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Diffusion and Heat Transport in a Dense Partially Ionized Plasma

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Abstract

Balance equations for the density, momentum and energy of a dense plasma are derived on the basis of quantum kinetic theory. The influence of many-body effects on ionization/recombination reactions, diffusion and thermal conductivity are discussed. It is shown that (microscopic) many-particle effects lead to nonlinear macroscopic relaxation behaviour. For illustration, we solve the coupled density-temperature balance equations for a dense partially ionized hydrogen plasma.

1 Introduction

The relaxation of chemical composition and temperature in dense plasmas are of special interest in ultrashort laser experiments [1, 2]. Recently it became possible to measure electron densities up to $10^{23} cm^{-3}$ and to investigate the dynamics of the expanding plasma [3].

In such dense plasmas, many-particle effects, as screening, self-energy, bound states, and lowering of the ionization energy, have particular influence on the nonequilibrium behaviour. From the theoretical point of view, the relaxation process can be described by generalized quantum kinetic equations including the many-particle effects mentioned [4] - [9]. On the hydrodynamic level of discription, the plasma relaxation is determined by equations of change for the density, mean velocity and energy. Now, the transport and rate coefficients follow from the kinetic equations and we found quantum statistical expressions for these quantities.

It is of special importance for the investigation of dense laser produced plasmas to include reactive processes such as impact ionization and three-body recombination.

In the present paper, we consider a spatially inhomogenous plasma and we will describe diffusion and heat transport in connection with chemical reactions. In earlier papers [10, 11] reaction-diffusion equations were described for the isothermal case. Here, we investigate a nonisothermal dense plasma and look at the coupled system of equations for density and temperature. The influence of many-body effects on the transport coefficients and on the evolution process is demonstrated.

2 Hydrodynamic Equations for Dense Plasmas

To obtain hydrodynamic equations for nonideal partially ionized plasmas, we start from generalized quantum kinetic equations. Such kinetic equations for quasiparticles were derived in Refs. [4 - 9]. Many-particle effects, such as screening of the Coulomb interaction, self-energy, Pauli blocking, formation and decay of bound states and pressure ionization (Mott effect) are included in those equations. Using the concept of quasiparticles, we can describe important many-particle effects in a simple manner. In this picture, the single-particle energy (quasiparticle energy) is given by the dispersion relation (a labels different species)

$$\varepsilon_a(\mathbf{p}\mathbf{r}t) = \frac{p^2}{2m} + Re\Sigma_a^R(\omega\mathbf{p}\mathbf{r}t)|_{\hbar\omega=\varepsilon_a(\mathbf{p}\mathbf{r}t)}, \tag{1}$$

where $\Sigma_a^R(\omega\mathbf{p}\mathbf{r}t)$ is the retarded selfenergy function of Green's function theory [12]. This function describes the modification of the energy of a particle due to the influence of the surrounding plasma. For bound particles we have to include the binding energy in the expression of the quasiparticle energy (1).

While the kinetic equation allows to describe relaxation processes on microscopic (kinetic) and macroscopic scales, we are interested here only in the hydrodynamic relaxation. Then it is convenient to derive hydrodynamic balance equations for the macroscopic quantities density, mean velocity and energy density, which are related to the Wigner distribution function f_a by

$$\begin{aligned}
n_a(\mathbf{r}t) &= \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} f_a(\mathbf{p}\mathbf{r}t), &(2)\\
\mathbf{u}_a(\mathbf{r}t) &= \frac{1}{n_a(\mathbf{r}t)} \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \frac{\partial \varepsilon_a(\mathbf{p}\mathbf{r}t)}{\partial \mathbf{p}} f_b(\mathbf{p}\mathbf{r}t), &(3)\\
\frac{E_a(\mathbf{r}t)}{V} &= \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \frac{p^2}{2m_a} f_a(\mathbf{p}\mathbf{r}t) + \frac{1}{2} \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} Re\Sigma_a^R(\hbar\omega = \varepsilon_a, \mathbf{p}\mathbf{r}t) f_a(\mathbf{p}\mathbf{r}t). &(4)
\end{aligned}$$

The energy density (4) contains a kinetic part (first integral), which will be related to the temperature below, and an interaction contribution (second integral). The hydrodynamic equations are derived from the kinetic equations using standard methods [13]

$$\begin{aligned}
\frac{\partial}{\partial t} n_a(\mathbf{r}t) + \frac{\partial}{\partial \mathbf{r}} \mathbf{j}_a^D(\mathbf{r}t) + \frac{\partial}{\partial \mathbf{r}} [n_a(\mathbf{r}t)\mathbf{u}(\mathbf{r}t)] &= W_a(\mathbf{r}t), &(5)\\
\frac{\partial}{\partial t} \rho_a(\mathbf{r}t) u_{ai}(\mathbf{r}t) + \frac{\partial}{\partial r_j} \Pi_{aij}(\mathbf{r}t) &= \mathbf{R}_{ai}(\mathbf{r}t), &(6)\\
\frac{\partial}{\partial t} \left[\frac{E_a(\mathbf{r}t)}{V}\right] + \frac{\partial}{\partial \mathbf{r}} Q_a(\mathbf{r}t) &= U_a(\mathbf{r}t). &(7)
\end{aligned}$$

Let us discuss the terms in eqs. (5) – (7) more in detail. Consider first the drift terms on the l. h. s. of eqs. (5) – (7). In eq. (5), $\mathbf{j}_a^D$ is the diffusion current, defined as

$$\mathbf{j}_a^D(\mathbf{r}t) = n_a(\mathbf{u}_a - \mathbf{u}), \tag{8}$$

with the average mass velocity $\mathbf{u} = 1/\rho \sum_a \rho_a \mathbf{u}_a$ and the mass densities $\rho_a = n_a m_a$, $\rho = \sum_a \rho_a$. The third term on the l. h. s. of eqs. (5) is the convective current. In eq. (6), we introduced the pressure tensor,

$$\frac{\partial}{\partial r_j} \Pi_{aij} = \frac{\partial}{\partial r_j} \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} p_i \frac{\partial \varepsilon_a}{\partial p_j} f_a + \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \frac{\partial \varepsilon_a}{\partial r_j} f_a \delta_{ij}, \tag{9}$$

which contains many–body correlations due to the selfenergy. In eq. (7), Q_a is the energy flux,

$$Q_a(\mathbf{r}t) = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \varepsilon_a(\mathbf{p}\mathbf{r}t) \frac{\partial \varepsilon_a(\mathbf{p}\mathbf{r}t)}{\partial \mathbf{p}} f_a(\mathbf{p}\mathbf{r}t). \tag{10}$$

Now, we consider the source terms on the r. h. s. of eqs. (5) – (7), which are given by

$$W_a(\mathbf{r}t) = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \sum_c I_{abc}(\mathbf{p}\mathbf{r}t), \tag{11}$$

$$\mathbf{R}_a(\mathbf{r}t) = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3}\mathbf{p}\left[\sum_b I_{ab}(\mathbf{p}\mathbf{r}t) + \sum_{bc} I_{abc}(\mathbf{p}\mathbf{r}t)\right], \tag{12}$$

$$U_a(\mathbf{r}t) = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3}\varepsilon_a(\mathbf{p}\mathbf{r}t)\left[\sum_b I_{ab}(\mathbf{p}\mathbf{r}t) + \sum_{bc} I_{abc}(\mathbf{p}\mathbf{r}t)\right]. \tag{13}$$

W_a describes the change of particle number n_a due to inelastic three–particle collisions (the two–particle integrals I_{ab} are density conserving). $\mathbf{R}_a$ and U_a describe the effect of collisions on the momentum and energy balance, respectively. The source terms for the bound particles in the balance equations are

$$\sum_j W^j_{(ab)}(\mathbf{r}t) = \sum_j \int \frac{d\mathbf{P}}{(2\pi\hbar)^3}\sum_c I^j_{(ab)c}(\mathbf{P}\mathbf{r}t), \tag{14}$$

$$\sum_j \mathbf{R}^j_{(ab)}(\mathbf{r}t) = \sum_j \int \frac{d\mathbf{P}}{(2\pi\hbar)^3}\mathbf{P}\sum_c I^j_{(ab)c}(\mathbf{P}\mathbf{r}t), \tag{15}$$

$$\sum_j U^j_{(ab)}(\mathbf{r}t) = \sum_j \int \frac{d\mathbf{P}}{(2\pi\hbar)^3}\varepsilon_a(\mathbf{P}\mathbf{r}t)\sum_c I^j_{(ab)c}(\mathbf{P}\mathbf{r}t), \tag{16}$$

where $\mathbf{P}$ is the center of mass momentum und j comprises the quantum numbers of the levels of the bound particles. Explicit expressions for the collision integrals I_{ab}, I_{abc} and $I^j_{(ab)c}$ can be found in Refs. [4] and [5].

The balance equations (5) – (7) are generally valid for partially ionized nonideal plasmas. Simplifications are possible in the case of a three–component plasma consisting of electrons (e), z–fold charged ions (i) and atoms (ei). Furthermore, we will use simplifications for the selfenergy and for the pressure balance, which we discuss now.

1. *Momentum independent energy shifts:* The retarded selfenergy function $\Sigma^R_a(\omega\mathbf{p}\mathbf{r}t)$ depends on the distribution function (for a discussion see Ref. [10]). Therefore, in principle, it has to be determined self–consistently with the solution of the kinetic equations. The solution of the hydrodynamic equation with self–consistently calculated energy shifts would be very difficult. Therefore we use, for the energy shifts, the rigid shift approximation. Here $\Sigma^R_a(\omega\mathbf{p}\mathbf{r}t)$ is replaced by momentum independent shifts [14]

$$\varepsilon_a(\mathbf{p}\mathbf{r}t) = \frac{p^2}{2m_a} + \Delta_a(\mathbf{r}t). \tag{17}$$

The shift $\Delta_a(\mathbf{r}t)$ has to be determined from a condition, which reproduces the correct normalization to the density. In first order follows

$$\Delta_a(\mathbf{r}t) = \left(\int \frac{d\mathbf{p}}{(2\pi\hbar)^3} Re\Sigma^R_a(\omega\mathbf{p}\mathbf{r}t)|_{\hbar\omega=\varepsilon_a}\frac{\partial}{\partial\mu^{id}_a}f_a(\mathbf{p}\mathbf{r}t)\right) \Big/ \left(\int \frac{d\mathbf{p}}{(2\pi\hbar)^3}\frac{\partial}{\partial\mu^{id}_a}f_a(\mathbf{p}\mathbf{r}t)\right). \tag{18}$$

The thermally averaged energy shift is connected with the chemical potential by

$$\mu_a(\mathbf{r}t) = \mu^{id}_a(\mathbf{r}t) + \Delta_a(\mathbf{r}t), \tag{19}$$

and is equal to the interaction part of the chemical potential. The analytical calculation of $\Delta_a(\mathbf{r}t)$ is only possible in simple cases. For example, in the nondegenerate low density case, we get ($a = e, i$)

$$\Delta_a(\mathbf{r}t) = -\frac{e^2}{2r_0}, \quad \frac{1}{r_0^2} = \kappa^2 = 4\pi\sum_a\frac{n_a z_a^2 e_a^2}{k_B T_a}, \tag{20}$$

with the screening length r_0 and the screening parameter κ. In eq. (20), $\Delta_a(\mathbf{r}t)$ is the Debye shift, which represents the limiting law for systems with Coulomb interactions.

2. *Elimination of the momentum balance equation:* Explicit expressions for the diffusion current j_a^D can be derived from the momentum balance (6). If further the system is close to local equilibrium we have $(\mathbf{u}_a - \mathbf{u}) \ll (k_BT/m_a)^{1/2}$ and the distribution functions can be taken in linear approximation

$$f_a = f_a^0\left[1+\frac{\mathbf{c}_a(\mathbf{u}_a-\mathbf{u})}{k_BT}\right], \qquad f_a^0 = n_a\Lambda_a^3\exp\left[-\frac{(\mathbf{p}_a - m_a\mathbf{u})^2}{2m_ak_BT}\right], \tag{21}$$

where Λ_a is the thermal wavelength. A similar expression follows for the distribution functions of the bound states. Neglecting contributions nonlinear in u, we obtain from eq. (6) for the mass average velocity

$$\rho\frac{\partial}{\partial t}\mathbf{u} \approx -\nabla P, \tag{22}$$

and for the pressure

$$\nabla p_a - \frac{\rho_a}{\rho}\nabla P = \mathbf{S}_a = \mathbf{R}_a - \mathbf{u}_a m_a W_a, \tag{23}$$

where we used $\partial\Pi_{aij}/\partial r_j = \nabla p_a\delta_{ij}$. According to eq. (9) and using momentum independent energy shifts (17), the pressure gradients are given by

$$\nabla P(\mathbf{r}t) = \nabla\sum_a p_a(\mathbf{r}t), \qquad \nabla p_a(\mathbf{r}t) = \nabla p_a^{id}(\mathbf{r}t) + n_a\nabla\Delta_a(\mathbf{r}t). \tag{24}$$

The pressure p_a is not the pure ideal partial pressure because of the interaction contributions contained in the energy shift $\Delta_a(\mathbf{r}t)$ (for details see Ref. [10]).

eq. (23) connects the thermodynamic forces of the nonideal plasma with the momentum transfer due to the collision processes. If we restrict ourselves to elastic contributions, we get for the r. h. s. of eq. (23)

$$\mathbf{S}_a = \mathbf{R}_a^{el} = \sum_b \frac{k_BT}{n_\sigma\mathcal{D}_{ab}}\left(n_a\mathbf{j}_b^D - n_b\mathbf{j}_a^D\right), \tag{25}$$

where n_σ is the total number density. The explicit expression for the diffusion coefficients can be found in Ref. [10]. Now we can solve eq. (23) with expression (25) in standard way

$$\mathbf{j}_b^D = \frac{n_\sigma}{\rho k_BT}\sum_{b\neq a} m_bD_{ab}\left(\nabla p_b - \frac{\rho_b}{\rho}\nabla P\right). \tag{26}$$

D_{ab} are the multicomponent diffusion coefficients, which can be expressed in terms of the binary diffusion coefficients $\mathcal{D}_{ab}$

$$D_{ab} = \mathcal{D}_{ab}\left(1+\frac{n_c[\mathcal{D}_{ac}(m_c/m_b) - \mathcal{D}_{ab}]}{n_a\mathcal{D}_{ab}+n_b\mathcal{D}_{ac}+n_c\mathcal{D}_{ab}}\right). \tag{27}$$

Expression (26) is an important generalization of the ideal gas result because it contains nonideality contributions in terms of the energy shift.

3. *Ambipolar diffusion regime:* In the following, we want to study the diffusion process in ambipolar diffusion regime. This leads to a steady state with charge neutrality and equal electron and ion number fluxes

$$z_en_e(\mathbf{r}t) + z_in_i(\mathbf{r}t) = 0, \qquad z_e\mathbf{j}_e^D(\mathbf{r}t) + z_i\mathbf{j}_i^D(\mathbf{r}t) = 0. \tag{28}$$

Further we suppose $\nabla P \approx 0$. With eq. (22), $\mathbf{u} = const$, and we can consider the system in a moving frame where $\mathbf{u} \approx 0$. As a result we get $n = n_e + n^1_{(ei)}$, and the system of reaction–diffusion equations in a three–component plasma reduces to one equation

$$\frac{\partial}{\partial t} n_e = W_e + \nabla D_{AMB} \nabla n_e. \tag{29}$$

Here we introduced the ambipolar diffusion coefficient in a three–component plasma, which is given by [15, 16]

$$D_{AMB} = D_0 \frac{n_e}{k_b T} \left(\frac{\partial \mu_e}{\partial n_e} + \frac{\partial \mu_i}{\partial n_i} \right), \tag{30}$$

$$D_0 = \frac{n_\sigma}{\rho} \frac{m_i D_{ei} m_H D_{iH} + m_e D_{ie} m_H D_{eH} - m_e D_{ie} m_i D_{ei}}{m_e D_{ie} + m_i D_{ei}}. \tag{31}$$

4. *Plasma temperature balance:* In many cases, one anticipates a multi-stage 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 the temperature mentioned and of the chemical composition of the plasma in connection with diffusion and heat conductivity. The plasma temperature T is given by

$$\frac{3}{2} n_\sigma(\mathbf{r}t) k_B T(\mathbf{r}t) = \sum_a \int \frac{d^3p}{(2\pi\hbar)^3} \frac{p^2}{2m_a} f_a(\mathbf{pr}t). \tag{32}$$

Summing up the eq. (7) over the components in a three–component plasma, we get

$$\frac{\partial T}{\partial t} = \left(\frac{3}{2} n_\sigma k_B + \frac{1}{4} \frac{e^2 n_e}{r_0 T} \right)^{-1} \left[\nabla \lambda \nabla T - \left(\frac{3}{2} k_B T + |E_1| - \frac{3}{4} \frac{e^2}{r_0} \right) W_e \right] \tag{33}$$

Here we introduced the thermal conductivity λ.

We reduced the system of balance equations (5) – (7) to the eqs. (29) and (33). These equations are strongly coupled. Before we solve the system of eqs. (29) and (33), we will discuss the source function, ambipolar diffusion and thermal conductivity, respectively.

3 Many–Particle Effects in the Transport Coefficients

3.1 Source Function

To study nonideality effects on the relaxation kinetics in a simple example, we consider in the following partially ionized hydrogen, consisting of electrons, protons and atoms. If we introduce impact ionization coefficients α_j^c and three–body recombination coefficients β_j^c, corresponding to atomic level j, we can transform the source terms (11) into

$$W_e = W_p = -\sum_j W_H^j = \sum_{c=e,p} \sum_j (\alpha_j^c n_c n_j - \beta_j^c n_c n_e n_p). \tag{34}$$

Explicit expressions for the ionization and recombination coefficients can be found in Refs. [4] and [17]. Now we restrict ourselves to atoms in the ground state. Since the impact ionization by ions is much less effective as compared to electron impact ionization, it is usually sufficient to consider the latter process. The electron impact ionization coefficient was calculated with an approximate impact ionization cross section, which is given in Ref. [17]. Then we obtain an analytic expression for the ionization coefficient

$$\alpha_1 = \alpha_1^{id} \exp[(\Delta_1 - \Delta_e - \Delta_p)/k_B T], \qquad \alpha_1^{id} = \alpha_0 \, g\left(\frac{|E_1|}{k_B T} \right). \tag{35}$$

Here α_0 and g are defined by

$$\alpha_0 = \frac{(10\pi a_B^2 |E_1|^{1/2})}{(2\pi m_e)^{1/2}}, \qquad g(x) = x^{1/2} \int_x^\infty (e^{-t}/t)dt. \tag{36}$$

The ionization coefficient has a strong dependence on the density, because the ionization is a process with a threshold energy. In the approximation of thermally averaged shifts, the ionization and the recombination coefficients are coupled by the relation

$$\beta_j = \alpha_j \Lambda_e^3 \exp(I_j^{eff}/k_B T), \qquad I_j^{eff} = |E_j| - \Delta_1 + \Delta_e + \Delta_p, \tag{37}$$

with I_j^{eff} being the effective ionization energy. The influence of many-body effects on the recombination coefficient is weaker in comparison to the ionization coefficient (cf. the results for nonideal hydrogen plasma [18, 19], for alkali plasma [20] and for carbon plasma [21]). We, therefore, use here $\beta_1 \approx \beta_1^{id}$, in accordance with eqs. (35) and (37).

3.2 Ambipolar Diffusion

The ambiploar diffusion coefficient was given by eq. (30). This density-dependent coefficient leads to nonlinear diffusion caused by many-body effects. In a hydrogen plasma the ambipolar diffusion coefficient was calculated in Refs. [10] and [15]. It was shown, that the classical result $D_{AMB} = 2\mathcal{D}_{pH}$ occurs only for electron densities below $10^{15} cm^{-3}$. For higher densities, the many-body effects cause a minimum. Below $T = 17500K$ even negative values of D_{AMB} may occur as a direct consequence of the "van der Waals loop" in the plasma chemical potential. A discussion of the negative diffusion is found in Ref. 11. In this paper we concentrate on densities and temperatures, where D_{AMB} is positiv.

3.3 Thermal Conductivity

The total thermal conductivity in low density hydrogen plasmas was measured by many scientists, for example see Refs. [22] and [23]. Theoretical calculations were made also for low density hydrogen plasmas [24, 25]. In dense plasmas many-body effects lead to deviations from these results. We use the Chapmann-Enskog-Burnett theory for the determination of the total thermal conductivity [13]. In this theory the total thermal conductivity is expressed in terms of transport cross sections [25]

$$\lambda' = -\frac{75 k_B}{8} \frac{\sqrt{2\pi k_B T}}{|\,\mathbf{q}\,|} \begin{vmatrix} \mathbf{q}_{ij}^{00} & \mathbf{q}_{ij}^{01} & \mathbf{q}_{ij}^{02} & 0 \\ \mathbf{q}_{ij}^{10} & \mathbf{q}_{ij}^{11} & \mathbf{q}_{ij}^{12} & n_i \\ \mathbf{q}_{ij}^{20} & \mathbf{q}_{ij}^{21} & \mathbf{q}_{ij}^{22} & 0 \\ 0 & n_j/m_j^{1/2} & 0 & 0 \end{vmatrix} \qquad \mathbf{q}_{ij}^{mp} = \begin{matrix} q_{ee}^{mp} & q_{ep}^{mp} & q_{eH}^{mp} \\ q_{pe}^{mp} & q_{pp}^{mp} & q_{pH}^{mp} \\ q_{He}^{mp} & q_{Hp}^{mp} & q_{HH}^{mp} \end{matrix}, \tag{38}$$

where $\mathbf{q}_{ij}^{mp}$ is an array of elements q_{ij}^{mp} and $|\,\mathbf{q}\,|$ is formed from the explicitly given determinant by deleting the last row and the last column. The terms q_{ij}^{mp} are sums over the transport cross sections [25]. The thermal conductivity λ is usually defined as the coefficient of the temperature gradient term when all diffusion velocities are zero. Because we do not consider thermal diffusion effects (these effects are very small in the considered situations), the term λ' is equal to the usual thermal conductivity.

The transport cross sections of the p–H ,H–p and H–H scattering were calculated with effective hard sphere diameters. For the dominating interactions (e–p ,p–e and e–e) the transport cross sections were determined from scattering phase shift calculations. The elastic scattering of electrons on H–atoms was computed from the close coupling equations [26]. The p–p scattering is much less effective and is therefore not included. In Fig. 1, the

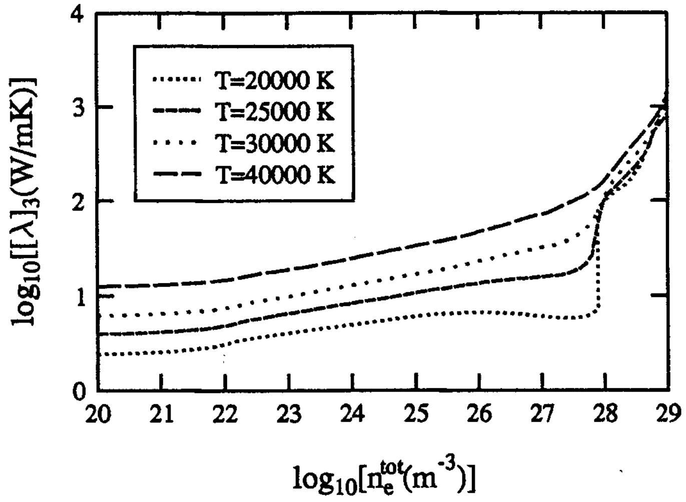

Figure 1: Total thermal conductivity in a dense hydrogen plasma for different temperatures.

total thermal conductivity is shown in a partially ionized hydrogen plasma in equilibrium. The chemical composition was calcutated from the nonideal Saha equation. One clearly sees a density dependence of the total thermal conductivity. For low temperatures we observe a minimum, which is a consequence of the formation of H-atoms. At even higher densities, close to the Mott density, the thermal conductivity increases drastically due to pressure ionization. A similar behaviour was already found in Ref. [27] for the electronic part of the thermal conductivity.

4 Numerical Solutions

We now solve the system of equations (29) and (33) for partially ionized hydrogen. We use the ambipolar diffusion coefficient (30), the heat conductivity (38), the ionization coefficient (35) and the recombination coefficient (37). We use momentum independent energy shifts given by eq. (20). It is convenient to introduce dimensionless variables for time, length, plasma density, temperature and diffusion

$$\tau = t/t_0, \quad x = r/l_0, \quad c = n_e/n, \quad \theta = k_B T/|E_1|, \quad D = D_{AMB}/D_0. \tag{39}$$

The time and length scales are defined as $t_0 = (\alpha_0 n)^{-1}$ and $l_0^2 = D_0 t_0$, where n is the total electron density and D_0 is given by eq. (31). Then we can rewrite eqs. (29) and (33) in the new variables (one dimensional case)

$$\frac{\partial c}{\partial \tau} = \nabla_x D(c,\theta,n)\nabla_x c + c\, g(\theta) f(c,\theta,n), \tag{40}$$

$$\frac{\partial \theta}{\partial \tau} = \left(\frac{3}{2} D_0(\theta,n) n k_B \left\{1 + c\left[1+\gamma(\theta,n)\sqrt{c}/6\right]\right\}\right)^{-1} \nabla_x \lambda(c,\theta,n)\nabla_x\theta - \frac{[2/3 + \theta - \gamma(\theta,n)\theta\sqrt{c}/2]}{\{1 + c[1+\gamma(\theta,n)\sqrt{c}/6]\}} c\, g(\theta) f(c,\theta,n). \tag{41}$$

The term $g(\theta)$ is given by eq. (36). The function $f(c,\theta,n)$ can be written as $f(c,\theta,n) = (1-c)\exp[\gamma(\theta,n)\sqrt{c}] - c^2\Gamma(\theta,n)$, where $\gamma(\theta,n) = 2e^3/(\theta \mid E_1 \mid) \times [(2\pi n)/(\theta \mid E_1 \mid)]^{1/2}$ and

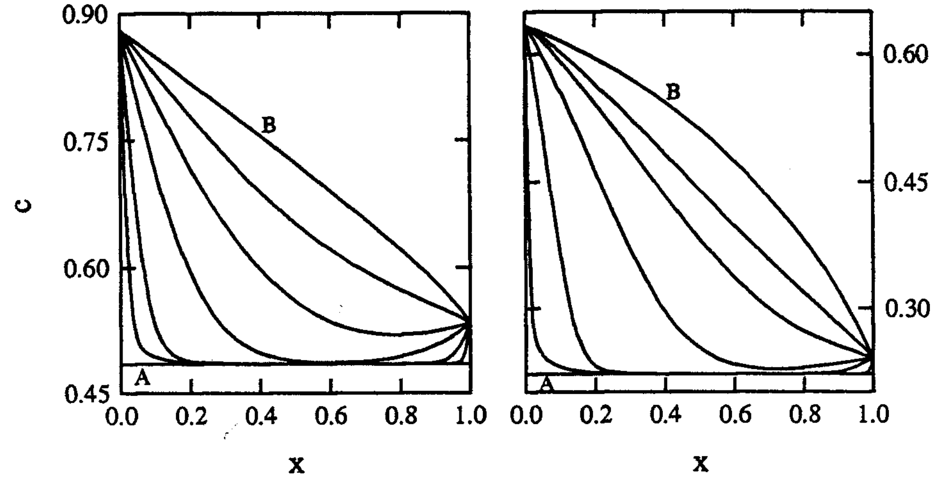

Figure 2: Solution of the coupled equations (29) and (33). The density is $n = 5\times10^{21}cm^{-3}$. x is the dimensionless length, c the degree of ionization and θ the dimensionless temperature. Fixed boundary concentrations and temperatures are used. The relaxation starts with profiles (A) and ends in profiles (B). The stationary density profile is reached at $\tau = 5\times10^{-1}$ and the temperature profile at $\tau = 2.5\times10^{-2}$ ($1\tau = 3.7\times10^{-15}$s).

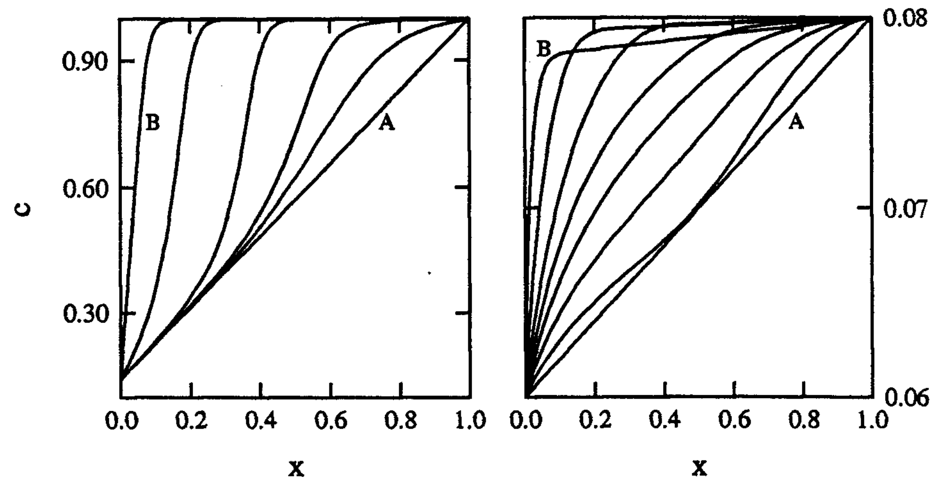

Figure 3: Same as Fig. 2, but with different boundary conditions and density of $n = 2\times10^{23}cm^{-3}$. The stationary profiles for both density and temperature are reached at $\tau = 3\times10^{-2}$.

$\Gamma(\theta, n) = \lambda_e^3 n \exp(1/\theta)$. In Fig. 2, the system is initially in a stable state of homogeneous density and temperature (profiles A). The values of this state were calculated from the nonideal Saha equation. At time $\tau = 0$, on the boundaries higher values of c and θ are switched on (they are solutions of the Saha equation too), which are kept constant during the relaxation. We see that in the stationary state (B) density and temperature change in a nonlinear way between the boundaries.

While for the parameters of Fig. 2 the influence of the chemical reactions is small, in Fig. 3 we show a different situation. The density is increased by two orders of magnitude, what corresponds to the vicinity of the Mott point. Therefore the relaxation process is strongly affected by ionization of H–atoms. A remarkable feature of this situation is that the relaxation times of density and temperature are approximately equal, because the relaxation is dominated by the chemical reactions.

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