Relaxation of temperature and chemical composition in nonideal plasmas

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Rate equations for the coupled evolution of density and temperature in nonideal partially ionized plasmas are presented. The equations are derived from generalized quantum kinetic equations that include many-particle effects, such as screening, self-energy and lowering of the binding energy. The equations are solved for a three-component plasma. The influence of many-body effects on the density–temperature relaxation is demonstrated. © *1995 American Institute of Physics.*

I. INTRODUCTION

In a recent paper,[1] reaction and diffusion processes in partially ionized dense plasmas have been considered. In particular, the influence of many-body effects, such as screening, self-energy, and lowering of the ionization energy on these processes has been studied. This required a quantum statistical foundation of reaction–diffusion equations (RDE) as well as of the coefficients of impact ionization and diffusion. The RDE and expressions for these coefficients have been derived from generalized quantum kinetic equations. It was shown, that the many-body effects lead to a strong density dependence of the rate and diffusion coefficients. The result in the plasma kinetics are nonlinear phenomena, such as nonlinear diffusion, running ionization fronts, droplet growth, and bistability.

One essential limitation of Ref. 1 was that only density relaxation processes at homogeneous constant temperature were considered. This is valid in cases where the temperature relaxation proceeds much faster (e.g., if we consider relaxation of densities and temperatures in connection with an electrical field[2]), or, if the plasma is embedded in a thermostat. However, in many cases temperature and density relax on similar time scales. This situation will be studied in the following.

In this paper we aim to compare the relaxation properties of nonideal and ideal plasmas. In particular, we study the relaxation of plasma composition and temperature. To make the nonideality effects transparent, we, as a first step, focus on the spatially homogeneous case. In Sec. II we derive hydrodynamic equations from generalized kinetic equations for quasiparticles. Of special interest is how nonideality effects manifest themselves in the rate equations. In Sec. III we give numerical results for the solution of the coupled equation of density and temperature.

II. HYDRODYNAMIC EQUATIONS FOR NONIDEAL PLASMAS

To obtain hydrodynamic equations for nonideal partially ionized plasmas, we start from generalized quantum kinetic equations (see Refs. 3 and 4) for the Wigner distribution function f_a of the free particles of species (a)

$$\left(\frac{\partial}{\partial t}+\frac{\partial\epsilon_a}{\partial p}\frac{\partial}{\partial r}-\frac{\partial\epsilon_a}{\partial r}\frac{\partial}{\partial p}\right)f_a(p,r,t)$$

$$=\sum_b I_{ab}(p,r,t)+\sum_{bc} I_{abc}(p,r,t). \tag{1}$$

The right-hand side (RHS) of the kinetic equation (1) describes the collisions between quasiparticles. The integrals I_{ab} and I_{abc} contain all possible two- and three-body scattering processes, respectively. In particular, the integrals I_{abc} take into account the formation and decay of bound states by recombination and ionization reactions. Similar to Eq. (1) one can derive an equation for the bound particles. In contrast to Eq. (1), it contains on the RHS collision integrals of the form $I_{(ab)c}$, describing the scattering of bound states on free particles and bound states, respectively. This equation can be found in Refs. 4 and 5. Explicit expressions for the collision integrals are given in the Appendix.

Many-body effects enter the kinetic expression (1) via the quasiparticle energy ϵ_a

$$\epsilon_a(prt)=\frac{p^2}{2m_a}+\mathrm{Re}\,\Sigma_a^R(p\omega rt)|_{\hbar\omega=\epsilon_a(prt)}. \tag{2}$$

In the second term of Eq. (2), $\Sigma_a^R(p\omega rt)$ is the retarded self-energy function. This function describes the modification of the energy of a particle due to the influence of the surrounding plasma; Σ_a^R itself depends on the distribution function (for a discussion see Ref. 1). Therefore, in principle, it has to be determined self-consistently with the solution of the kinetic equations.

The hydrodynamic equations, we are interested in here, are the density and energy balance equations for the different components. They can be derived in the usual manner by multiplying the kinetic equations for the free particles (1) and bound particles[4,5] with 1 and the quasiparticle energies, respectively, and subsequent integration with respect to the momentum. The number density of species (b) is given by

$$n_b=\int\frac{d^3p}{(2\pi\hbar)^3}f_b. \tag{3}$$

We keep in mind, further, that the variation of the total energy density of a quasiparticle system due to an infinitesimally small change of the distribution functions is given by[6]

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$$\frac{\delta E}{V}=\sum_a \int \frac{d^3p}{(2\pi\hbar)^3}\,\epsilon_a(p)\,\delta f_a=\sum_a \frac{\delta E_a}{V}. \tag{4}$$

As a result, the system of hydrodynamic equations for a homogeneous plasma, consisting of free particles (a) and bound particles (AB), reduces to the following equations:

$$\frac{\partial n_a}{\partial t}=W_a, \tag{5}$$

$$\frac{\partial n_{(AB)}}{\partial t}=\sum_j W^j_{(AB)}, \tag{6}$$

$$\frac{\partial}{\partial t}\left(\frac{E_a}{V}\right)=\int \frac{d^3p}{(2\pi\hbar)^3}\,\epsilon_a(prt)\left(\sum_b I_{ab}+\sum_{bc} I_{abc}\right), \tag{7}$$

$$\frac{\partial}{\partial t}\left(\frac{E_{(AB)}}{V}\right)=\sum_j \int \frac{d^3p}{(2\pi\hbar)^3}\left(\frac{p^2}{2m_{(AB)}}+E_j\right)\sum_c I_{(AB)c}. \tag{8}$$

The total number density of atoms is $n_{(AB)}=\Sigma_j n^j_{(AB)}$. The term W_a is the source function of the free particles and describes the change of the density n_a due to the ionization and recombination processes; $W^j_{(AB)}$ is the source function of the bound particles.[7] The source functions follow from the RHS of the kinetic equations. They are defined by the three-particle collision integrals only, since the two-particle integrals conserve density.

Let us now make the choice of the plasma more specific. We will consider in the following a system consisting of electrons (e), singly charged ions (i), and atoms (AB). Then we obtain for the electrons

$$W_e=\sum_{c=e,i}\sum_j (\alpha^c_j n_c n_j-\beta^c_j n_c n_e n_i). \tag{9}$$

Here the summation is over the impact particles and the quantum numbers of the atom; α^c_j and β^c_j are, respectively, the coefficients of impact ionization and three-body recombination of the atomic level j. Explicit expressions for these rate coefficients are given in the Appendix. The source functions for the components are related by $W_e=W_i=-\Sigma_j W^j_{(AB)}$.

If we sum up Eqs. (5), (6) and (7), (8), respectively, for the components, it can be shown, that the density $n=n_e+n_{(AB)}$ and the total energy $E=E_e+E_i+E_{(AB)}$ are conserved. Some details are discussed in the Appendix.

Let us consider the energy balance equations (7) and (8) more in detail. The energy density of the free particles is given in the framework of Green's functions by the exact relation[8]

$$\frac{E_a}{V}=\int \frac{d^3p}{(2\pi\hbar)^3}\frac{d\omega}{2\pi}\frac{(p^2/2m_a)+\hbar\omega}{2}(\pm i)g^<_a(p\omega t). \tag{10}$$

With the one-particle correlation function $g^<_a$ in quasiparticle approximation

$$(\pm i)g^<_a(p\omega t)=2\pi\hbar\,\delta[\hbar\omega-\epsilon_a(pt)]f_a(pt), \tag{11}$$

we get

$$\frac{E_a}{V}=\int \frac{d^3p}{(2\pi\hbar)^3}\frac{p^2}{2m_a}f_a(pt)+\frac{1}{2}\int \frac{d^3p}{(2\pi\hbar)^3}\,\mathrm{Re}\,\Sigma^R_a(p,\omega=\epsilon_a,t)f_a(pt). \tag{12}$$

For a nondegenerate system, which shall be considered in the following, the temperature can be defined by

$$\frac{3}{2}n_b k_B T_b=\int \frac{d^3p}{(2\pi\hbar)^3}\frac{p^2}{2m_b}f_b. \tag{13}$$

Explicit expressions for the interaction part in Eq. (12) can be obtained in local thermodynamic equilibrium. Using $Re\Sigma^R_a$ in the so-called V^s approximation, we get in lowest order[9,10]

$$\int \frac{d^3p}{(2\pi\hbar)^3}\,\mathrm{Re}\,\Sigma^R_a(p,\omega=\epsilon_a,t)f_a(p,t)=-\frac{e^2n_a}{2r_0}. \tag{14}$$

The screening length r_0 is

$$\frac{1}{r_0^2}=4\pi\sum_b \frac{n_b z_b^2 e^2}{k_B T_b}, \tag{15}$$

with z_b being the charge number of species b. The energy shift of bound states is assumed to be negligibly small.[1] Then the system of hydrodynamic equations reads

$$\frac{\partial n_a}{\partial t}=W_a, \tag{16}$$

$$\frac{\partial n_{(AB)}}{\partial t}=\sum_j W^j_{(AB)}, \tag{17}$$

$$\frac{\partial}{\partial t}\left(\frac{3}{2}n_a k_B T_a-\frac{e^2n_a}{4r_0}\right)=\int \frac{d^3p}{(2\pi\hbar)^3}\,\epsilon_a(prt)\left(\sum_b I_{ab}+\sum_{bc} I_{abc}\right), \tag{18}$$

$$\frac{\partial}{\partial t}\left(\frac{3}{2}n_{(AB)}k_B T_{(AB)}+\sum_j E_j n^j_{(AB)}\right)=\sum_j \int \frac{d^3p}{(2\pi\hbar)^3}\left(\frac{p^2}{2m_{(AB)}}+E_j\right)\sum_c I_{(AB)c}. \tag{19}$$

With Eqs. (16)–(19) we can describe the relaxation of the densities and temperatures of the plasma species. This relaxation is driven by the chemical reactions only. In many cases, one anticipates a multistage process, where first a common nonequilibrium temperature T of the whole plasma is established. We will consider here the second stage, i.e., the coupled relaxation of this temperature and of the chemical composition of the plasma. The plasma temperature T is given by

$$\frac{3}{2}n_\sigma k_B T=\sum_b \int \frac{d^3p}{(2\pi\hbar)^3}\frac{p^2}{2m_b}f_b, \tag{20}$$

with $n_\sigma=\Sigma_b n_b$ and $b=e,i,A$. Summing up Eqs. (16)–(19) over the components, we obtain

$$\frac{\partial n_\sigma}{\partial t}=\frac{\partial n_e}{\partial t}=-\sum_j W^j_{(AB)}, \tag{21}$$

$$\frac{\partial T}{\partial t}=\sum_j \left(\frac{\frac{3}{2}k_BT+|E_j|-\frac{3}{4}(e^2/r_0)}{\frac{3}{2}n_\sigma k_B+\frac{1}{4}(e^2n_e/r_0T)} \right) W^j_{(AB)}. \tag{22}$$

Nonideality effects enter these equations via the atomic source function $W^j_{(AB)}$ and the screening length r_0. As we will see below, this leads to significant deviations of the relaxation in comparison to the ideal case. Equations (21) and (22) are quite general for three-component partially ionized plasmas. Specific microscopic properties of the plasma lead, of course, to different expressions for the source function and the screening length. The expressions for the rate coefficients are given in the Appendix (A14) and (A15). Their calculation requires the knowledge of the quasiparticle energies. This is a very complicated problem which has been solved so far only within certain approximations. As in Ref. 1, we can use here the so-called rigid shift approximation,[9] in which the quasiparticle energies are given by momentum-independent shifts

$$\epsilon_a(pt)=\frac{p^2}{2m_a}+\Delta_a(t), \tag{23}$$

with

$$\Delta_a(t)=\frac{\int d^3p \text{ Re } \Sigma^R_a(p,r,t)(\partial/\partial\mu^{id}_a)f_a(p,r,t)}{\int d^3p(\partial/\partial\mu^{id}_a)f_a(p,r,t)},$$
$$\approx\frac{1}{n_a}\int\frac{d^3p}{(2\pi\hbar)^3}\text{ Re }\Sigma^R_af_a. \tag{24}$$

Thus this shift is a thermally averaged quasiparticle shift. It is related to the chemical potential by

$$\mu_a=\mu^{id}_a+\Delta_a. \tag{25}$$

Similar to (14), we have

$$\Delta_a=-\frac{e^2}{2r_0}. \tag{26}$$

The shifts Δ_a describe the influence of the surrounding plasma on the single-particle properties.

On the other hand, nonideality effects influence two-particle properties also. The major effect here is the lowering of the ionization energy of bound states, such as atoms. The effective binding energy (effective ionization energy) of atoms in state $|j\rangle$ is given by

$$I^{\text{eff}}_j=|E_j|-\Delta_j+\Delta_e+\Delta_i. \tag{27}$$

Neglecting the small shift of the ground state energy ($\Delta_1\approx 0$), we obtain

$$I^{\text{eff}}_1=|E_1|-\frac{e^2}{r_0}. \tag{28}$$

From Eq. (28), the lowering of the ionization energy with increasing plasma density and/or decreasing temperature is obvious. At the so-called Mott line (see Figs. 2–4), the binding energy vanishes. That means, as a result of the Coulomb interaction between the plasma particles, bound states break up.

To study nonideality effects on the relaxation kinetics in a simple example, we consider in the following partially ionized hydrogen. Furthermore, we restrict ourselves to atoms in the ground state. Since the impact ionization by ions is much less effective compared to electron impact ionization, one usually can restrict to the latter process. The electron impact ionization coefficient was calculated with an approximate impact ionization cross section, which is given in Ref. 11. Then we obtain an analytic expression for the ionization coefficient

$$\alpha_1=\alpha^{id}_1\exp[(\Delta_1-\Delta_e-\Delta_p)/k_BT], \tag{29}$$

$$\alpha^{id}_1=\alpha_0 g\left(\frac{|E_1|}{k_BT}\right); \tag{30}$$

α_0 and g are defined by

$$\alpha_0=\frac{(10\pi a_B^2|E_1|^{1/2})}{(2\pi m_e)^{1/2}}, \tag{31}$$

$$g(x)=x^{1/2}\int_x^\infty\left(\frac{e^{-t}}{t}\right)dt. \tag{32}$$

The ionization coefficient has a strong dependence on the density, because the ionization is a process with a threshold energy [see Eq. (27)]. In the approximation of thermally averaged shifts, the ionization and the recombination coefficients are dependent due to the relation

$$\beta_j=\alpha_j\lambda_e^3\exp(I^{\text{eff}}_j/k_BT), \tag{33}$$

with λ_e being the thermal wavelength. The influence of many-body effects on the recombination coefficient is smaller in comparison to the ionization coefficient (cf. the results for nonideal hydrogen plasma[5,7] and for alkali plasma[12]). In the simple approximation used here, we obtain from Eq. (33) with Eq. (29) $\beta_1=\beta^{id}_1$, i.e., the three-body recombination coefficient is independent of the density.

III. NUMERICAL RESULTS

Let us now investigate the influence of nonideality effects on the kinetics of density and temperature in a dense hydrogen plasma. We start from the spatially homogeneous hydrodynamic equations (21) and (22), with the ionization and recombination coefficients (29) and (33) and the screening length (15). Furthermore, we assume local charge neutrality ($n_e=n_i$). We consider a closed system with constant total number of electrons $n=n_e+n_A=\text{const}$. For numerical purposes, it is convenient to use dimensionless variables for density, time, and temperature

$$c=\frac{n_e}{n},\quad \tau=\frac{t}{t_0},\quad \theta=\frac{k_BT}{|E_1|}, \tag{34}$$

c is the degree of ionization, n the total electron density, τ the dimensionless time, and θ the dimensionless temperature. The energy (temperature) unit is the Rydberg energy, time unit is $t_0=(\alpha_0 n)^{-1}$. In contrast to the characteristic time in

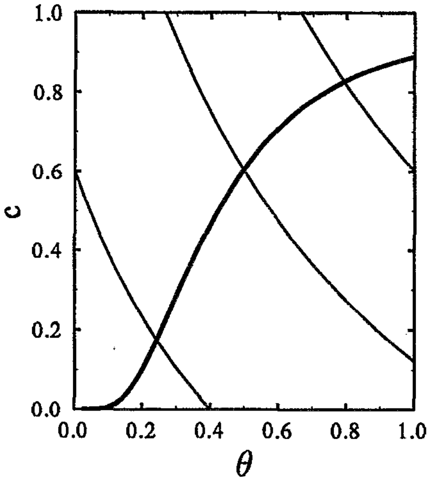

FIG. 1. Stationary solutions (thick line) of the ideal coupled density–temperature equations in the (θ-c) plane for a hydrogen plasma (c—degree of ionization, θ—dimensionless temperature). The thin lines are the solutions of Eq. (39) for different initial values. The total electron number density is $n=7.692\times10^{27}$ m^{-3}.

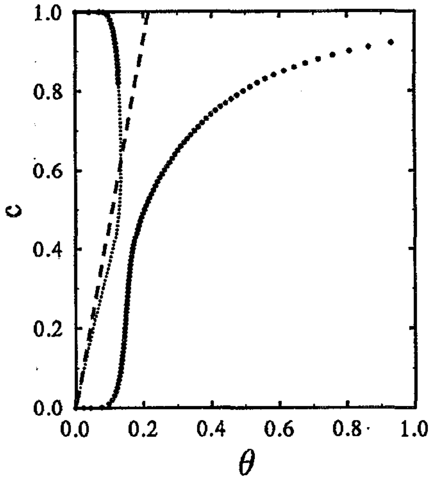

FIG. 2. Stable (filled circles) and unstable (small dots) stationary solutions of the nonideal coupled density–temperature equations in the (θ-c) plane for a hydrogen plasma. The dashed line is the Mott line. The total electron number density is $n=7.2\times10^{27}$ m^{-3}. n is less than the critical density $n_{\mathrm{cr}}=7.692\times10^{27}$ m^{-3}.

Ref. 1 we had to choose a slightly different definition for t_0, that is independent of the temperature [cf. definition of α_0 in Eq. (31)]. Now we can transform Eqs. (21) and (22) into dimensionless form

$$\frac{\partial c}{\partial \tau}=cg(\theta)f(c,\theta,n), \tag{35}$$

$$\frac{\partial \theta}{\partial \tau}=-\frac{(\frac{2}{3}+\theta-\frac{1}{2}\gamma(\theta,n)\theta\sqrt{c})}{[1+c(1+\frac{1}{6}\gamma(\theta,n)\theta\sqrt{c})]}cg(\theta)f(c,\theta,n). \tag{36}$$

The function $f(c,\theta,n)$ is

$$f(c,\theta,n)=(1-c)e^{\gamma(\theta,n)\sqrt{c}}-c^2\lambda(\theta,n), \tag{37}$$

where $\gamma(\theta,n)$ and $\lambda(\theta,n)$ are given by

$$\gamma(\theta,n)=\frac{2e^3}{\theta|E_1|}\left(\frac{2\pi n}{\theta|E_1|}\right)^{1/2}, \quad \lambda(\theta,n)=\Lambda_e^3 n e^{1/\theta}. \tag{38}$$

The corresponding expressions for an ideal hydrogen plasma follow from Eqs. (35) and (36), if we set $\gamma=0$.

Prior to the numerical solution, let us discuss some properties of the system (35) and (36). In our model, the source function of electrons is $W_e(c,\theta,n)=cf(c,\theta,n)$. This function appears in both Eqs. (35) and (36). The solutions of these coupled equations are essentially determined by the source function W_e. In particular, the stationary solutions (c_s,θ_s) are given by the zeros of the source function. First, we find the trivial zero $c_s=0$ (θ arbitrary), which is always unstable. Further zeros can be derived from the equation $f(c_s,\theta_s,n)=0$ which yields the Saha equation for a nonideal dense hydrogen plasma (see below).

In the case of an ideal plasma, the Saha equation has one solution, given by a line $\theta_s^{id}(c_s)$ in the density–temperature plane (thick line in Fig. 1). This line gives simultaneously the equilibrium plasma composition and temperature. It depends parametrically on the total electron number density n. Let us consider now the relaxation process of density and temperature, starting with initial (nonequilibrium) values $c(\tau=0)$, $\theta(\tau=0)$. Obviously, the relaxation process will end on the line $\theta_s^{id}(c_s)$. Before solving Eqs. (35) and (36), it is instructive to consider its properties in the ($\theta-c$) phase space. This allows one to calculate the phase trajectory $\theta(c)$ and to find the stationary solutions of Eqs. (35) and (36). Indeed, dividing the second equation by the first, one can eliminate time. In the ideal case, we obtain

$$\frac{\partial \theta}{\partial c}=-\frac{(\frac{2}{3}+\theta)}{(1+c)}. \tag{39}$$

The solution is easily found

$$\theta^{id}(c;\theta_0)=\frac{(\frac{2}{3}+\theta_0)}{(1+c)}-\frac{2}{3}. \tag{40}$$

It describes a family of noncrossing lines, that cover the whole plane; $\theta_0=\theta(c=0)$ is the crossing with the θ axis. These lines are monotonically decreasing, i.e., growth of the

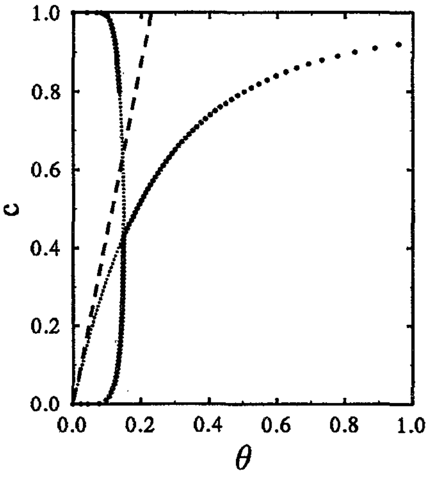

FIG. 3. Same as Fig. 2, with $n=7.692\times10^{27}$ m$^{-3}=n_{\mathrm{cr}}$.

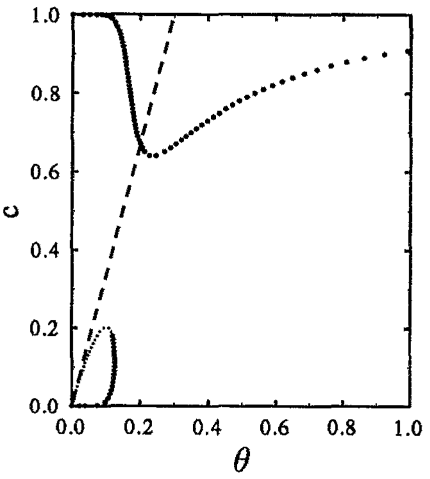

FIG. 4. Same as Fig. 2, with $n=1\times10^{28}\ \mathrm{m}^{-3}>n_{\mathrm{cr}}$.

degree of ionization is always associated with decreasing temperature and vice versa. These lines are also shown in Fig. 1. The choice of the initial values $\theta(\tau=0)$, $c(\tau=0)$ picks the corresponding line. The crossing of this line with $\theta_s^{id}(c_s)$ will be the final point of the relaxation. If the initial point lies below (above) the line $\theta_s^{id}(c_s)$, the relaxation leads to a decrease (increase) of temperature and to an increase (decrease) of the degree of ionization.

The situation is more complicated for strongly coupled plasmas. Due to nonideality effects, at low temperatures, the ideal line $\theta_s^{id}(c_s)$ splits into two lines. This property is closely related to the anticipated plasma phase transition in equilibrium.[13] In the n-T plane there exists a whole region where the source function has multiple zeros with a critical point $(n_{\mathrm{cr}},T_{\mathrm{cr}})$.[1] For our problem, there arise three different situations, depending on whether the total electron density is lower, equal or greater than n_{cr}. They are shown in Figs. 2–4. In these figures, also the Mott line, i.e., the line where $I^{\mathrm{eff}}=0$, is shown. Above this line, there are no bound states possible. In the same way as in the ideal case, we can eliminate the time from the rate equations and find the trajectory in $(\theta$-$c)$ phase space that is now defined by

$$\frac{\partial\theta}{\partial c}=-\frac{(\frac{2}{3}+\theta-\frac{1}{2}\gamma(\theta,n)\theta\sqrt{c})}{[1+c(1+\frac{1}{6}\gamma(\theta,n)\theta\sqrt{c})]}. \qquad (41)$$

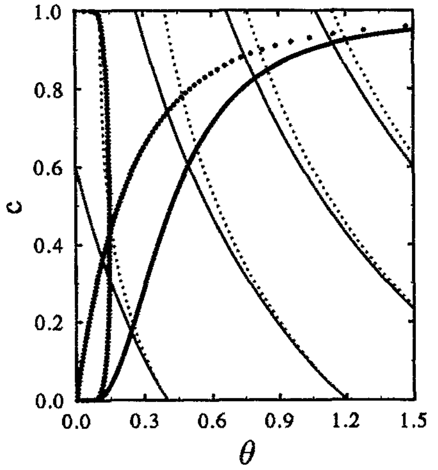

FIG. 5. Comparison of the ideal and nonideal solutions of the coupled density–temperature equations (35) and (36). The thick line marks the stationary solution for the ideal plasma. The corresponding stationary solutions of the nonideal system are marked by filled circles (for details cf. Fig. 3). The solutions in phase $(\theta$-$c)$ space are also shown. The ideal solutions of Eq. (39) are marked by thin solid lines, the nonideal ones [Eq. (41)] by dots. $n=7.692\times10^{27}\ \mathrm{m}^{-3}$, cf. also Figs. 1 and 3.

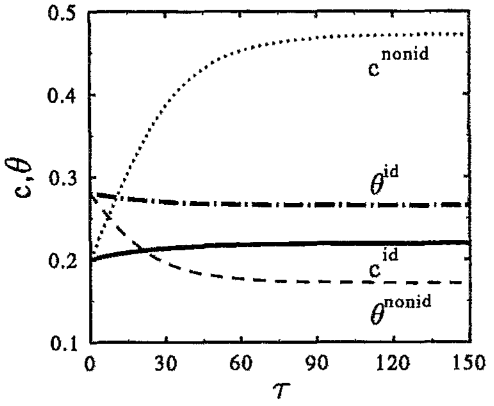

FIG. 6. Solution of the coupled density–temperature equations (35) and (36) for an ideal and nonideal plasma, respectively. The total electron density is $n=7.692\times10^{27}\ \mathrm{m}^{-3}$.

The solution of Eq. (41) is shown in Fig. 5 together with the corresponding results for the ideal case. Due to the lowering of the ionization energy, the lines $\theta_s(c_s)$ lie above the corresponding ideal lines. As one expects, the largest deviations from the ideal result occur at low temperature and high degree of ionization, where nonideality effects are strong.

The relaxation of temperature and the degree of ionization calculated from Eqs. (35) and (36) is shown in Figs. 6–8 for different initial conditions. One clearly sees that it is essential to take the nonideality effects into account. They lead to significant modifications of the relaxation process compared to that of ideal plasmas. In particular, the final values of density and temperature in a nonideal plasma may

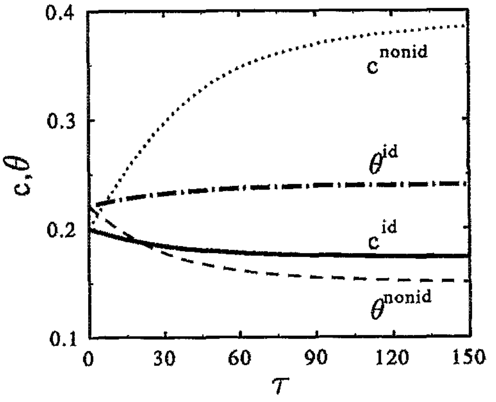

FIG. 7. Same as Fig. 6, but for different initial conditions.

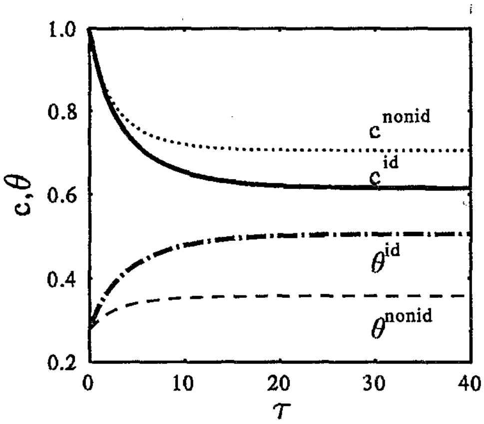

FIG. 8. Same as Fig. 6, but for different initial conditions.

deviate essentially from those in an ideal one. In Fig. 6 the nonideal relaxation leads to bigger changes of density and temperature. This is, however, not a general trend, but depends on the location of the initial point with respect to the stationary solutions $\theta^{id}(c_s)$ and $\theta^{nid}(c_s)$, respectively. So, if one picks the initial values in between both lines, the ideal and nonideal relaxations will go in different directions, cf. Fig. 7. In Fig. 8 another situation is shown. Here we start with a fully ionized system. The ideal relaxation leads to bigger changes of density and temperature.

Concerning the relaxation times, we first confirm the simultaneous character of density and temperature relaxation. This is understandable since the only driving force of the relaxation are the chemical reactions and the related consumption/production of the ionization energy. Furthermore, the nonideality effects seem not to change the relaxation time drastically.

IV. CONCLUSIONS

In this paper we continued previous investigation on the influence of (microscopic) nonideality effects on the dynamics of macroscopic quantities. Starting from generalized quantum kinetic equations for quasiparticles, we derived rate equations for dense partially ionized plasmas. Our main result is the temperature balance equation (22) for a nonideal plasma. This equation reflects the total energy conservation of nonideal systems. Thus we have nonideality corrections, which lead to an additional density dependence of the temperature relaxation. For the case of spatially homogeneous systems, we investigated in detail the coupled relaxation of density and plasma temperature. Nonideality effects lead to significant modifications of the relaxation process. Starting from the same initial state, the final state of the plasma may strongly deviate from that of an ideal plasma.

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APPENDIX: SUMMATION OF THE COLLISION TERMS

In this appendix, the summation of the collision integrals of the hydrodynamic equations (5)–(8) is shown. We have to calculate sums of the form

$$J^{(\psi)}=\sum_b J_b^{(\psi)}=\sum_b \int \frac{d^3p_b}{(2\pi\hbar)^3}\,\psi_b I_b, \tag{A1}$$

where the summation is over all components, and I_b is the sum of all collision integrals in the kinetic equation of species "b." The function $\psi_b=1$, $\epsilon_b(prt)$ in the case of free particles ($b=A,B$) and $\psi_b=1$, $(P_b^2/2m_b+E_j)$ in the case of bound states $[b=(AB)]$ for the density and energy balance, respectively. In a three-component plasma, the sum (A1) can be expressed in terms of the two- and three-particle collision integrals

$$\begin{aligned}J^{(\psi)}=&\int \frac{d^3p_A}{(2\pi\hbar)^3}\,\psi_A\Big(\sum_a I_{Aa}+\sum_{ab} I_{Aab}\Big)\\&+\int \frac{d^3p_B}{(2\pi\hbar)^3}\,\psi_B\Big(\sum_a I_{Ba}+\sum_{ab} I_{Bab}\Big)\\&+\sum_j\int \frac{d^3P_{(AB)}}{(2\pi\hbar)^3}\,\psi^j_{(AB)}\sum_a I_{(AB)a}.\end{aligned} \tag{A2}$$

We have the following collision integrals in Eq. (A2).

(i) The two-particle collision integrals ($c=A,B$), describing elastic scattering processes, are given by

$$\begin{aligned}I_{ca}=&\frac{1}{\hbar V}\int \frac{d^3p_a}{(2\pi\hbar)^3}\frac{d^3\bar{p}_c}{(2\pi\hbar)^3}\frac{d^3\bar{p}_a}{(2\pi\hbar)^3}\\&\times|\langle p_cp_a|T_{ca}|\bar{p}_c\bar{p}_a\rangle|^2 2\pi\delta(E_{ca}-\bar{E}_{ca})[\bar{f}_c\bar{f}_a(1\pm f_c)\\&\times(1\pm f_a)-(1\pm\bar{f}_c)(1\pm\bar{f}_a)f_cf_a].\end{aligned} \tag{A3}$$

(ii) The three-particle collision integrals I_{cab} with $c=A,B$ are[4]

$$I_{cab}=\sum_{k=0}^{3}(I_{cab}^{0k}+I_{c(ab)}^{1k}), \tag{A4}$$

with

$$\begin{aligned}I_{cab}^{0k}=&\frac{1}{2\hbar V}\int \frac{d^3p_a}{(2\pi\hbar)^3}\frac{d^3\bar{p}_b}{(2\pi\hbar)^3}\,d^3(k\bar{\alpha})\\&\times|\langle p_cp_ap_b|T_{cab}^{0k}|k\bar{\alpha}\rangle|^2 2\pi\delta(E_{cab}-\bar{E}_k)\\&\times(\bar{f}_kN_0-\bar{N}_kf_af_bf_c),\end{aligned} \tag{A5}$$

$$\begin{aligned}I_{c(ab)}^{1k}=&\frac{1}{2\hbar V}\sum_j\int \frac{d^3P_{(ab)}}{(2\pi\hbar)^3}\,d^3(k\bar{\alpha})\\&\times|\langle p_cP_{(ab)}j|T_{c(ab)}^{1k}|k\bar{\alpha}\rangle|^2 2\pi\delta(E_{c(ab)j}-\bar{E}_k)\\&\times(\bar{f}_kN_1-\bar{N}_kf_cf_{j(AB)}).\end{aligned} \tag{A6}$$

These integrals describe all possible three-body scattering processes involving three free particles or one free and one bound particle (explanation of k see below).

(iii) The integrals $I_{(AB)a}$ contain the scattering of bound states on free particles ($a=A,B$), as they appear in the kinetic equation of the atoms,

$$I_{(AB)a}=\sum_{k=0}^{3} I^{1k}_{(AB)a}, \tag{A7}$$

where we have, similar to $I^{1k}_{c(ab)}$,

$$I^{1k}_{(AB)a}=\frac{1}{\hbar V}\sum_{j}\int\frac{d^3p_a}{(2\pi\hbar)^3}\,d^3(k\bar{\alpha})$$
$$\times|\langle p_aP_{(AB)}j|T^{1k}_{(AB)a}|k\bar{\alpha}\rangle|^2 2\pi\delta(E_{a(AB)j}-\bar{E}_k)$$
$$\times(\bar{f}_kN_1-\bar{N}_kf_af_{j(AB)}). \tag{A8}$$

Here k is the channel number. The scattering states $|k\alpha\rangle$, channel energies E_k and the Pauli blocking factors N_k are given in Ref. 1.

Now we consider the sum in Eq. (A2) separately for the different types of collision integrals describing elastic scattering, excitations, rearrangements, and reactions.

(1) The sum over the elastic two-particle scattering terms is

$$\int\frac{d^3p_A}{(2\pi\hbar)^3}\,\psi_A\sum_a I_{Aa}+\int\frac{d^3p_B}{(2\pi\hbar)^3}\,\psi_B\sum_a I_{Ba}$$
$$=\sum_{c=A,B}\sum_a\int\frac{d^3p_c}{(2\pi\hbar)^3}\,\psi_cI_{ca}. \tag{A9}$$

This sum can be transformed in standard manner into

$$\sum_{ca}\int\frac{d^3p_c}{(2\pi\hbar)^3}\,\psi_cI_{ca}$$
$$=\frac{1}{4\hbar V}\sum_{ca}\int\frac{d^3p_c}{(2\pi\hbar)^3}\frac{d^3p_a}{(2\pi\hbar)^3}\frac{d^3\bar{p}_c}{(2\pi\hbar)^3}\frac{d^3\bar{p}_a}{(2\pi\hbar)^3}$$
$$\times(\psi_c+\psi_a-\bar{\psi}_c-\bar{\psi}_a)|\langle p_cp_a|T_{ca}|\bar{p}_c\bar{p}_a\rangle|^2 2\pi\delta(E_{ca}$$
$$-\bar{E}_{ca})(\bar{f}_c\bar{f}_a(1\pm f_c)(1\pm f_a)-(1\pm\bar{f}_c)(1\pm\bar{f}_a)f_cf_a). \tag{A10}$$

This expression vanishes, because of the conservation of mass and energy in elastic two-particle collisions (of course, mass conservation is fulfilled already by each elastic collision integral separately). Therefore, the sum over the elastic two-particle collisions does not contribute to the total density and energy balance.

The elastic collisions between three free particles [integrals I^{00}_{cab} with $c=A,B$, cf. (ii) above] can be considered in the same way as the elastic two-particle collisions. Thus, the sum over these terms does not contribute to the total density and energy balance also.

(2) Now we consider the terms involving the collision integrals $I^{11}_{Aab}, I^{11}_{Bab}$ in Eq. (A4) and $I^{11}_{(AB)a}$ in Eq. (A7). These integrals describe scattering of free particles on a bound state and include both elastic scattering and excitation (deexcitation). The sum over the corresponding terms in Eq. (A2), can be written as

$$\int\frac{d^3p_A}{(2\pi\hbar)^3}\,\psi_A\sum_{ab}I^{11}_{Aab}+\int\frac{d^3p_B}{(2\pi\hbar)^3}\,\psi_B\sum_{ab}I^{11}_{Bab}+\sum_j\int\frac{d^3P_{(AB)}}{(2\pi\hbar)^3}\,\psi^j_{(AB)}\sum_a I^{11}_{(AB)a}$$
$$=\frac{1}{2\hbar V}\sum_c\sum_j\sum_{\bar{j}}\int\frac{d^3p_c}{(2\pi\hbar)^3}\frac{d^3P_{(AB)}}{(2\pi\hbar)^3}\frac{d^3\bar{p}_c}{(2\pi\hbar)^3}\frac{d^3\bar{P}_{(AB)}}{(2\pi\hbar)^3}(\psi_c+\psi^j_{(AB)}-\bar{\psi}_c-\bar{\psi}^{\bar{j}}_{(AB)})|\langle p_cP_{(AB)}j|T^{11}_{(AB)c}|\bar{p}_c\bar{P}_{(AB)}\bar{j}\rangle|^2$$
$$\times 2\pi\delta(E_{c(AB)j}-\bar{E}_{c(AB)\bar{j}})(\bar{f}_c\bar{f}_{\bar{j}(AB)}(1\pm f_c)(1+f_{j(AB)})-(1\pm\bar{f}_c)(1+\bar{f}_{\bar{j}(AB)})f_cf_{j(AB)}). \tag{A11}$$

Obviously, each integral separately conserves density. For the case of total energy balance, the sum (A11) vanishes again, because of the properties of the delta function.

Applying the same considerations to the case of rearrangement reactions [$I^{12}_{Aab}, I^{13}_{Aab}, I^{12}_{Bab}, I^{13}_{Bab}, I^{12}_{(AB)a}, I^{13}_{(AB)a}$, see Eq. (A2)], one can show that these terms also do not contribute to the total density and energy balance.

(3) Now we consider the remaining terms of the sum (A2) consisting of all ionization/recombination processes. Collecting the corresponding integrals, we can use similar transformations as above, yielding

$$\int\frac{d^3p_A}{(2\pi\hbar)^3}\,\psi_A\sum_{ab}[I^{01}_{Aab}+I^{02}_{Aab}+I^{03}_{Aab}+I^{10}_{Aab}]+\int\frac{d^3p_B}{(2\pi\hbar)^3}\,\psi_B\sum_{ab}[I^{01}_{Bab}+I^{02}_{Bab}+I^{03}_{Bab}+I^{10}_{Bab}]+\sum_j\int\frac{d^3P_{(AB)}}{(2\pi\hbar)^3}\,\psi^j_{(AB)}\sum_a I^{10}_{(AB)a}$$
$$=\frac{1}{\hbar V}\sum_c\sum_j\int\frac{d^3p_c}{(2\pi\hbar)^3}\frac{d^3P_{(AB)}}{(2\pi\hbar)^3}\frac{d^3\bar{p}_c}{(2\pi\hbar)^3}\frac{d^3\bar{p}_A}{(2\pi\hbar)^3}\frac{d^3\bar{p}_B}{(2\pi\hbar)^3}(\psi^j_{(AB)}+\psi_c-\bar{\psi}_c-\bar{\psi}_A-\bar{\psi}_B)|\langle p_cP_{(AB)}j|T^{10}_{c(AB)}|\bar{p}_c\bar{p}_A\bar{p}_B\rangle|^2$$
$$\times 2\pi\delta(E_{c(AB)j}-\bar{E}_{cAB})(\bar{f}_c\bar{f}_A\bar{f}_B(1\pm f_c)(1+f_{j(AB)})-(1\pm\bar{f}_c)(1\pm\bar{f}_A)(1\pm\bar{f}_B)f_cf_{j(AB)}). \tag{A12}$$

For the total density balance, i.e., $\psi=1$, the sum (A12), and hence the sum $J^{(1)}$ in (A1) simplifies to

$$J^{(1)}=-\sum_j W^j_{(AB)},$$

$$=\sum_{c=A,B}\sum_j (\alpha^c_j n_c n_j-\beta^c_j n_c n_A n_B). \tag{A13}$$

Here, the impact ionization and recombination coefficients have been introduced. They are defined as

$$\alpha^c_j=\frac{1}{\hbar V}\int\frac{d^3p_c}{(2\pi\hbar)^3}\frac{d^3P_{(AB)}}{(2\pi\hbar)^3}\frac{d^3\bar{p}_c}{(2\pi\hbar)^3}\frac{d^3\bar{p}_A}{(2\pi\hbar)^3}\frac{d^3\bar{p}_B}{(2\pi\hbar)^3}$$

$$\times|\langle p_cP_{(AB)}j|T^{10}_{c(AB)}|\bar{p}_c\bar{p}_A\bar{p}_B\rangle|^2 2\pi\delta(E_{c(AB)j}-\bar{E}_{cAB})$$

$$\times\frac{f_c}{n_c}\frac{f_{j(AB)}}{n_{j(AB)}}(1\pm\bar{f}_c)(1\pm\bar{f}_A)(1\pm\bar{f}_B), \tag{A14}$$

$$\beta^c_j=\frac{1}{\hbar V}\int\frac{d^3p_c}{(2\pi\hbar)^3}\frac{d^3P_{(AB)}}{(2\pi\hbar)^3}\frac{d^3\bar{p}_c}{(2\pi\hbar)^3}\frac{d^3\bar{p}_A}{(2\pi\hbar)^3}\frac{d^3\bar{p}_B}{(2\pi\hbar)^3}$$

$$\times|\langle p_cP_{(AB)}j|T^{10}_{c(AB)}|\bar{p}_c\bar{p}_A\bar{p}_B\rangle|^2 2\pi\delta(E_{c(AB)j}-\bar{E}_{cAB})$$

$$\times\frac{f_c}{n_c}\frac{f_A}{n_A}\frac{f_B}{n_B}(1\pm f_c)(1+f_{j(AB)}). \tag{A15}$$

From Eq. (A13) follows

$$\frac{\partial}{\partial t}(n_A+n_B+n_{(AB)})=-\sum_j W^j_{(AB)} \tag{A16}$$

and thus the number density $n=n_A+n_{(AB)}$ is conserved [cf. Eqs. (5) and (6)]. Consider now the total energy balance, i.e., $\psi_a=\epsilon_a(prt)$ with $(a=A,B,c)$ and $\psi_{(AB)}=(P^2_{(AB)}/2m_{(AB)}+E_j)$. The energy conserving delta function with momentum-dependent quasiparticle energies is given by

$$\delta(E_{c(AB)j}-\bar{E}_{c(AB)})$$

$$=\delta\left(\frac{P^2_{(AB)}}{2m_{(AB)}}+E_j+\epsilon_c(p_c)-\epsilon_c(\bar{p}_c)-\epsilon_A(\bar{p}_A)-\epsilon_B(\bar{p}_B)\right). \tag{A17}$$

Thus it is obvious that the contribution (A12) vanishes. We have $J^{(\epsilon)}=0$ and the system of hydrodynamic equations (5)–(8) conserves the total energy.

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[13] The plasma phase transition arises from the monotonically decreasing part of the plasma chemical potential of the free particles as a function of density. As a result, below a critical temperature (here $\theta_{cr}\approx 0.15$), the source function has three zeros (besides $c=0$) which are shown in Figs. 2–4. This effect occurs also if one uses better approximations for the quasiparticle shifts.[1] If one, on the other hand, takes into account the formation of H_2 molecules, the multistability vanishes in equilibrium. However, it can possibly appear in nonequilibrium relaxation processes. This is still an open question.