Energy transfer and potential energy contributions in dense two-temperature plasmas

2006 J. Phys. A: Math. Gen. 39 4739

(http://iopscience.iop.org/0305-4470/39/17/S67)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) 4739–4742 doi:10.1088/0305-4470/39/17/S67

Energy transfer and potential energy contributions in dense two-temperature plasmas

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

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

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

Received 19 September 2005, in final form 8 December 2005
Published 7 April 2006
Online at stacks.iop.org/JPhysA/39/4739

Abstract
We investigate the relaxation of nonideal plasmas and demonstrate the connection between the energy transfer rate and potential energy contributions. A quantum-statistical approach is used to determine how the energies of the electron and ion subsystems can be defined. In particular, it is shown that the electron–ion potential energy term must be split equally between both subsystems. We finally demonstrate that this treatment is consistent with the transfer of total energy between the subsystems as it is for instance considered within the coupled mode approach.

PACS numbers: 05.30.−d, 52.25.Kn, 52.25.Gj, 71.10.−w

1. Introduction

The relaxation of dense two-temperature plasmas has received new interest since modern pump–probe experiments allow for very intense and short pulses as well as small, but well defined, time delays for probe pulses. With these techniques, the relaxation stage when electrons and ions have already established Fermi/Maxwell distributions but the different species temperatures have not equilibrated is now experimentally accessible.

Early theoretical descriptions of temperature equilibration considered exclusively the energy transfer through binary electron–ion collisions in hot plasmas [1, 2]. For weakly coupled plasmas, numerical simulations could confirm the results of the Landau–Spitzer (LS) approach [3, 4]. Using the Fermi-golden-rule approach, and thereby also considering collective excitations, LS-like relaxation rates could be obtained for both classical plasmas [5] and systems with degenerate electrons [6]. However, several experiments showed strong indications for a much smaller energy transfer between electrons and ions in dense plasmas [7–9]. Such reduced energy transfer rates were also theoretically predicted by an approach that considered the coupling between the collective excitations in the electron and ion subsystems

[10], whereas a fully quantum mechanical treatment of binary electron–ion collisions without arbitrary cut-off procedures yields larger energy transfers [11, 12].

In addition to the modified energy transfer rates, equation of state effects, i.e. potential energy contributions, can strongly influence the temperature equilibration process in dense plasmas. The importance of the time-dependent binding energy in partially ionized plasmas was demonstrated in [13–15], where the correlations between the carriers were included on the lowest level with a Debye shift. Strong ion–ion correlations were also shown to result in a much slower ion heating in systems with hot electrons and high ionization degree [16].

However, all these investigations used some *ad hoc* ansatz for the correlation energies of the subsystems. While the relaxation process in weakly coupled (ideal) plasmas is mainly determined by the energy transfer rates Z_{ei}, e.g. for classical plasmas by

$$\frac{3}{2}n_{\mathrm{e}}k_{\mathrm{B}}\frac{\partial}{\partial t}T_{\mathrm{e}} = Z_{\mathrm{ei}} \qquad \text{and} \qquad \frac{3}{2}n_{\mathrm{i}}k_{\mathrm{B}}\frac{\partial}{\partial t}T_{\mathrm{i}} = -Z_{\mathrm{ei}}, \tag{1}$$

it is not obvious how to define the energies of the electron and ion subsystems in dense plasmas due to the electron–ion term in the potential energy. Furthermore, it has to be determined how the energy transfer between the subsystems gets redistributed between the kinetic and potential energy terms and, therefore, how the temperature evolution is influenced by strong correlations. In this paper, we will use a quantum-statistical approach to answer these questions. In particular, we show how the assignment of the correlation energy terms and the approximation for the electron–ion energy transfer rate are interconnected.

2. General quantum-statistical description of relaxing plasmas

We investigate the evolution of the mean kinetic and potential energies of species 'a' for a coupled systems of electrons and ions. These energies are here defined by[3]

$$\langle K_a(t)\rangle = \mathrm{Tr}_1\{H_a\rho_a(t)\} \qquad \text{and} \qquad \langle V_a(t)\rangle = \frac{1}{2}\sum_b \mathrm{Tr}_{1,2}\{V_{ab}\rho_{ab}(t)\}. \tag{2}$$

The energy of species 'a' is determined by the one- and two-particle density operators ρ_a and ρ_{ab}, respectively. These operators satisfy the following equations of motion [17]:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\rho_a = [H_a, \rho_a] + \sum_b \mathrm{Tr}_2\{V_{ab}, \rho_{ab}\}, \tag{3}$$

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\rho_{ab} = \left[H^0_{ab}, \rho_{ab}\right] + [V_{ab}, \rho_{ab}] + \sum_c \mathrm{Tr}_3\{(V_{ac} + V_{bc}), \rho_{abc}\}. \tag{4}$$

It is our goal to determine the evolution of the species temperatures or the kinetic energies $\langle K_a(t)\rangle$. If Z_{ab} denotes the transfer rate of total energy between the subsystems 'a' and 'b', we have to find expressions of the form

$$\frac{\partial}{\partial t}\langle K_a(t)\rangle + \frac{\partial}{\partial t}\langle V_a(t)\rangle = \sum_b Z_{ab}. \tag{5}$$

To this end, we apply the equation of motion of the one-particle density operator (3) in the definition of the kinetic energy (2) and obtain by using the cyclical invariance of the trace

$$\begin{aligned}\frac{\partial}{\partial t}\langle K_a\rangle &= \frac{1}{\mathrm{i}\hbar}\mathrm{Tr}_1\{H_a[H_a, \rho_a]\} + \frac{1}{\mathrm{i}\hbar}\sum_b \mathrm{Tr}_{1,2}\{H_a[V_{ab}, \rho_{ab}]\} \\ &= \frac{1}{2\mathrm{i}\hbar}\sum_b \mathrm{Tr}_{1,2}\{(H_a + H_b)[V_{ab}, \rho_{ab}]\} + \mathrm{Tr}_{1,2}\{(H_a - H_b)[V_{ab}, \rho_{ab}]\}.\end{aligned} \tag{6}$$

[3] While the first definition is obvious, the second has to be further justified.

We will now show that the first term in the second line can be identified with the time derivative of the potential energy of species 'a' as defined by equation (2) and that the second term is the energy transfer rate Z_{ab}.

3. Identifying the potential energy contribution

Now we show that the first term in equation (6) can be identified with the negative time derivative of the potential energy of species 'a'. To this goal, we use the equation of motion for the two-particle density operator (4) and find

$$\begin{aligned}
\frac{1}{2\mathrm{i}\hbar}\sum_b \mathrm{Tr}_{1,2}\{(H_a+H_b)[V_{ab},\rho_{ab}]\} &= -\frac{1}{2\mathrm{i}\hbar}\sum_b \mathrm{Tr}_{1,2}\{V_{ab}[(H_a+H_b),\rho_{ab}]\}\\
&= +\frac{1}{2\mathrm{i}\hbar}\sum_b \mathrm{Tr}_{1,2}\{V_{ab}[V_{ab},\rho_{ab}]\} + \frac{1}{2\mathrm{i}\hbar}\sum_{b,c}\mathrm{Tr}_{1,2,3}\{V_{ab}[(V_{ac}+V_{bc}),\rho_{abc}]\}\\
&\quad -\frac{1}{2}\frac{\partial}{\partial t}\sum_b \mathrm{Tr}_{1,2}\{V_{ab}\rho_{ab}\} \equiv -\frac{\partial}{\partial t}\langle V_a\rangle. \qquad (7)
\end{aligned}$$

The first term in the second line vanishes due to the cyclical invariance of the trace and the second due to a combination of the trace properties and the summation over particle species 'b' and 'c'.

For classical systems, it is often convenient to relate the potential energy of the species 'a' to the time-dependent pair distribution function $g_{ab}(t)$:

$$\langle V_a(t)\rangle = \frac{1}{2}\sum_b n_a n_b \int \mathrm{d}\mathbf{r} V_{ab}[g_{ab}(r,t)-1]. \qquad (8)$$

Analytic expressions for the pair distribution exist only for weakly coupled plasmas [18]; otherwise, it has to be calculated numerically, e.g. by generalized integral equations.

4. Identifying the electron–ion energy transfer rate

Now the second term of equation (6) is transformed into a more convenient form. Obviously, the terms with $a=b$ vanish. For the further calculation, it is useful to separate the correlation part of the density operator, i.e.,

$$\rho_{ab} = \rho_a\rho_b + \rho_{ab}^{\mathrm{corr}} = \rho_a\rho_b + \mathrm{i}\hbar L_{ab}^{<}(t,t')|_{t=t'}, \qquad (9)$$

where $\mathrm{i}\hbar L_{ab}^{<}(t,t') = \langle \delta\varrho_b(2t')\delta\varrho_a(1t)\rangle$ is the density–density correlation function. Using the equation of motion for this correlation function and the commutation relations of the field operators, we obtain for homogeneous plasmas

$$\begin{aligned}
Z_{ab} &\equiv \frac{1}{2\mathrm{i}\hbar}\mathrm{Tr}_{1,2}\{(H_a(1)-H_b(2))[V_{ab},\rho_{ab}]\}\\
&= \frac{\mathrm{i}\hbar}{2}\mathrm{Tr}_{1,2}V_{ab}\left\{\left(\frac{\partial}{\partial t}-\frac{\partial}{\partial t'}\right)L_{ab}^{<}(t,t')\right\}\Bigg|_{t=t'}. \qquad (10)
\end{aligned}$$

Evaluating the trace in coordinate space and introducing the Fourier transform with respect to the relative coordinate r_1-r_2 and time difference $t-t'$, we finally obtain

$$Z_{ab}(t) = 2\mathcal{V}\,\mathrm{Im}\int\frac{\mathrm{d}^3q}{(2\pi\hbar)^3}\int_0^\infty\frac{\mathrm{d}\omega}{2\pi}\omega V_{ab}(q)\mathrm{i}\hbar L_{ab}^{<}(\mathbf{q};\omega,t). \qquad (11)$$

This is a very general form for the energy transfer rates.

There exist well-known approximation schemes for the density response function L_{ab} [17]. In the lowest order approximation, we have $L^<_{\mathrm{ei}} = \mathcal{L}^<_{\mathrm{e}} V_{\mathrm{ei}} \mathcal{L}^A_{\mathrm{i}} + \mathcal{L}^R_{\mathrm{e}} V_{\mathrm{ei}} \mathcal{L}^<_{\mathrm{i}}$. With the connection to the density of states given by $\mathrm{i}\hbar\mathcal{L}^<_a = \mathcal{A}_a(\omega, T_{\mathrm{i}}) n_{\mathrm{B}}(\omega/T_a)$ and $-2\,\mathrm{Im}\,\mathcal{L}^R_a(\omega, T_a) = \mathcal{A}_a(\omega, T_a)$, one obtains the well-known Fermi-golden-rule formula. The effects of coupled collective modes (see also [10]) can be described applying a more general approximation for $L^<_{ab}$ in equation (11).

Obviously, we have obtained the desired form (5) for the evolution of the species energies. It is demonstrated that a consistent description of equilibration in dense plasmas must include potential energy contributions in the form (2). Such a treatment should also be applied to tackle problems like the rapid build-up of correlations and screening in the beginning of the relaxation.

References

[1] Landau L D 1936 *Phys. Z. Sowjetunion* **10** 154
[2] Spitzer L 1956 *Physics of Fully Ionized Gases* (New York: Interscience)
[3] Hansen J-P and McDonald I R 1983 *Phys. Lett.* A **97** 42
[4] Reimann U and Toepffer C 1990 *Laser Part. Beams* **8** 771
[5] Hazak G, Zinamon Z, Rosenfeld Y and Dharma-wardana M W C 2001 *Phys. Rev.* E **64** 66411
[6] Gericke D O 2005 *J. Phys. (Conf. Section)* **11** 111
[7] Celliers P, Ng A, Xu G and Forsman A 1992 *Phys. Rev. Lett.* **68** 2305
[8] Ng A, Celliers P, Xu G and Forsman A 1995 *Phys. Rev.* E **52** 4299
[9] Riley D *et al* 2000 *Phys. Rev. Lett.* **84** 1704
[10] Dharma-wardana M W C and Perrot F 1998 *Phys. Rev.* E **58** 3705
Dharma-wardana M W C and Perrot F 1998 *Phys. Rev.* E **63** 69901
[11] Zhdanov V M 2002 *Transport Processes in Multicomponent Plasma* (London: Taylor and Francis)
[12] Gericke D O, Murillo M S and Schlanges M 2002 *Phys. Rev.* E **65** 036418
[13] Ohde Th, Bonitz M, Bornath Th, Kremp D and Schlanges M 1996 *Phys. Plasmas* **3** 1241
[14] Bornath Th, Schlanges M and Prenzel R 1998 *Phys. Plasmas* **5** 1485
[15] Grubert G K, Schlanges M, Bornath Th and Gericke D O 2005 *J. Phys. (Conf. Section)* **11** 124
[16] Gericke D O and Murillo M S 2004 *Proc. Int. Conf. on Inertial Fusion Science and Applications (Monterey)* ed B A Hammel, D D Meyerhofer, J Meyer-ter-Vehn and H Azechi (La Grange Park: American Nuclear Society) p 2002
[17] Kremp D, Schlanges M and Kraeft W-D 2005 *Quantum Statistics of Nonideal Plasmas* (Berlin: Springer)
[18] Cauble R and Rozmus W 1995 *Phys. Rev.* E **52** 2974