Energy relaxation in dense two-temperature plasmas

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SFB 652: Strong Correlations and Collective Effects in Radiation Fields:

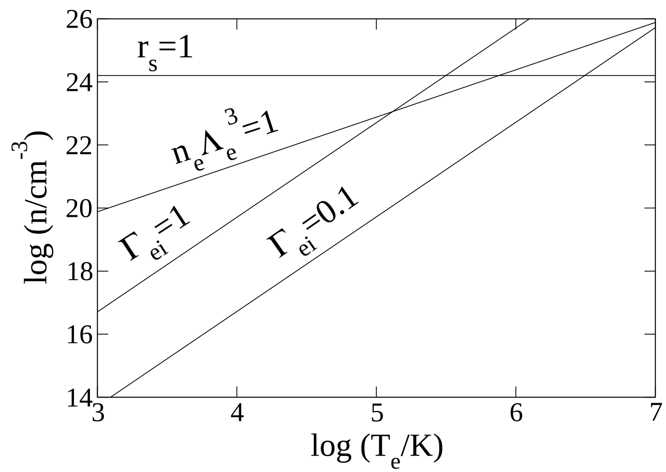
Coulomb Systems, Clusters and Particles

Outline

- Introduction
- Energy balance equation, energy transfer rate
- Two-temperature plasmas, internal energies
- Temperature relaxation, discussion of different models
- Conclusion

Introduction

High energy density matter produced by intense laser or ion beams
$\longrightarrow$ dense plasmas in nonequilibrium states with correlation and quantum effects



Characteristic parameters

$\Gamma_{ei}{=}e^2 Z_i/dk_B T_e, \quad d{=}(\frac{4}{3\pi}n)^{-1/3}$

$r_s{=}d/a_B$

$\Lambda_e{=}(2\pi\hbar^2/m_e k_B T_e)^{1/2}$

Important process : Energy relaxation

Standard approach

$$\frac{dT_e}{dt} = (T_i - T_e)/\tau_{ei}^{LS}$$

$$\tau_{ei}^{LS} = \frac{3m_e m_i}{8\sqrt{2\pi}n_i Z_i^2 e^4 \ln\Lambda}\left(\frac{k_B T_e}{m_e} + \frac{k_B T_i}{m_i}\right)^{3/2}$$

Problems:

- Correlation and quantum effects in the energy transfer rates
- Kinetic and potential energy contributions in the balance equations

The energy balance equation

Mean kinetic and the mean potential energy of species "a"

$$\begin{aligned} \langle K_a(t)\rangle &= \mathrm{Tr}_1\{H_a \rho_a(t)\} \\ \langle V_a(t)\rangle &= \frac{1}{2}\sum_b \mathrm{Tr}_{1,2}\{V_{ab}\,\rho_{ab}(t)\}. \end{aligned}$$

Reduced density operators are determined by the quantum BBGKY hierarchy

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\rho_a &= [H_a, \rho_a] + \sum_b \mathrm{Tr}_2[V_{ab}, \rho_{ab}]\,, \\ i\hbar\frac{\partial}{\partial t}\rho_{ab} &= [H_{ab}, \rho_{ab}] + \sum_c \mathrm{Tr}_3[(V_{ac} + V_{bc}), \rho_{abc}]\,. \end{aligned}$$

Balance equation for mean energy

$$\frac{\partial}{\partial t}\langle K_a\rangle + \frac{\partial}{\partial t}\langle V_a\rangle = \sum_b Z_{ab}\,,$$

with the energy transfer rate Z_{ab} between species "a" and "b" ($Z_{ab} = -Z_{ba}$)

$$Z_{ab} = \frac{1}{2}\mathrm{Tr}_{1,2}\frac{1}{i\hbar}\{(H_a - H_b)[V_{ab}, \rho_{ab}]\}\,,$$

The energy transfer rate

$$Z_{ab} = \frac{1}{2}\mathrm{Tr}_{1,2}\,\frac{1}{i\hbar}\{(H_a - H_b)[V_{ab}, \rho_a\rho_b + \rho_{ab}^{\mathrm{corr}}]\}\,.$$

It is useful to apply the following relation $(b \neq a)$

$$\langle 12|\rho_{ab}^{\mathrm{corr}}(t)|2'1'\rangle = i\hbar L_{ab}^{<}(11't, 22't')\Big|_{t=t'}\,,$$

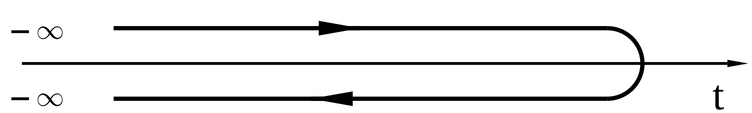
with $i\hbar L_{ab}^{<}(11't,22't') = \langle \delta\hat{\rho}_b(22',t')\,\delta\hat{\rho}_a(11',t)\rangle \qquad \delta\hat{\rho}_a = \psi_a^\dagger\psi_a - \langle\psi_a^\dagger\psi_a\rangle\,.$

For spatially homogeneous systems then follows that

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

$L_{ab}^{<}$ can be obtained within real-time Green's functions
equation for L_{ab} defined on the Keldysh time contour

$$L_{ab}(t_1,t_2) = \Pi_{ab}(t_1,t_2) + \sum_{c,d}\int_C d\bar{t}\,\Pi_{ac}(t_1,\bar{t})\,V_{cd}\,L_{db}(\bar{t},t_2)\,.$$



The energy transfer rate

Two-component plasma: electron (n_e) and ions (n_i, Z_i); approximation: $\Pi_{ab} = \Pi_a \delta_{ab}$

$$L^<_{ei}(\mathbf{q};\omega,t) \quad = \quad \frac{\mathcal{P}^<_{ei}(\mathbf{q};\omega,t)}{\left|1 - \mathcal{L}^R_e(\mathbf{q};\omega,t)\, V_{ei}(q)\, \mathcal{L}^R_i(\mathbf{q};\omega,t) V_{ie}(q)\right|^2}\,,$$

where $\mathcal{P}^<_{ei} = \mathcal{L}^<_e\, V_{ei}\, \mathcal{L}^A_i + \mathcal{L}^R_e\, V_{ei}\, \mathcal{L}^<_i$ and $\mathcal{L}^R_a = \Pi^R_a + \Pi^R_a V_{aa} \mathcal{L}^R_a$.

energy transfer rate for two-temperature plasma, T_e and T_i,
(*Dharma-wardana, Perrot (1998), Vorberger et al. (2009)*)

$$\begin{aligned} Z_{ei}(t) \quad &= \quad -4\mathcal{V} \int \frac{d^3q}{(2\pi\hbar)^3} \int_0^\infty \frac{d\omega}{2\pi}\, \hbar\omega\, [V_{ei}(q)]^2 \\ &\times \quad \frac{\mathrm{Im}\mathcal{L}^R_e(\mathbf{q};\omega,t)\, \mathrm{Im}\mathcal{L}^R_i(\mathbf{q};\omega,t) \Big[n_B(\omega/T_e) - n_B(\omega/T_i)\Big]}{\left|1 - \mathcal{L}^R_e(\mathbf{q};\omega,t)\, V_{ei}(q)\, \mathcal{L}^R_i(\mathbf{q};\omega,t) V_{ie}(q)\right|^2}\,. \end{aligned}$$

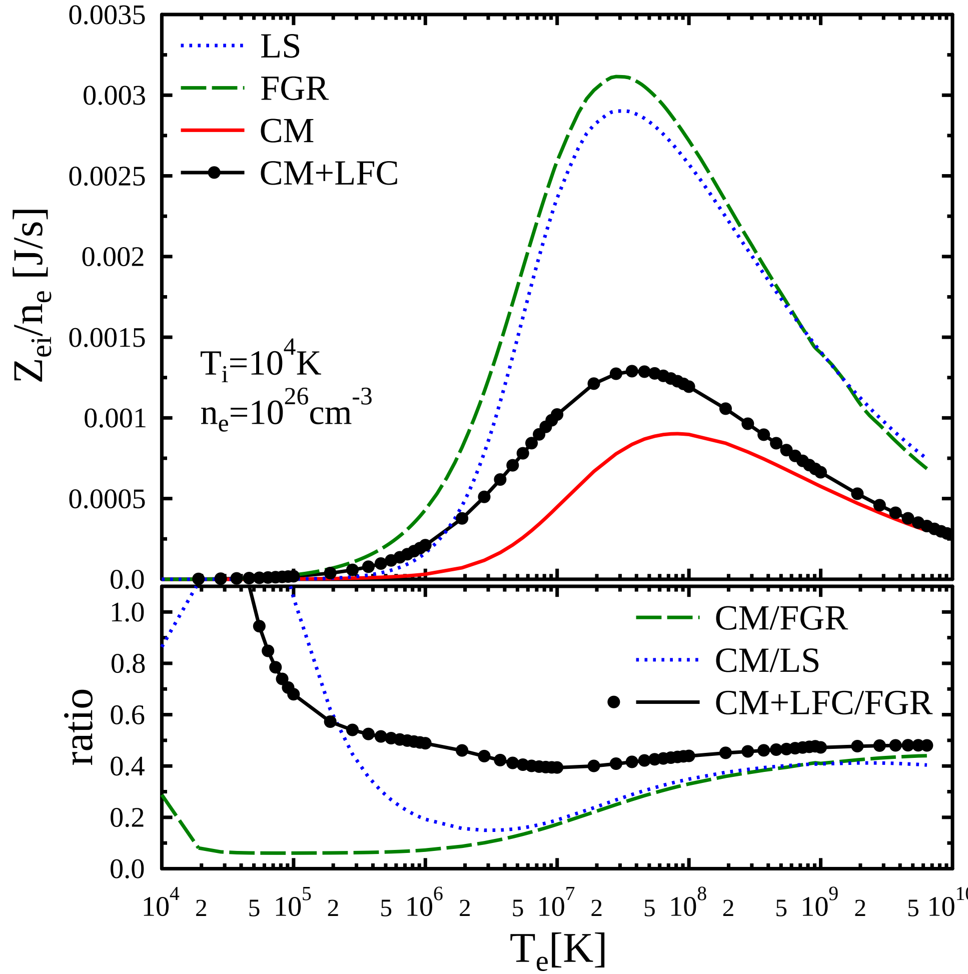
Denominator: coupling of electronic and ionic modes,

Correlation effects in the subsystems via local field corrections (LFC)

$$\mathcal{L}^R_a(\mathbf{q};\omega,t) = \frac{\Pi^0_a(\mathbf{q};\omega,t)}{1 - V_{aa}(q)\,[1 - G_a(\mathbf{q},t)]\, \Pi^0_a(\mathbf{q};\omega,t)}\,.$$

Different approximations: Fermi Golden Rule (FGR), Coupled modes (CM), CM+LFC

Results for the energy transfer rates



Energy transfer rates for hydrogen in different approximations: Landau-Spitzer (LS), Fermi Golden Rule (FGR), Coupled Mode (CM), and Coupled Mode including ionic local field corrections (CM+LFC)

Two-temperature relaxation, internal energies

Mean total energy of species "a"

$$\langle K_a \rangle + \langle V_a \rangle = U_a(T_e, T_i)$$

Coupled set of From the energy balance equations leads to

$$\frac{dT_e}{dt} = Z_{ei}(T_e, T_i) \frac{\frac{\partial U_e}{\partial T_i} + \frac{\partial U_i}{\partial T_i}}{\frac{\partial U_e}{\partial T_e}\frac{\partial U_i}{\partial T_i} - \frac{\partial U_e}{\partial T_i}\frac{\partial U_i}{\partial T_e}}$$

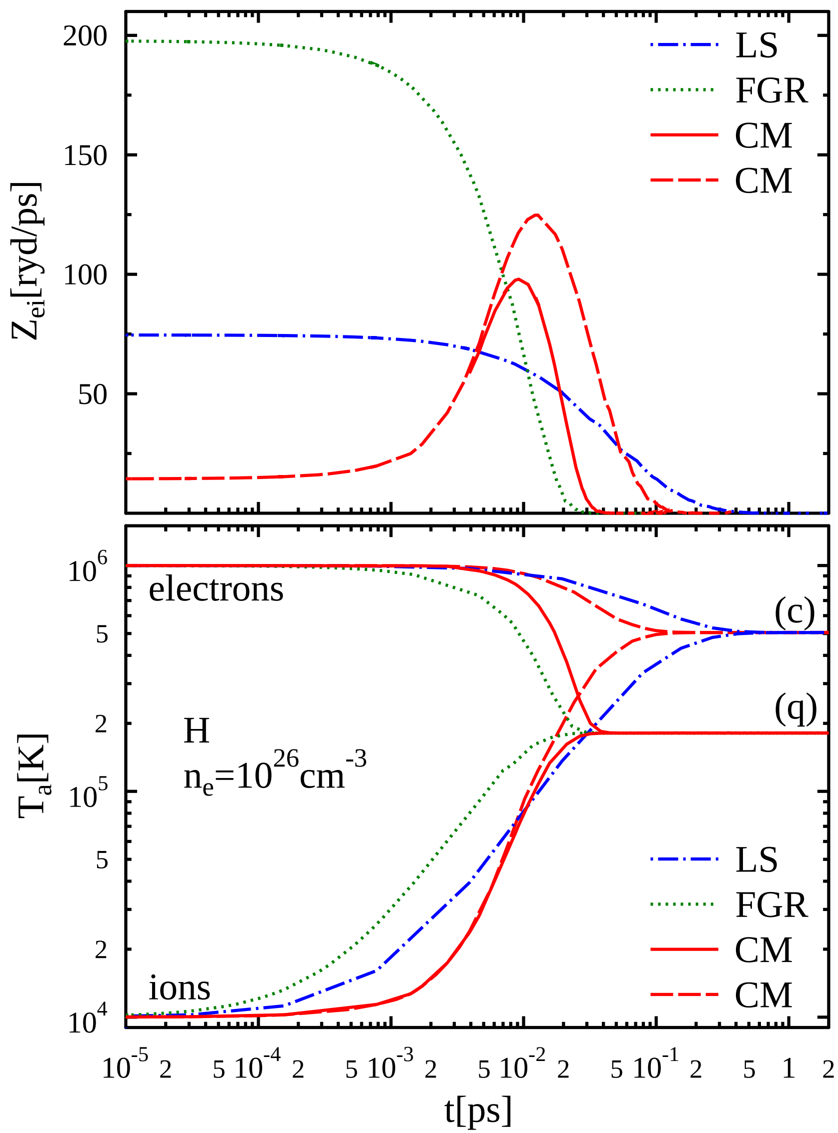
Internal energies of the dense quantum plasma

$$\begin{aligned} U_e &= U_e^{id} + U_e^{HF} + U_e^{MW} + U_e^{e^4}, \qquad U_e^{id} = \frac{3k_B T_e}{\Lambda_e^3} I_{3/2}(\mu_e/k_B T_e) \\ U_i &= \frac{3}{2} n_i k_B T_i + U_i^{corr} \\ U_i^{corr} &= \frac{n_i^2}{2} \int_0^\infty d^3r \left[g_{ii}(r, n_i, T_e, T_i) - 1 \right] \phi_{ii}(r, n_e, T_e) \,. \end{aligned}$$

Effective one-component model $\phi_{ii}(r, n_e, T_e) = \frac{Z_i^2 e^2}{r} e^{-\kappa_e(n_e, T_e) r}$

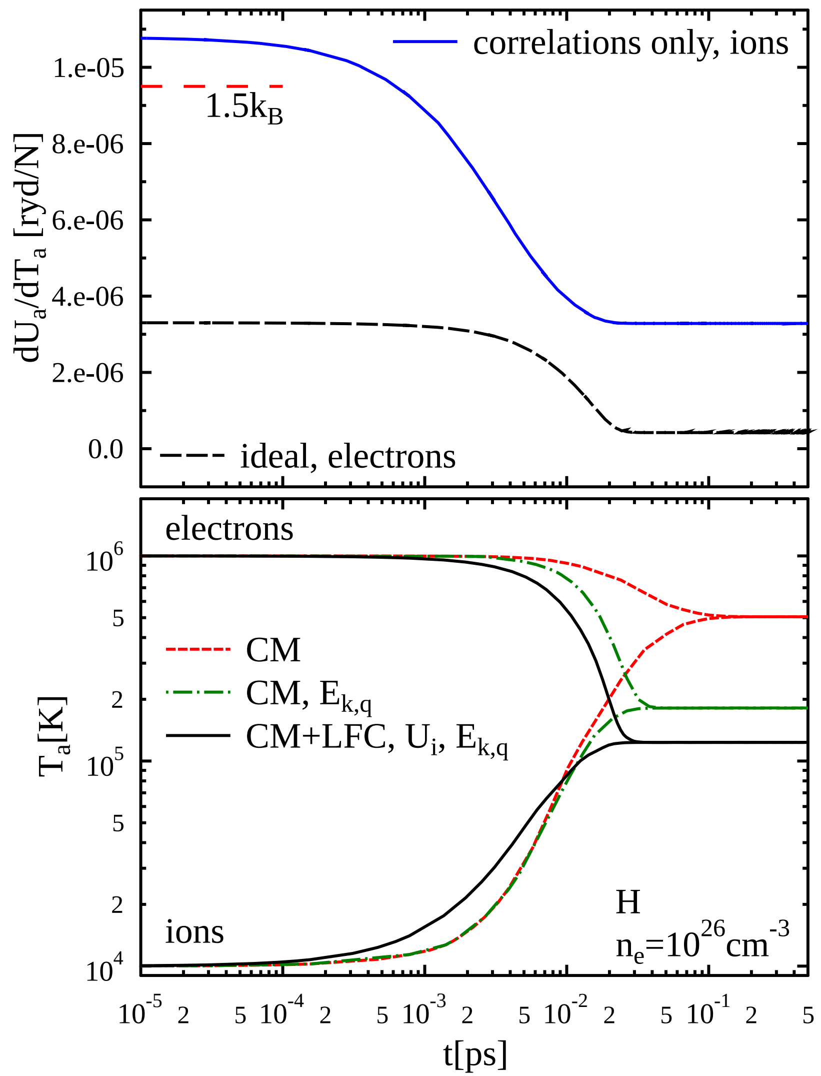
with $\kappa_e^2 = (4e^2 m_e/\pi\hbar^3) \int_0^\infty dp f_e(p, T_e)$

Two-temperature relaxation in dense hydrogen



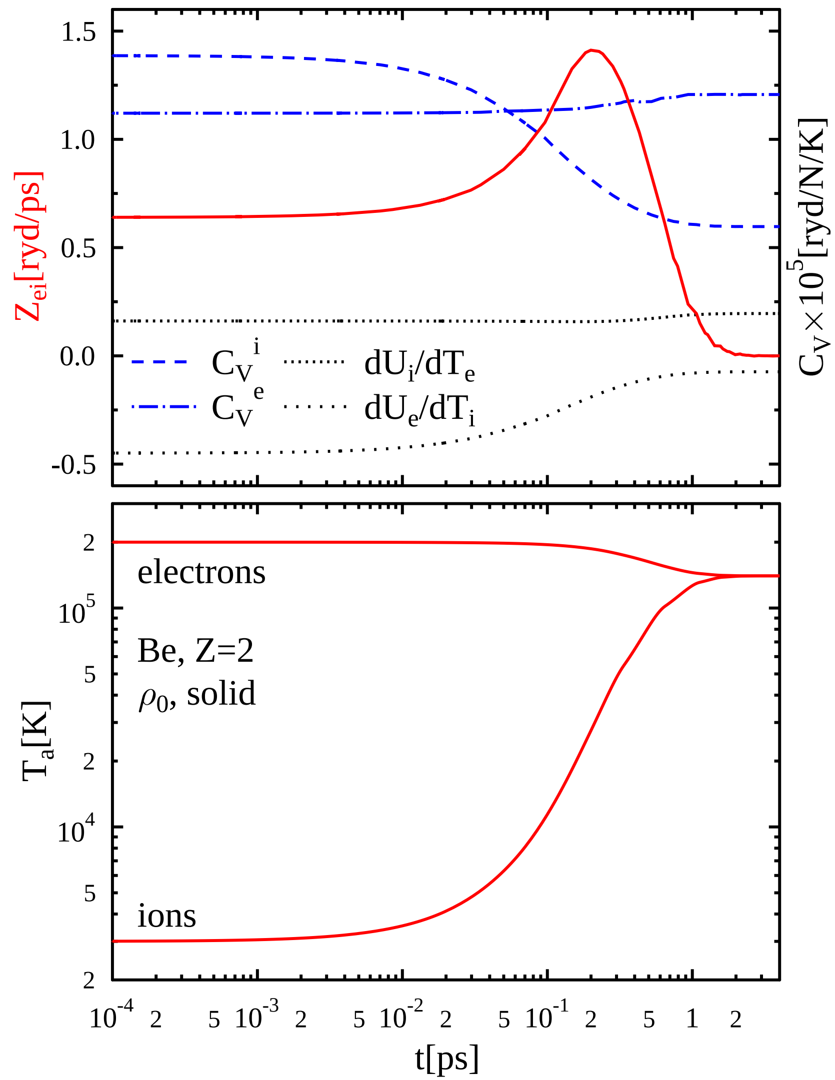
Temperature relaxation in a laser produced ideal hydrogen plasma. The heat capacities are taken for the ideal gas, in classical approximation (c) or for the quantum case (q).

Two-temperature relaxation in dense hydrogen



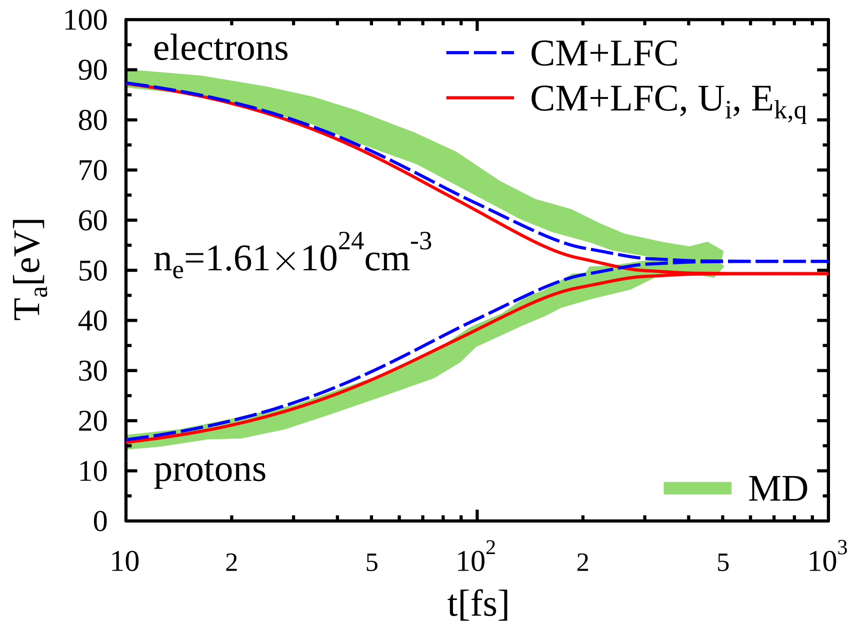
Temperature relaxation in a nonideal hydrogen plasma: Contributions to the heat capacities (upper panel), temperature evolution subject to different transfer rates and nonideal contributions to the heat capacities (lower panel).

Relaxation in a laser produced beryllium plasma



Temperature relaxation in a dense laser produced solid state density beryllium plasma as considered experimentally by Glenzer et al. PRL 98 (2007).

Comparison with Molecular Dynamics Simulations

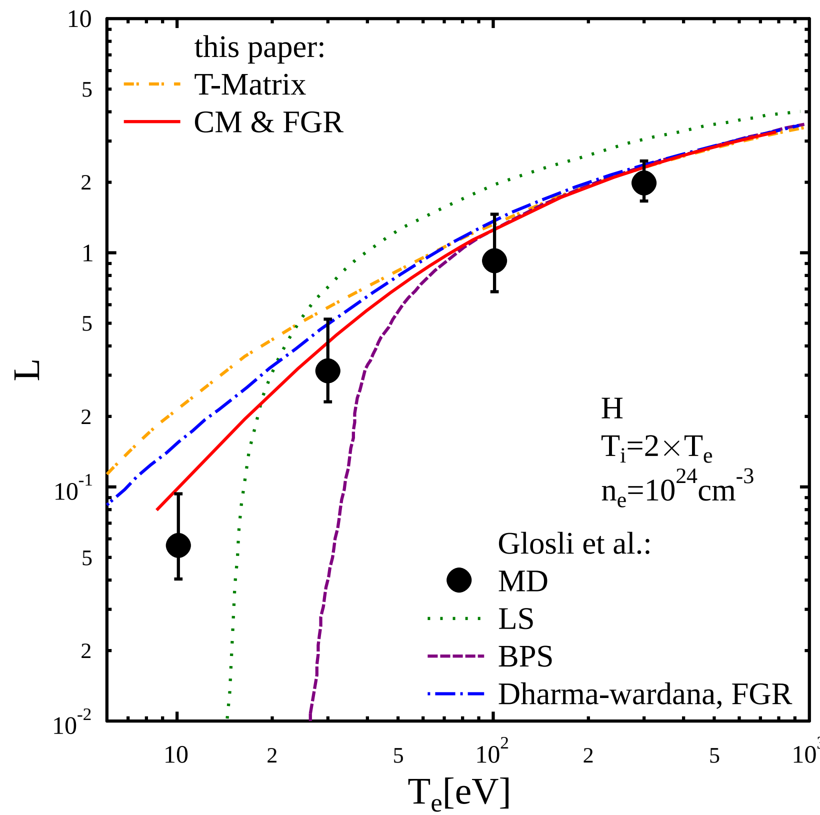


Temperature relaxation for a dense nonideal hydrogen plasma. A comparison is given between our results and the results from MD simulations obtained by Glosli et al, PRE (2008).

Summary

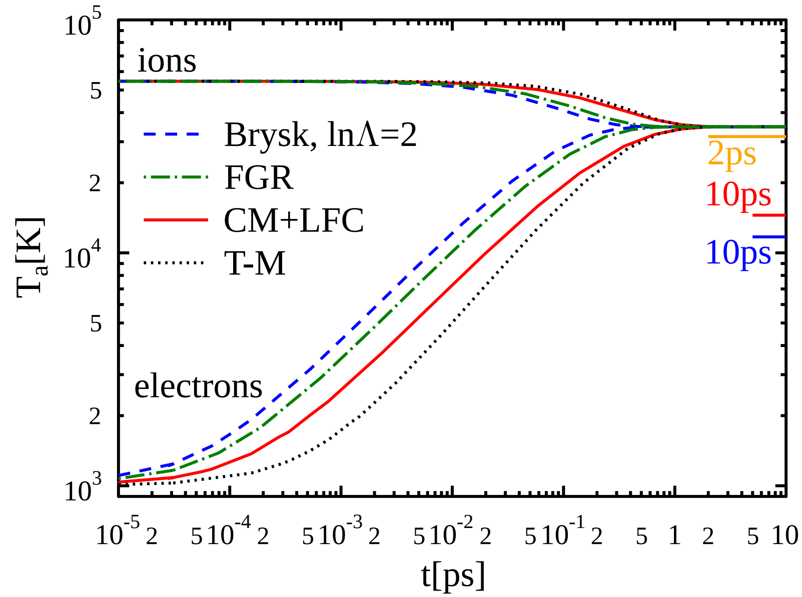
- Derivation of balance equations for the energy relaxation.
- Potential energy contributions due to correlations between the particles.
- Included correlations in the heat capacity of the ion subsystem (integral equation methods).
- Quantum statistical perturbation approach to the internal energy for the electrons.
- In cases with dominant electron degeneracy, relaxation times are significantly shorter than for an ideal case.
- Ion correlations tend to increase relaxation times but their main influence is the change of final temperature.
- Comparisons with recent classical MD simulations show reasonable agreement.
- Did not find extremely large relaxation times.
- T-Matrix effects have however to be included additionally.

Comparison with Molecular Dynamics Simulations



Comparison of energy transfer rates for dense nonideal hydrogen with results obtained from MD simulations by Glosli et al, PRE (2008) and with results from some analytical theories.

Relaxation in a shock produced silicon plasma



Temperature relaxation in a dense shock produced silicon with Z=4 and $n_e = 5.36 \times 10^{23} cm^{-3}$ as considered experimentally by Ng et al., PRE (1995). The line and times at the right axis indicate the final temperatures and relaxation times in special approximations.