Collisional absorption in strong laser fields

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Abstract. Collisional absorption of dense fully ionized plasmas in strong high-frequency laser fields is investigated in the non-relativistic case. Quantum statistical methods are used as well as molecular dynamics simulations. In the quantum statistical expressions for the electrical current density and the electron-ion collision frequency – valid for arbitrary field strength – strong correlations are taken into account. In addition, molecular dynamic simulations were performed to calculate the heating of dense plasmas in laser fields. Comparisons with the analytic results for different plasma parameters are given. Isothermal plasmas as well as two–temperature plasmas are considered.

1. Introduction

An important question in almost all experiments with interaction of intense laser pulses with matter is the calculation of the energy deposition and the description of the heating connected with that. If a solid target is irradiated by such an intense laser pulse, dense plasmas can be created. One of the important mechanisms of energy deposition is inverse bremsstrahlung, i.e., laser light absorption via collisional processes between the plasma particles usually described in terms of the electron-ion collision frequency.

In several papers, various approaches were used to calculate the electron-ion collision frequency and the dynamic conductivity, respectively, for classical plasmas under different conditions [1, 2]. An essential further development of the theory has been given also by Klimontovich [3, 4]. Klimontovich used his powerful technique of second quantization in phase space to investigate density-density and microfield fluctuations in low- and in high-frequency fields. He was able to derive collision integrals for classical plasmas in strong fields which take into account dynamical screening and to derive a complete theory of transport processes [4, 5]. A result of central importance is an expression for the collisional heating rate and the electron-ion collision frequency in terms of the imaginary part of the dielectric function [4]. Rather recently, expressions of the same form were derived again [7].

Quantum mechanical treatments were given by several authors, e.g. [8, 9, 10, 11]. Rigorous quantum kinetic approaches, however, to the inverse bremsstrahlung absorption in dense plasmas were missing until recently. Kremp et al. [12, 13] derived a quantum kinetic equation for dense plasmas in strong laser fields using nonequilibrium Green's function techniques. In this approach, the different interaction processes can be taken into account by appropriate approximations of the generalized field-dependent scattering rates including nonlinear field effects such as

multiphoton processes and higher harmonics generation. Time-dependent phenomena were studied by numerical solution of this equation [14, 15] in statically screened Born approximation.

Quantum expressions for the collision term and the electron–ion collision frequency including dynamic screening were given in [16]. A quantum theory based on the dielectric approximation [17] lead to similar results.

Generalizations in order to study effects of strong electron–electron and ion–ion correlations on the collisional absorption rate were given in [18, 19] and in [20].

Simulations of inverse-bremstrahlung absorption were performed by Pfalzner and Gibbon [21] who used molecular dynamics enforcing a single temperature for electrons and ions. Heating rates were investigated also in a classical test particle approach [22].

In this paper we will describe collisional absorption within the analytical approach we developed recently. Results are given for the important case of a two-temperature plasma. Especially the influence of strong coupling effects on collisional absorption is discussed. Furthermore, we have performed molecular dynamics simulations. The simulation results agree qualitatively well with those from the analytical approach.

2. Collision frequency in dense laser plasmas

This is a short summary of the theory we developed elsewhere [16, 18, 19]. For the investigation of collisional absorption by the dense plasma, it is obvious to start from the balance equation for the energy and the electrical current resulting from a generalized non-Markovian kinetic equation. The energy balance reads

$$\frac{dW^{\rm kin}}{dt} - \mathbf{j} \cdot \mathbf{E} = \sum_{a,b} \int \frac{d^3k_a}{(2\pi\hbar)^3} \frac{k_a^2}{2m_a} I_{ab}(\mathbf{k}_a) \,. \tag{1}$$

It was shown that the r.h.s. of Eq. (1) with a non-Markovian collision integral gives just the contribution of the mean value of the potential energy [16]. Thus the energy balance (1) is given by

$$\frac{dW^{\rm kin}}{dt} + \frac{dW^{\rm pot}}{dt} = \mathbf{j} \cdot \mathbf{E} \,, \tag{2}$$

where the r.h.s. is in turn the energy loss of the electromagnetic field due to Poynting's theorem.

The electrical current density needed in the above equation follows from the general balance equation for the current density in the following form

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathbf{j}_{a}(t) - n_{a}\frac{e_{a}^{2}}{m_{a}}\mathbf{E}(t) = \sum_{b\neq a} \int \frac{\mathrm{d}^{3}q}{(2\pi\hbar)^{3}} \frac{e_{a}\mathbf{q}}{m_{a}} V_{ab}(q) L_{ab}^{<}(\mathbf{q};t,t)$$
(3)

where $i\hbar L_{ab}^{\leq}(t,t') = \langle \delta \rho_b(t') \delta \rho_a(t) \rangle$ denotes the correlation function of the density fluctuations which can be determined within nonequilibrium Green's functions methods.

In a plasma in a strong laser field, the coupling between species with different charges can be considered to be weak, whereas the coupling between particles with equal charges is not affected by the laser field. Therefore an approximation in lowest order of V_{ei} seems to be appropriate. The subsystems, however, may be strongly coupled.

We will assume in the following of this section that the subsystems are in local thermodynamic equilibrium with temperatures T_e and T_i , respectively. The dependence on the electric field can be made explicite. It has an exponential form and causes thus nonlinear effects like multi-photon absorption and the occurrence of higher harmonics in the current. For a harmonic electric field $\mathbf{E} = \mathbf{E}_0 \cos \omega t$ the exponential pre-factor can be expanded into a Fourier series. The current balance is given then by

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathbf{j}_{e}(t) - n_{e}\frac{e_{e}^{2}}{m_{e}}\mathbf{E}(t)
= \operatorname{Re} \int \frac{\mathrm{d}^{3}q}{(2\pi\hbar)^{3}} \frac{2\pi e_{e}\mathbf{q}}{m_{e}\hbar} V_{ei}^{2}(q) \sum_{m} \sum_{n} (-i)^{m+1} J_{n}\left(\frac{\mathbf{q}\cdot\mathbf{v}_{0}}{\hbar\omega}\right) J_{n-m}\left(\frac{\mathbf{q}\cdot\mathbf{v}_{0}}{\hbar\omega}\right) e^{im\omega t}
\times \int_{-\infty}^{\infty} \frac{\mathrm{d}\bar{\omega}}{2\pi} \left[\mathcal{S}_{ee}(\mathbf{q};\bar{\omega}-n\omega) \mathcal{L}_{ii}^{A}(\mathbf{q};\bar{\omega}) + \mathcal{L}_{ee}^{R}(\mathbf{q};\bar{\omega}-n\omega) \mathcal{S}_{ii}(\mathbf{q};\bar{\omega}) \right].$$
(4)

with the one-component structure factors and response functions S_{aa} and \mathcal{L}_{aa} , respectively [18, 19]. J_l is the Bessel function of *l*th order and $\mathbf{v}_0 = (e_e/m_e)\mathbf{E}_0/\omega$.

The ion dynamic structure factor S_{ii} and the response function \mathcal{L}_{ii} are localized in the lowfrequency region, i.e., for a high-frequency electric field, $\bar{\omega}$ can be neglected in comparison with $n\omega$. In this case, the first term in the brackets in Eq. (4) vanishes because $\int d\bar{\omega} \mathcal{L}_{ii}^A(\mathbf{q};\bar{\omega}) = 0$, and further the static structure factor $n_i S_{ii}(q) = \int d\bar{\omega} S_{ii}(\mathbf{q};\bar{\omega})$ can be introduced.

An important quantity is the cycle averaged dissipation of energy $\langle \mathbf{j} \cdot \mathbf{E} \rangle$ which is given by

$$\langle \mathbf{j} \cdot \mathbf{E} \rangle = n_i \int \frac{d^3 q}{(2\pi\hbar)^3} V_{ei}^2(q) \,\mathcal{S}_{ii}(\mathbf{q}) \,\sum_{n=-\infty}^{\infty} n\omega \,J_n^2\left(\frac{\mathbf{q} \cdot \mathbf{v}_0}{\hbar\omega}\right) \operatorname{Im} \mathcal{L}_{ee}^R(\mathbf{q};-n\omega) \,. \tag{5}$$

Often there is also the electron–ion collision frequency ν_{ei} discussed which is defined for the high-frequency case by (ω_p – plasma frequency)

$$\nu_{\rm ei} = \frac{\omega^2}{\omega_{\rm p}^2} \frac{\langle \mathbf{j} \cdot \mathbf{E} \rangle}{\langle \epsilon_0 \mathbf{E}^2 \rangle}.$$
 (6)

Equation (5) is a generalization of the theory developed in [16]. Approximating $S_{ii}(\mathbf{q}) \approx 1$ and using \mathcal{L}_{ee}^{R} in random phase approximation (RPA), one gets the results of Sec. IV in that former paper. Now there is included the static stucture factor of the ion component. Further the function \mathcal{L}_{ee}^{R} is the exact density response function of the electron subsystem, i.e., the electronelectron interaction can be included on a very high level. Appropriate approximations can be expressed via local field corrections (LFC), see e.g. [23, 24].

With equations (5) and (6), we are able to describe the collisional absorption for the important case of a two-temperature plasma. The influence of the ion component with temperature T_i is accounted for by the static ionic structure factor. Calculations [25] show a considerable influence of structure factor effects on collisional absorption especially for the case $T_i < T_e$. For high electron temperatures and $T_i \ll T_e$, the inclusion of the ion structur factor can reduce the collision frequency by about 25%.

For strong fields the electron-electron collisions are not efficient enough to establish a Maxwellian distribution [26]. This behaviour can be described by a so-called super-Maxwellian distribution [27]. Below we will present also results of calculations [28] with such a distribution function instead of a Maxwellian.

3. Molecular dynamics simulations

In an alternative approach we calculated the energy absorption with molecular dynamics simulations. The main difficulty in order to simulate a fully ionized plasma is to model the attractive electron–ion interaction: the pure Coulomb–potential has a singularity at the origin which causes a non-physical behaviour of the system. To avoid this divergence and to include quantum effects, we used the Kelbg-potential [29] which is given by

$$\Phi_{ij} = \frac{q_i q_j}{4\pi\epsilon_0 r} \left\{ 1 - \exp(-r^2/\lambda_{ij}^2) + \sqrt{\pi}r/\lambda_{ij} [1 - \operatorname{erf}(r/\lambda_{ij})] \right\}.$$
(7)

This potential has a finite value at the origin, and it is temperature dependent via the thermal wavelength $\lambda_{ij} = \hbar/\sqrt{2\mu_{ij}k_BT}$, where $\mu_{ij} = m_i m_j/(m_i + m_j)$ denotes the reduced mass of two particles of species *i* and *j*.

The external electric field was implemented as a homogeneous linearly polarized harmonic field. The temperature of the species a was defined as $\frac{3}{2}k_BT_a = E_{\text{therm}} = m_a(\langle v_a^2 \rangle - \langle v_a \rangle^2)/2$, where the angles denote an averaging over all particles of species a. This definition takes into account the undirected motion only. The MD-calculations were performed using periodic boundary conditions with Ewald summation. The number of particles was between 2000 and 5000.

At the beginning of the simulation, the electrons and ions have the same mean kinetic energy. The first stage of the simulation is the so-called establishment of correlations [12]. Due to the mass ratio of electrons and ions, the system can not relax to an equilibrium state in the following femtosecond, and a two-temperature plasma is produced. In order to have a defined equilibrium state, the system is thermalized by rescaling the velocities of the particles. The rescaling corresponds to a coupling to an external heat bath. Then the laser is switched on. The electrons move nearly collective in a directed motion driven by the external field. Due to collisions with ions, however, a fraction of the gained directed kinetic energy dissipates into random directions and the electrons are heated. The transfer of energy to ions is quite small, thus their temperature remains nearly constant and again a two-temperature plasma is formed.

The further development of the system is shown in figure 1 where the thermal energy of the electrons is plotted. The raw data (solid) show a steady increase of the temperature. The change

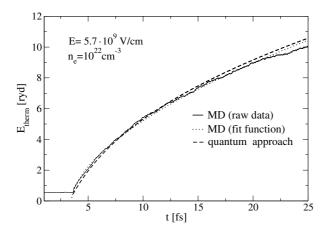


Figure 1. Time dependence of the thermal energy of the electrons in a hydrogen plasma under the influence of a strong laser field. Laser frequency: $\omega/\omega_p = 3$.

of thermal energy is associated with the electron–ion collision frequency for the high–frequency case via

$$\nu_{ei}(\omega) = \frac{\omega^2}{\omega_p^2} \frac{2}{\epsilon_0 E_0^2} \frac{\mathrm{d}E_{\mathrm{therm}}}{\mathrm{d}t} \,. \tag{8}$$

Thus the determination of heating rates and collision frequencies, respectively, from the simulation data requires the time derivative of the thermal energy. A fit of the form $E_{\text{therm}} =$

 $A(t-C)^B$ was used to get a smooth function for the thermal energy (dotted line in figure 1). Keeping in mind $E_{\text{therm}} \equiv 3/2k_BT_e$, one can extract now the collision frequency as a function of the electron temperature. Figure 1 shows that, for a constant field strength, the energy-input decreases in the region of high temperatures. For comparison, results from the kinetic approach are shown (dashed line). The agreement with the quantum kinetic approach which was obtained by time-integration of Eq. 8 is very good in this example. Larger deviations occur for higher coupling parameters.

In figure 2, the collision frequency normalized to the plasma frequency is plotted as a function of the coupling parameter $\Gamma = Ze^2(4\pi n/3)^{1/3}/(k_BT_e)$. The solid and dotted lines are results obtained from Eqs. (5) and (6). The solid line denotes the isothermal case with $T_i = T_e$, whereas the dotted line is the result for a two-temperature plasma with an ion temperature of 1000K.

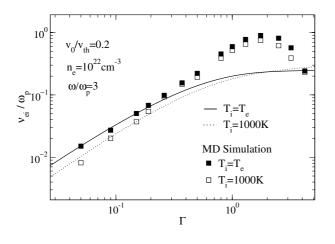


Figure 2. Electron-ion collision frequency as a function of the coupling parameter Γ for a hydrogen plasma in a laser field. Quantum statistical approach: — isothermal plasma $(T_i = T_e), \dots$ two-temperature plasma with $T_i = 1000$ K. The corresponding simulation data are denoted by \blacksquare and \Box , respectively.

The open squares are the corresponding simulation data for the two-temperature plasma. In addition, simulations were performed in which the temperature of the ions – by a rescaling of the ion's velocities at every time step – was forced to be the same as that of the electrons (filled squares). The simulation data as well as the analytic calculation show an increase of the collision frequency with increasing coupling. The agreement between the simulation and the quantum statistical results is quite good in the region of weak and moderate coupling (about $\Gamma = 0.3$). An important result is the lowering of the collision frequency for a two-temperature plasma with cold ions which is well confirmed by the MD-simulations. Physically this behaviour can be interpreted as follows: the cold ions are correlated, electrons do not interact with a single ion but with a (static) distribution of charges which contributes to screening.

In the region of higher coupling, $\Gamma > 0.3$, the deviations between the simulation and the analytic calculations are growing. One has to keep in mind that the analytic approach adopts weak coupling with respect to the electron-ion interaction. On the other hand, the effective potential used in the molecular dynamics has been derived for weak coupling with respect to quantum effects [29] what may lead to limitations of the range of applicability.

Figure 3 shows the energy absorption rate of a hydrogen plasma for different laser frequencies. Simulation results are compared with those of the analytic approach for an isothermal and a two-temperature plasma, respectively. Again, the simulations confirm the lowering of the absorption rate for a two-temperature plasma with cold ions. The heating rate depends strongly on the frequency. With increasing frequency the rate decreases very fast. For rather high frequencies, the agreement between the simulations and the analytic results is quite good. In the low-

frequency regime the deviations are bigger which is due to the limitation of the analytic approach to high frequencies whereas the MD simulations have no restriction regarding the frequency.

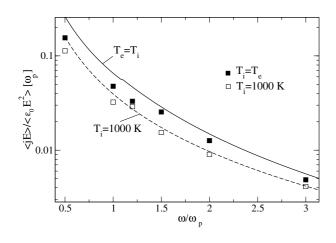


Figure 3. Energy absorption rate as a function of the laser frequency for a hydrogen plasma in the laser field for $\Gamma = 0.15, v_0/v_{\text{th}} =$ $0.2, n_e = 10^{22} \text{ cm}^{-3}$. Analytic results: — isothermal plasma, … twotemperature plasma with $T_i = 1000$ K. Corresponding simulation data are denoted by \blacksquare and \Box , respectively.

So far, results were presented for rather small field strength. The analytic model has – beside the restriction to the nonrelativistic case – no limitation on the strength of the field.

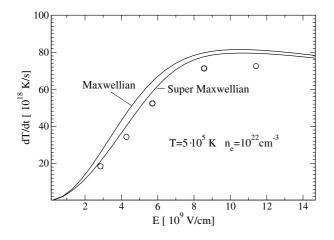


Figure 4. Heating rate of the electrons in a two-temperature hydrogen plasma ($T_i = 1000$ K) as a function of the field strength. The solid lines denote the analytic results for two different assumptions for the velocity distribution functions. The circles are MD–results.

Figure 4 shows simulation data of the heating of the electrons as a function of the applied field strength. These data are compared with results from the analytic approach for the corresponding two-temperature plasma where the ion temperature was 1000 K. For small field strengths, the heating rate is proportional to E_0^2 . For higher fields the well-known v_0^{-3} behaviour in the collision frequency [2] leads to a saturation and even a decrease of the heating rate. Calculations were performed with different assumptions for the velocity distribution function: we considered Maxwellian as well as super–Maxwellian distribution functions. There is a better agreement with the simulation data in the case of the super–Maxwellian indicating that the velocity distribution of the electrons does not remain Maxwellian under the influence of a laser field, c.f. the so-called Langdon effect [26].

In order to investigate this issue more in detail, the velocity distribution function was determined from simulations for different field strengths. Figure 5 shows the velocity distribution

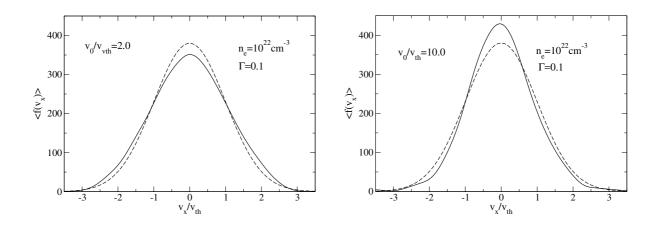


Figure 5. Velocity distribution function of the electrons (in field direction) under the influence of an intense laser field. The solid line denotes the simulation data for a field strength of E = 5.7 GV/cm (left figure) and E = 28.5 GV/cm (right figure), respectively. For comparison the Maxwell distribution (dashed) is plotted. The little asymmetry in the curves is a numerical artefact.

in the direction of the strong linearly polarized laser field for a weakly coupled hydrogen plasma. For a field strength of 5.7 GV/cm ($v_0/v_{\rm th} = 2$), one can see that the field leads to a broadening of the distribution function in comparison to the respective Maxwellian distribution function. This is in accordance with results of Pfalzner and Gibbon [21] who considered distribution functions for field strengths up to $v_0/v_{th} = 1$. If the field strength increases further, a different behaviour occurs which is in contrast to the Langdon effect. For a much higher field strength, 28.5 GV/cm ($v_0/v_{\rm th} = 10$), it can be observed that the distribution function is narrowed. It was proven that this narrowing is due to electron–ion collisions, however, there is no simple interpretation for this new effect.

Acknowledgments

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