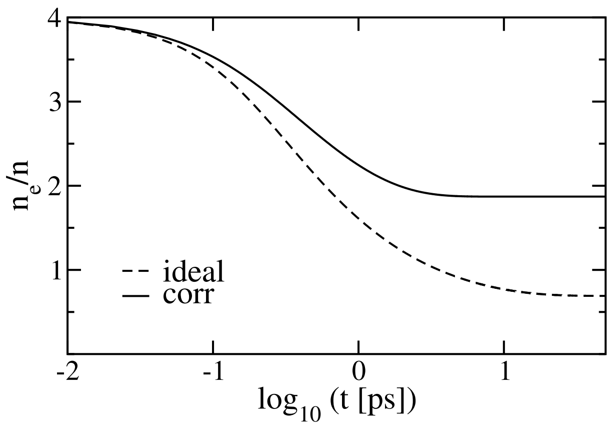

Figure 2. Evolution of the ionization degree for an initially fully ionized beryllium plasma with a density of the heavy particles of $n = 10^{22}\,\text{cm}^{-3}$. During the relaxation the temperature was kept constant at $T = 5\times10^4\,$K.

5.1. Ideal hydrogen plasmas

Let us first consider the most easy case of an ideal hydrogen plasma. As demonstrated by Ohde *et al.* [11], the reaction part on the r.h.s. of the temperature balance equation (3) can be expressed in terms of the rate coefficients α and β if the adiabatic approximation is used. Due to this approximation, the binding energy is fully contributed to the electron system and reactive processes do not directly influence the temperature of the heavy particles. If we assume that all heavy particles have the same temperature T_h, the system is described by

$$\begin{aligned} \frac{\partial}{\partial t} T_e &= \frac{2}{3 k_B n_e} \left\{ \left(\frac{3}{2} k_B T_e - E_1 \right) W^{1\to 0} + Z_{ei}(T_e, T_h) \right\} , \\ \frac{\partial}{\partial t} T_h &= \frac{2}{3 k_B n} \; Z_{ie}(T_e, T_h) \, , \\ W^{1\to 0} &= -\frac{\partial}{\partial t} n_e = n_e n_e n_1 \beta_0(T_e) - n_e n_0 \alpha_0(T_e) \, . \end{aligned} \tag{13}$$

The equilibration of an initially fully ionized hydrogen plasma described by these equations is shown in Fig. 3. Since the released binding energy flows completely into the electrons, the electron temperature rises in the first 30 femtoseconds where the relaxation is dominated by the density population. The temperature equilibration occurs then on a time scale of several picoseconds. During this time the ionization degree and the electron temperature are in equilibrium which results in the decreasing electron density with falling electron temperature.

Often (e.g. in Fig. 3) the composition changes only parametrically with electron temperature during the stage of temperature equilibration. This separation of time scales motivates a quasi-stationary ansatz for the plasma composition

$$\frac{\partial}{\partial t} n_a(t) = \frac{\partial}{\partial T_e} n_a(T_e) \; \frac{\partial}{\partial t} T_e(t) \, , \tag{14}$$

where $\partial n_a(T_e)/\partial T_e$ is calculated from the generalized Saha equation (12). Results from this approach are shown in Fig. 3, too. Of course, the quasi-stationary ansatz cannot describe the beginning of the relaxation correctly. However, we find a good agreement with the full approach (13) after the first recombination stage is completed. Furthermore, it gives the correct temperature evolution for the heavy particles.

5.2. Nonideal plasmas

In this section, we investigate the coupled density-temperature relaxation in nonideal plasmas. It is well known that kinetic equations for quasi-particles cannot describe the correlation

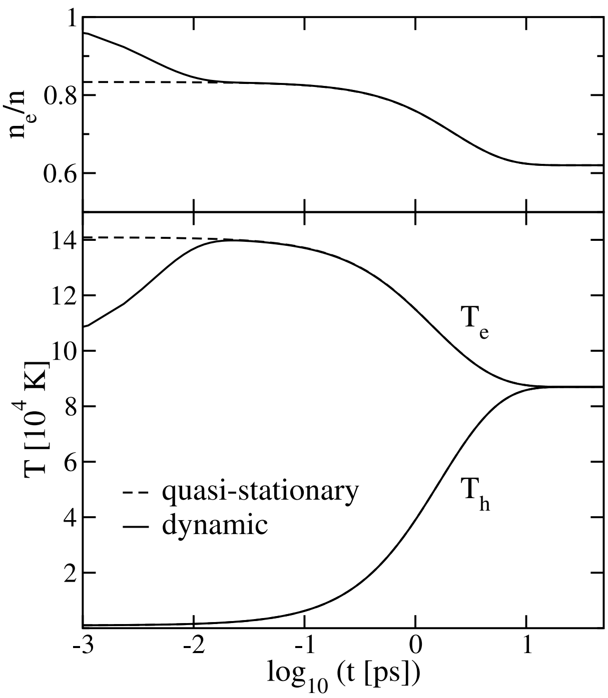

Figure 3. Relaxation of an initially fully ionized ideal hydrogen plasma with $n_e(0) = 10^{22}\,\mathrm{cm}^{-3}$, $T_e(0) = 10^5\,\mathrm{K}$, and $T_h(0) = 10^3\,\mathrm{K}$: the system is described with the full dynamic composition (13) and the quasi-stationary approach (14).

contributions to the total energy correctly [15]. Accordingly, the temperature equations, that result from the kinetic equation (1), lead to a violation of the energy conservation (only a half of the correlation energy is considered [11]). This problem might be avoided by the extended quasi-particle approximation [15], but no three-particle collision integral exists in that approximation yet. For this reason, we will use here a phenomenological ansatz to describe the relaxation in nonideal systems.

We start from the total energy of weakly coupled, nondegenerate plasmas [16]

$$\varepsilon = \sum_a \left(\frac{3}{2} n_a k_B T_a + n_a \Delta_a \right) + \sum_{i=0}^{Z-1} n_i E_i^{\mathrm{bound}} \,, \tag{15}$$

where E_i^{bound} denotes the binding energy per ion for a charged state of 'i' and Z is the charge of the ionic core. This approach allows also for a description of heavier elements than hydrogen. We now divide the total energy into an electron and an ion/atom part

$$\varepsilon_e = \frac{3}{2} n_e k_B T_e + n_e \Delta_e + \sum_{i=0}^{Z-1} n_i E_i^{\mathrm{bound}} \quad \text{and} \quad \varepsilon_\mathrm{h} = \frac{3}{2} \mathrm{n k_B T_h} + \sum_{\mathrm{i=1}}^{\mathrm{Z}} \mathrm{n_i \Delta_i} \,, \tag{16}$$

where we have assumed that all heavy particles have established a common temperature T_h. As for ideal plasmas, the binding energy is assigned to the electron part. The energy transfer between these subsystems defines then the change of total energy in the electron and ion subsystems. Using the self-energy shifts in Debye approximation (11), explicit equations for the species temperatures can be found

$$\begin{aligned} \frac{\partial}{\partial t} T_e &= \left[\frac{3}{2} n_e k_B - \frac{\Delta_e}{2} \frac{n_e}{T_e} \right]^{-1} \left\{ \sum_{i=1}^{Z} \left(\frac{3}{2} k_B T_e - E_i + \frac{3}{2} \Delta_e \right) W^{i \to i-1} + Z_{ei} \right\} , \\ \frac{\partial}{\partial t} T_h &= \frac{-2}{3 n k_B} \left\{ \frac{\Delta_e}{2} \sum_{i=1}^{Z} i^2 n_i \left(\frac{1}{n_e} \frac{\partial}{\partial t} n_e - \frac{1}{T_e} \frac{\partial}{\partial t} T_e + \frac{2}{n_i} \frac{\partial}{\partial t} n_i \right) + Z_{ei} \right\} . \end{aligned} \tag{17}$$

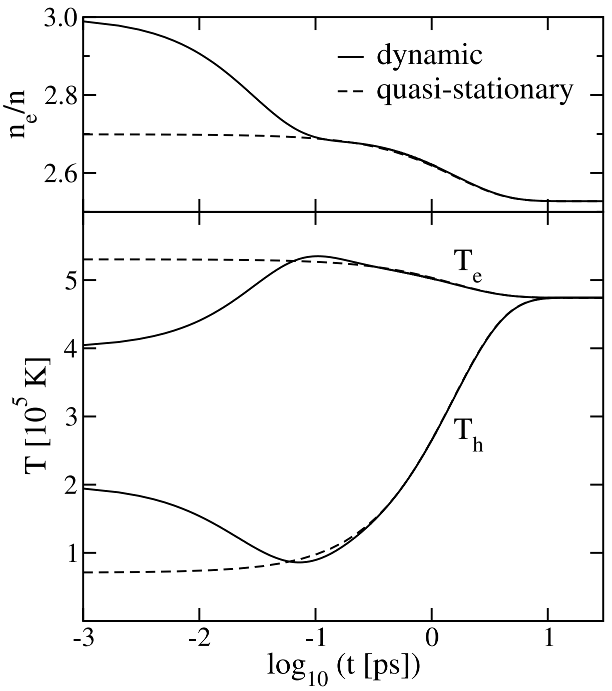

Figure 4. Coupled density-temperature relaxation in a nonideal beryllium plasma with a total ion density of $n = 5 \times 10^{22}\,\mathrm{cm}^{-3}$. The initial temperatures are $T_e(0) = 4 \times 10^5\,\mathrm{K}$ and $T_h(0) = 2 \times 10^5\,\mathrm{K}$.

In addition, the rate equations have to be solved selfconsistently. The full system consists therefore of $Z+2$ differential equations. As in the case of ideal plasmas, the time scales of the density population and the temperature equilibration are often very different. Therefore, the quasi-stationary approach (14) seems to be appropriate for nonideal plasmas, too.

In Fig. 4, the coupled relaxation of the densities and the temperatures in a nonideal beryllium plasma is shown using the full dynamic and quasi-stationary approach. One can clearly observe the separation of the relaxation phases in this case, too. The consideration of nonideality corrections leads here to a decrease of the ion temperature and a weaker increase of the electron temperature in the recombination phase. After this stage both the dynamic and the quasi-stationary approach principally coincide.

References

[1] Schlanges M, Bornath Th, and Kremp D 1988 *Phys. Rev.* A **38** 2174
[2] Ebeling W and Leike I 1991 *Physica A* **170** 285
[3] Bornath Th, Schlanges M, and Prenzel R 1998 *Phys. Plasmas* **5** 1485
[4] Murillo M S and Weisheit J C 1998 *Phys. Rep.* **302**
[5] Landau L D 1936 *Phys. Z. Sowjetunion* **10** 154
[6] Spitzer L 1956 *Physics of Fully Ionized Gases* (New York: Interscience)
[7] Dharma-wardana M W C and Perrot F 1998 *Phys. Rev.* E **58** 3705
[8] Zhdanov V M 2002 *Transport Processes in Mulitcomponent Plasma* (London, New York: Taylor & Francis)
[9] Gericke D O, Murillo M S, and Schlanges M 2002 *Phys. Rev.* E **65** 36418
[10] Klimontovich Yu L and Kremp D 1981 *Physica A* **109** 517
[11] Ohde Th, Bonitz M, Bornath Th, Kremp D, and Schlanges M 1996 *Phys. Plasmas* **3** 1241
[12] Klimontovich Yu L, Schlanges M, and Bornath Th 1990 *Contrib. Plasma Phys.* **30** 349
[13] Gericke D O *these proceedings*
[14] Seaton M J 1964 *Planet. Space Sci.* **12** 55
[15] Bornath Th, Kremp D, Kraeft W-D, and Schlanges M 1996 *Phys. Rev.* E **54** 3274
[16] Kraeft W-D, Kremp D, Ebeling W, and Röpke G 1986 *Quantum Statistics of Charged Particle Systems* (Berlin: Akademie-Verlag)