

# Transport and Optical Properties in Dense Plasmas



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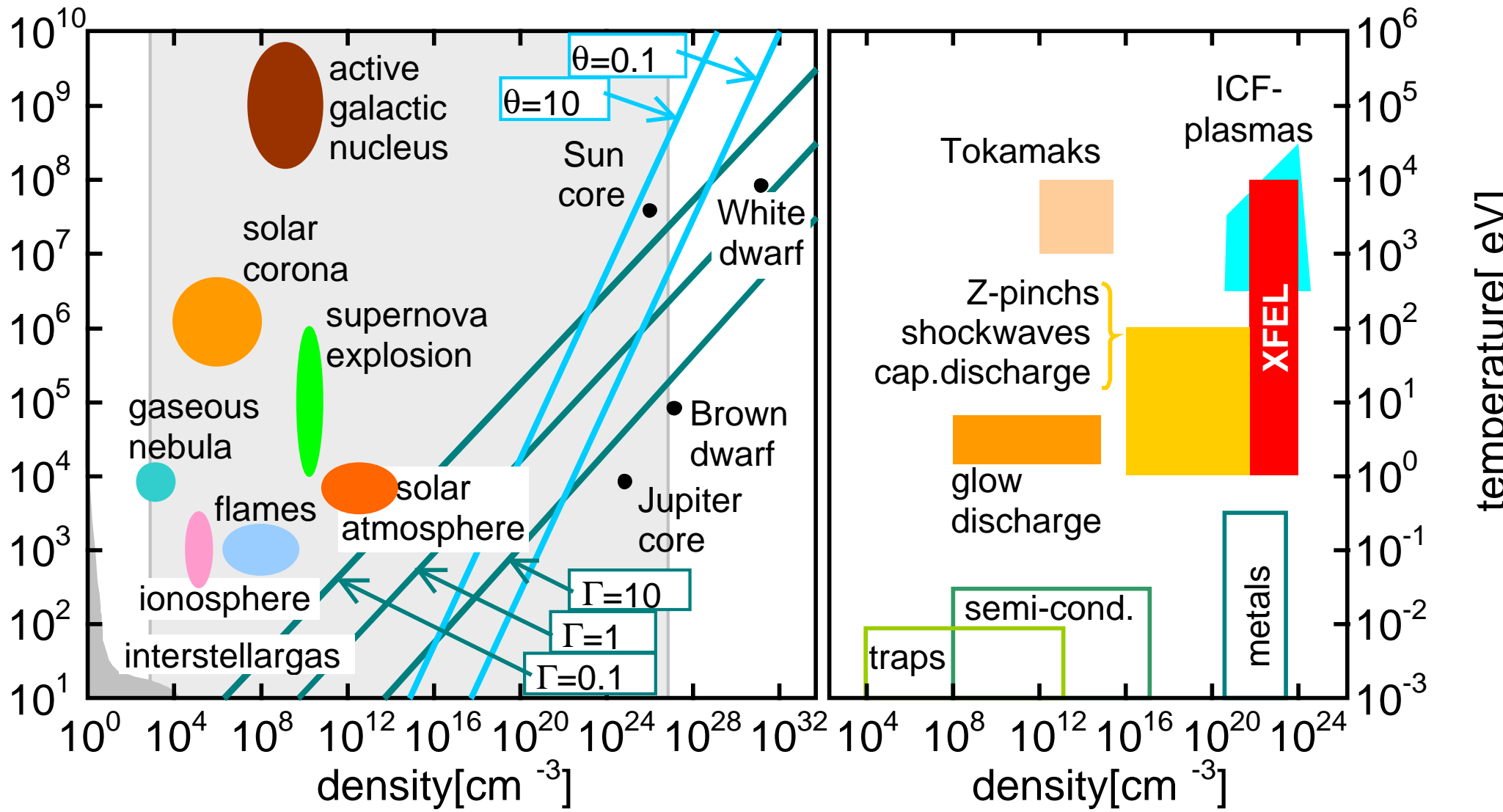
Dense Matter In Heavy Ion Collisions and Astrophysics

21.8.-1.9.2006, JINR, Dubna/Russia

# Outline

- Plasma in **electric** and **magnetic** fields, interaction with **radiation**  
⇒ production, excitation, **diagnostic tool**
- Many-particle theory
  - kinetic equations, linear response, molecular dynamics simulations  
⇒ dielectric function  $\epsilon(k, \omega)$ , dynamical **collision frequency**  $\nu(\omega)$
- Applications
  - ⇒ transport properties  
(**dc-conductivity**, thermopower, **Hall effect**)
  - ⇒ optical properties  
(dynamical conductivity, **reflectivity**, absorption,  
**Thomson scattering**, bremsstrahlung, spectral lines)

# Density-temperature regions



A. Höll, PhD thesis (Rostock, 2002)

# Electrical Conductivity $\sigma(\omega)$

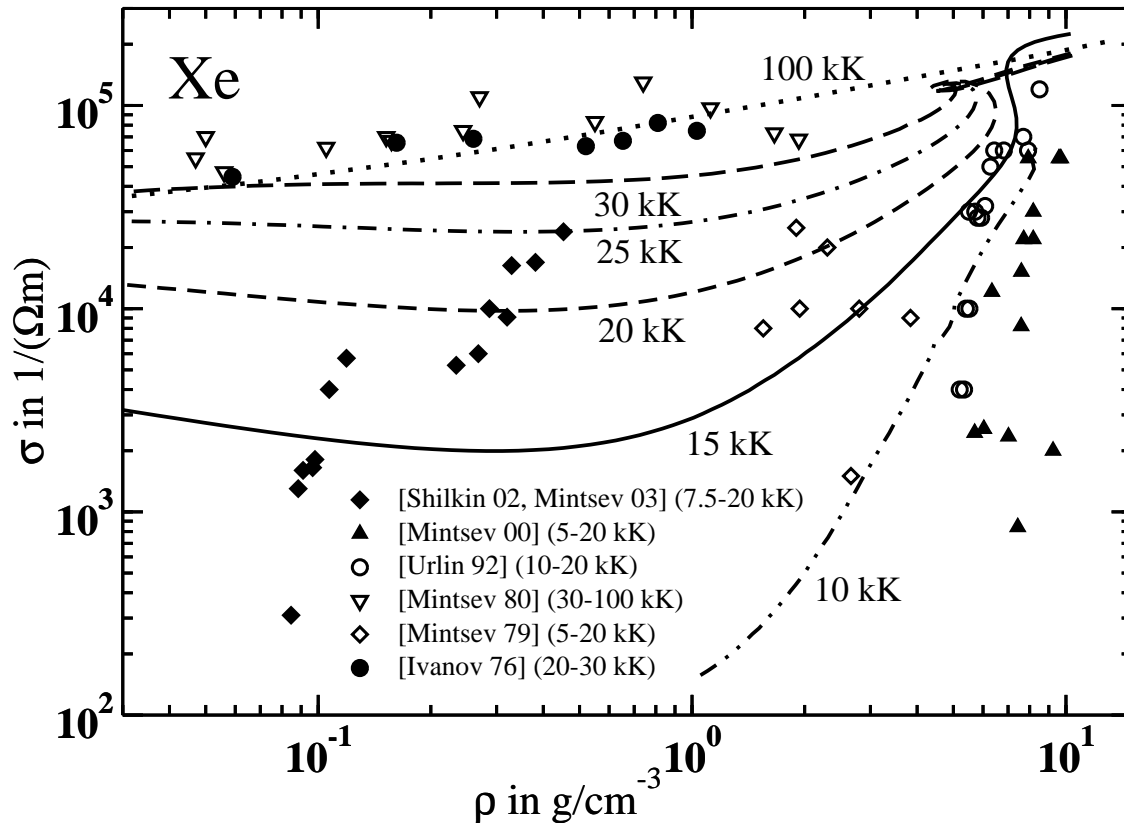
induced charge current density  $\vec{J}$  in many-particle system under the influence of electric field  $\vec{E}$

$$\vec{J} = \sigma \vec{E}$$

# Electrical Conductivity $\sigma(\omega)$

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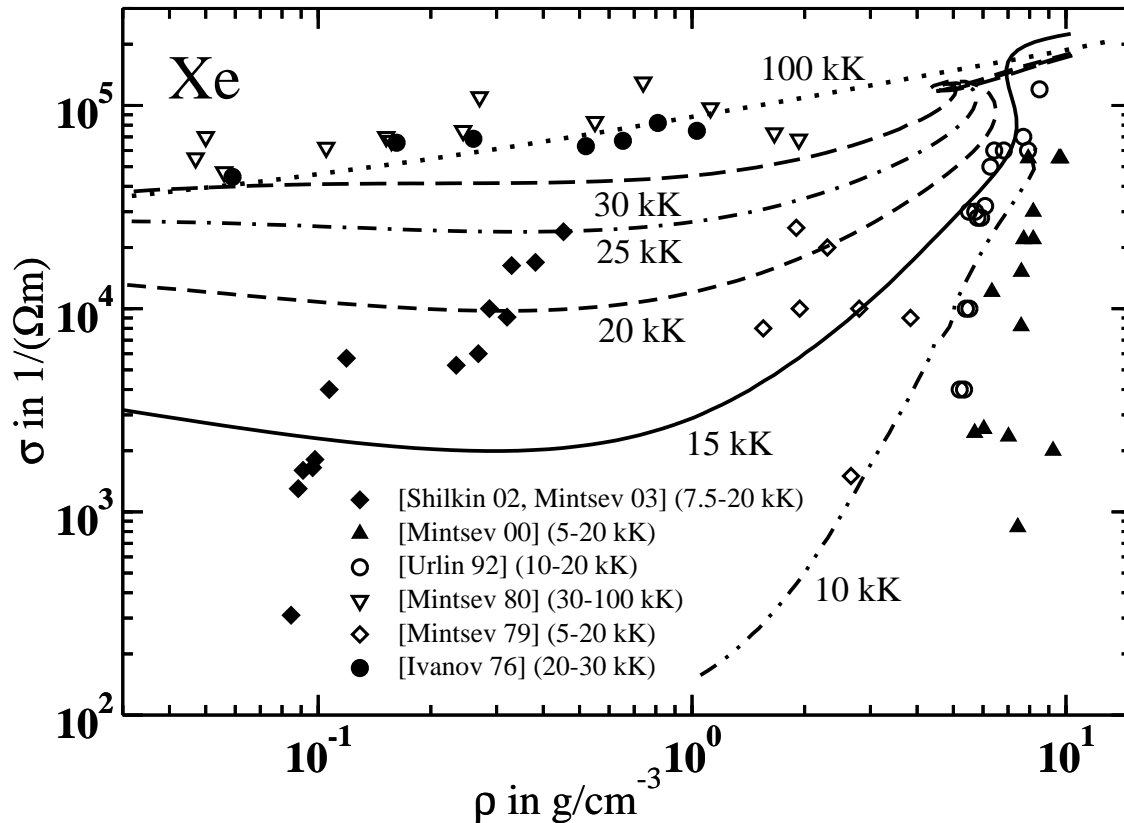
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# Electrical Conductivity $\sigma(\omega)$

induced charge current density  $\vec{J}$  in many-particle system under the influence of electric field  $\vec{E}$

$$\vec{J} = \sigma \vec{E} = \boxed{\text{Tr} \left\{ \hat{j} \hat{\rho} \right\}}$$



statistical operator  $\hat{\rho}$

current operator

$$\hat{j} = \frac{1}{\Omega} \sum_c \frac{e_c}{m_c} \hat{P}_c$$

# Linear response theory

- statistical operator for generalized grand canonical ensemble by introducing set of relevant observables  $\{B_n\}$

$$\rho_{\text{rel}} = \frac{1}{Z_{\text{rel}}} e^{-[\hat{\mathcal{H}} - \mu N + \sum_n \Phi_n B_n]} \quad \hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{eq}} - \sum_c e_c \vec{R}_c \vec{E}$$

- self-consistency condition for response parameter  $\Phi_n$

$$\boxed{\text{Tr}(B_n \rho_{\text{rel}}) = \text{Tr}(B_n \rho)} \quad \text{with statistical operator} \quad \rho = \rho_{\text{rel}} + \rho_{\text{irrel}}$$

- solution in **linear response**:

response equation containing equilibrium correlation functions/  
generalized BOLTZMANN equation

$$\langle B_m; \dot{\vec{R}}_c \rangle e_c \vec{E} = \sum_n \langle B_m; \dot{B}_n \rangle \Phi_n$$

$$\text{Tr} \{ B_n \rho \} = \sum_m (B_n; B_m) \Phi_n$$

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equilibrium correlation functions

$$\langle A; B \rangle_z = \int_0^\infty dt e^{izt} (A(t); B) = -\frac{i}{\beta} \int_{-\infty}^\infty \frac{d\omega}{\pi} \frac{1}{z - \omega} \frac{1}{\omega} \text{Im} G_{AB+}(\omega - i0)$$

$$(A(t); B) = \frac{1}{\beta} \int_0^\infty d\tau \text{Tr} [A(t - i\hbar\tau) B^+ \rho_0]$$

- 
- application to electrical current density using set  $\{B_n\} = \vec{P} = \dot{\vec{R}}$

$$\vec{J} = \langle \vec{j} \rangle = \text{Tr} \{ \rho \vec{j} \} = \frac{e}{\Omega} \text{Tr} \{ \rho \dot{\vec{R}} \} = \frac{e}{\Omega} \text{Tr} \{ \rho_{\text{rel}} \vec{P} \} = \sigma \vec{E}$$



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- solution for electrical conductivity

$$\sigma = \beta \Omega \langle j; j \rangle = \frac{\beta e^2}{\Omega m_e} \frac{(P; P)^2}{\langle \dot{P}; \dot{P} \rangle}$$

Kubo-Greenwood formula



force force correlation functions

$$(\dot{P} = F_{ei} + F_{ee} + F_{ea})$$

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*Röpke, Meister, Ann. Phys.* **36** (1979) 377; *Röpke, PRA* **38** (1988) 3001; *Reinholz et al., PRE* **52** (1995) 6368

# Dynamical conductivity

time dependent external field

$$\sigma(\omega) = \frac{\epsilon_0 \omega_{\text{pl}}^2}{-i\omega + \nu(\omega)}$$

$$\omega_{\text{pl}}^2 = \frac{e^2 n_e}{\epsilon_0 m_e}$$

generalized Drude formula

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$$\nu(\omega) = \frac{\beta}{n_e \Omega} \langle \dot{\vec{P}}; \dot{\vec{P}} \rangle_{\omega + i\eta}$$

*Reinholz, Redmer, Röpke, Wierling, PRE 62 (2000) 5648*

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- molecular dynamic simulations  
normalized current auto-correlation function (ACF)

$$\langle J; J \rangle_{\omega+i\eta} = \frac{\epsilon_0 \omega_{\text{pl}}^2}{\beta \Omega} \lim_{\epsilon \rightarrow 0} \int_0^{\infty} e^{i(\omega+i\epsilon)t} K(t) dt \quad K(t) = \frac{1}{\langle J^2 \rangle} \frac{1}{\delta} \int_0^{\delta} d\tau J(t+\tau) J(\tau)$$

# MD simulations

normalized current auto-correlation function (ACF)

$$K(t)^{L/T} = \frac{1}{\langle J^2 \rangle} \frac{1}{\delta} \int_0^\delta d\tau J^{z/x}(t + \tau) J^{z/x}(\tau)$$

with

$$\vec{J}(t) = \frac{1}{\Omega_0} \sum_c \sum_{\alpha=1}^N e_c \vec{v}_{c,\alpha}^z(t)$$

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equation of motion with **mean field**  $E^z$  due to

average current density  $\vec{j}(t) = j_z \vec{e}_z$

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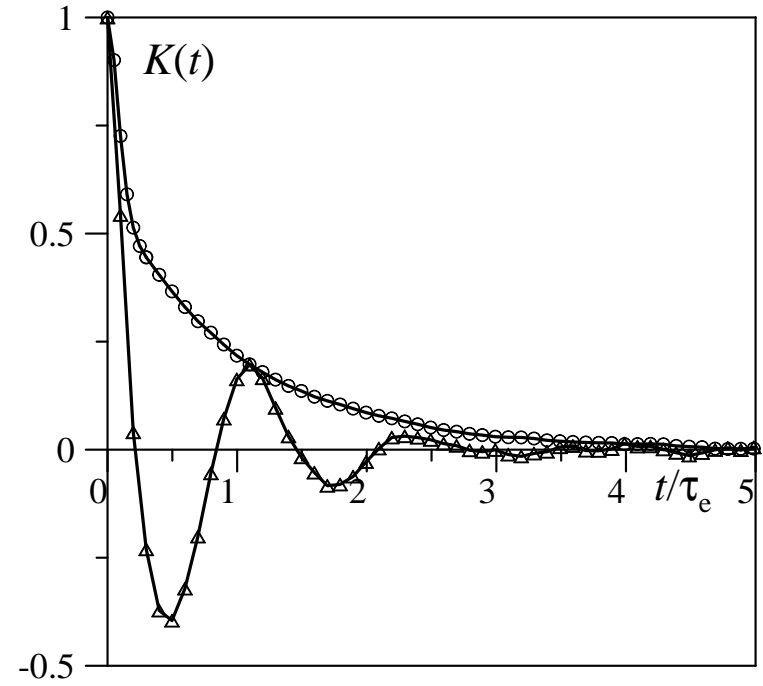
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**Kelbg pseudopotential**

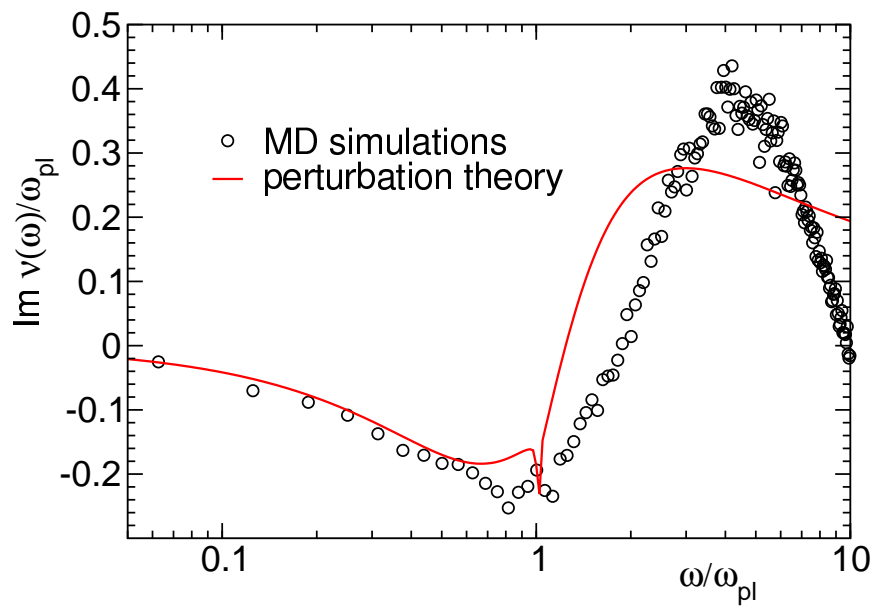
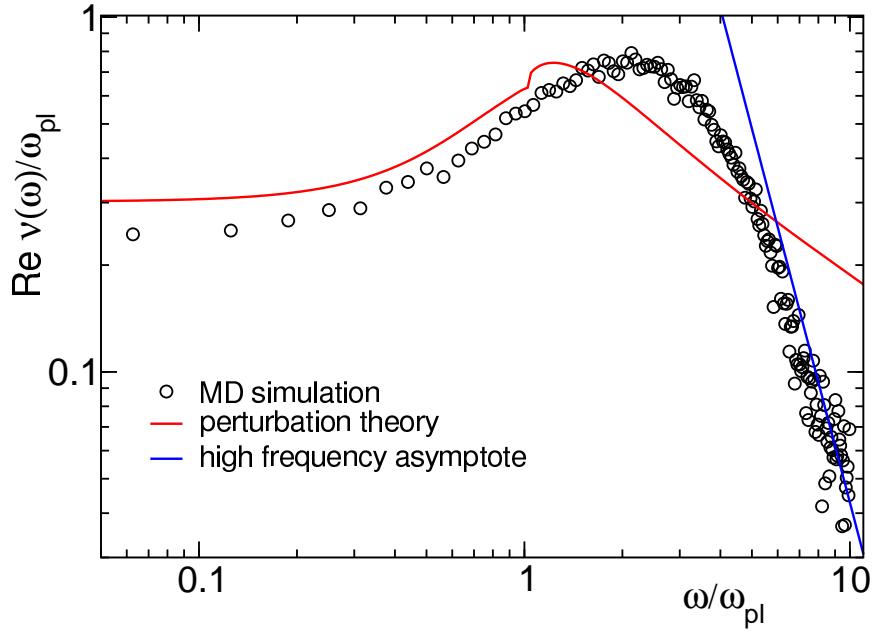
**Figure:** normalized current ACF for  $\Gamma = 1.28$ ,  $\tau_e = 2\pi/\omega_{pl}$  – period of electron plasma oscillations: MD simulations **without** (o) and **including** ( $\Delta$ ) an additional mean-field term

*Reinholz et al., PRE 69 (2004) 066412; Morozov et al. PRE 71 (2005) 066408*



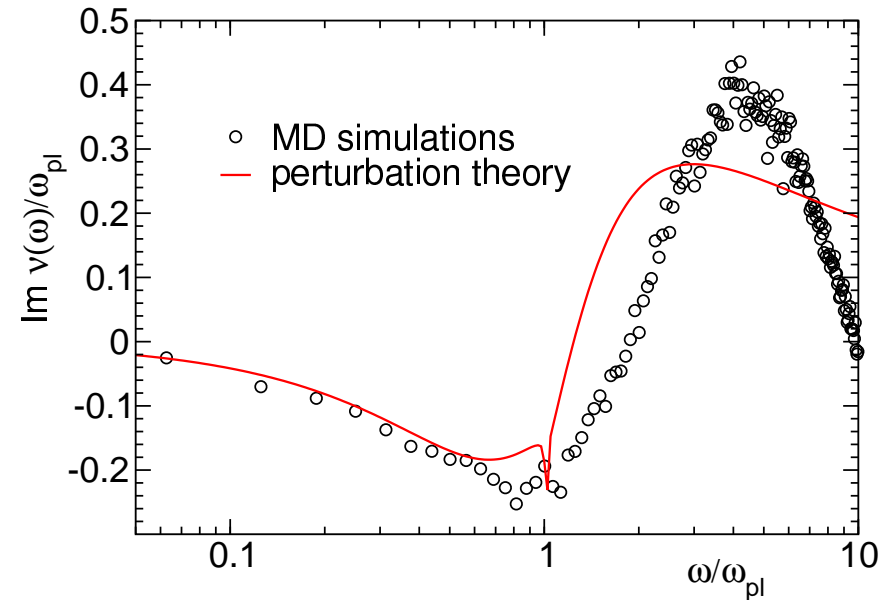
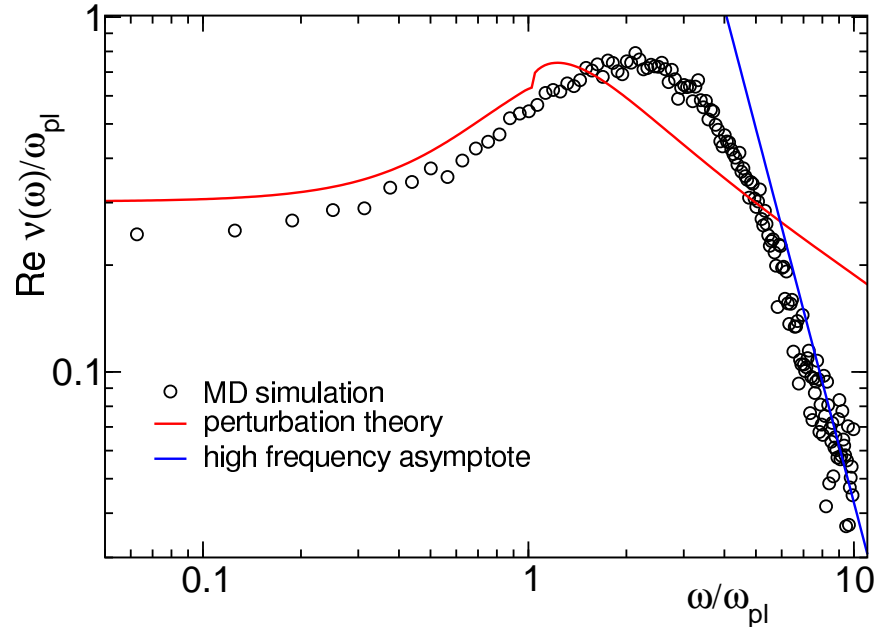
# Dynamical collision frequency

fully ionized plasma at  $n = 3.8 \times 10^{21} \text{ cm}^{-3}$ ,  $T = 33\,000 \text{ K}$ ,  $\Gamma = 1.28$ ,  $\Theta = 3.2$



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perturbation theory:

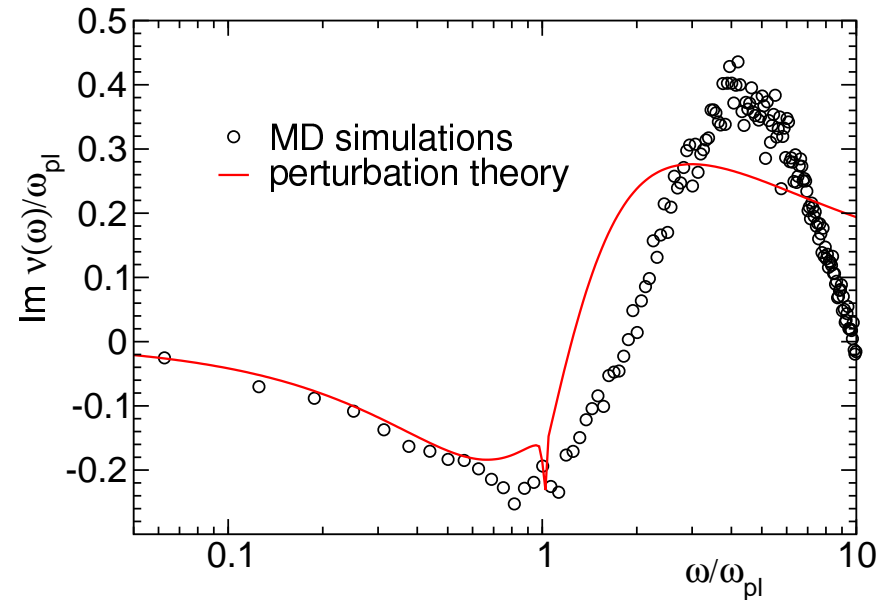
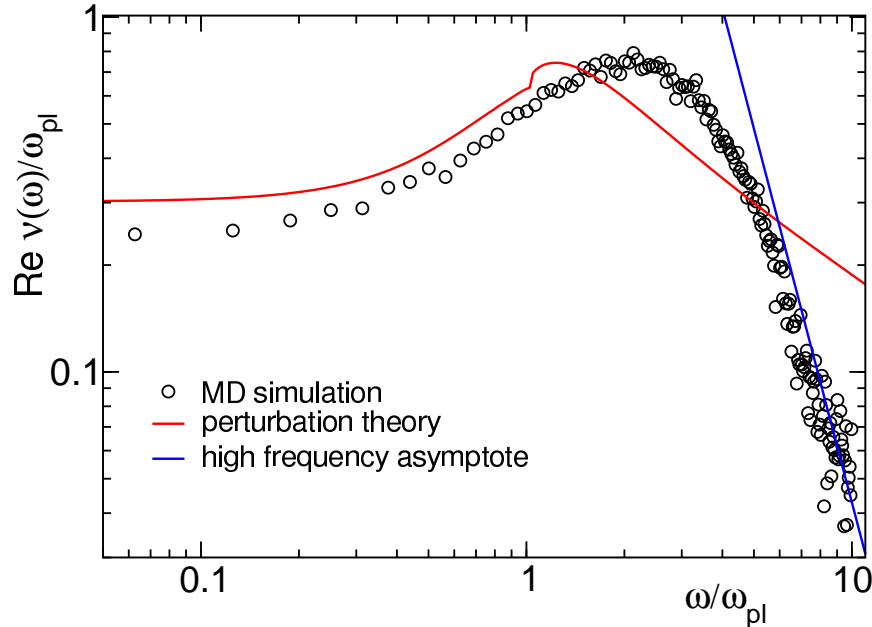
*Reinholz et al., PRE 62 (2000) 5648; PRE 69 (2004) 066412*

$$\nu(\omega) \approx r(\omega)\nu^{(P_0)}(\omega) = r(\omega)\nu^{\text{GD}}(\omega) = r(\omega)\left(\nu^{\text{ladder}}[\omega] - \nu^{\text{Born}}(\omega) + \nu^{\text{LB}}(\omega)\right)$$

dynamically screened binary collision approximation using [Gould-deWitt ansatz](#) (dynamical screening and strong collisions); higher moments of single-particle distribution function via [renormalization factor](#) (electron-electron interaction)

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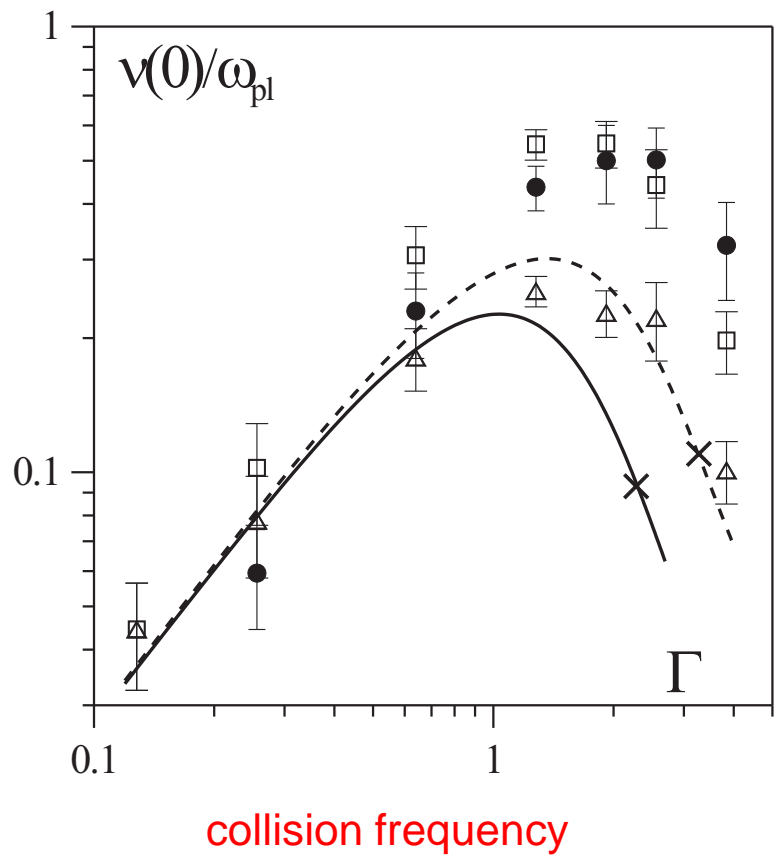
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high frequency asymptotes in Born approximation

$$\text{Re } \nu^{\text{Kelbg}}(\omega) \propto \omega^{-7/2}$$

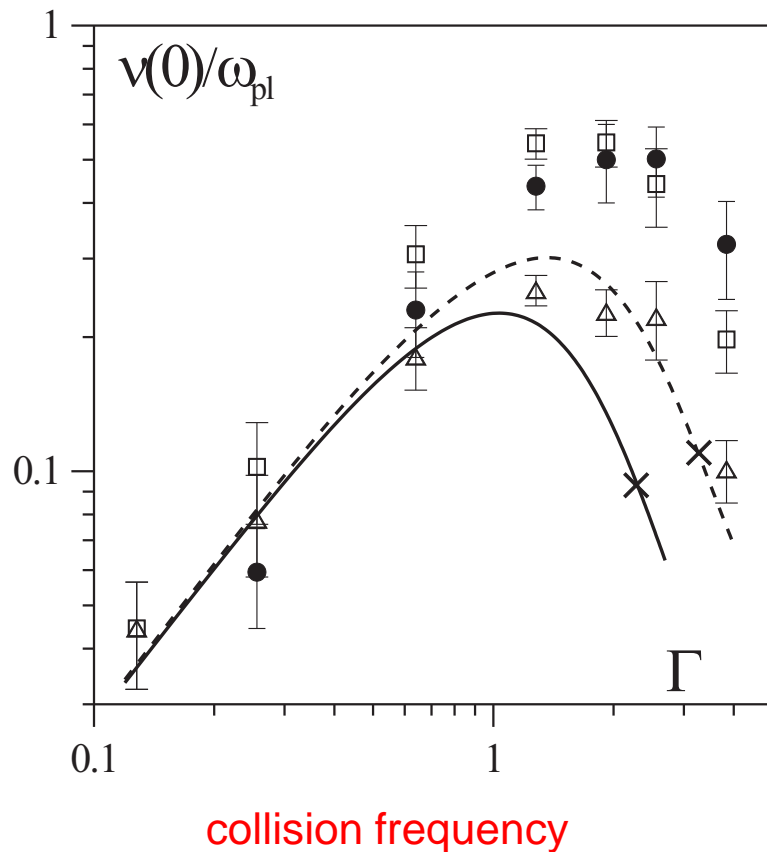
$$\nu^{\text{Coulomb}}(\omega) \propto \omega^{-3/2}$$

# DC Conductivity comparison



- from MD simulations at  $\omega_{pl}$
- collisional damping of Langmuir waves,  $\nu = 2\delta_c$   
(Morozov, Norman, JETP 100 (2005))

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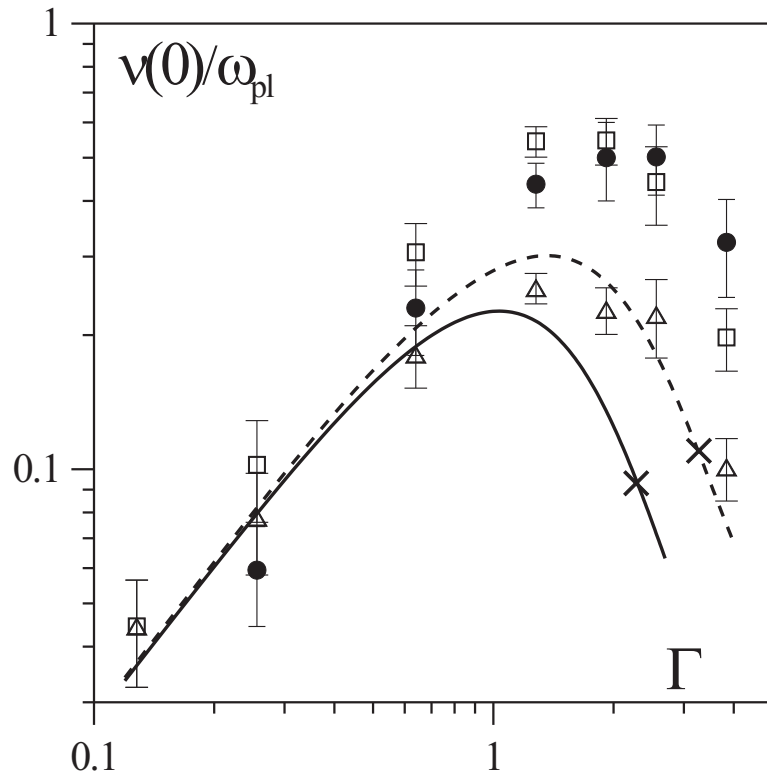


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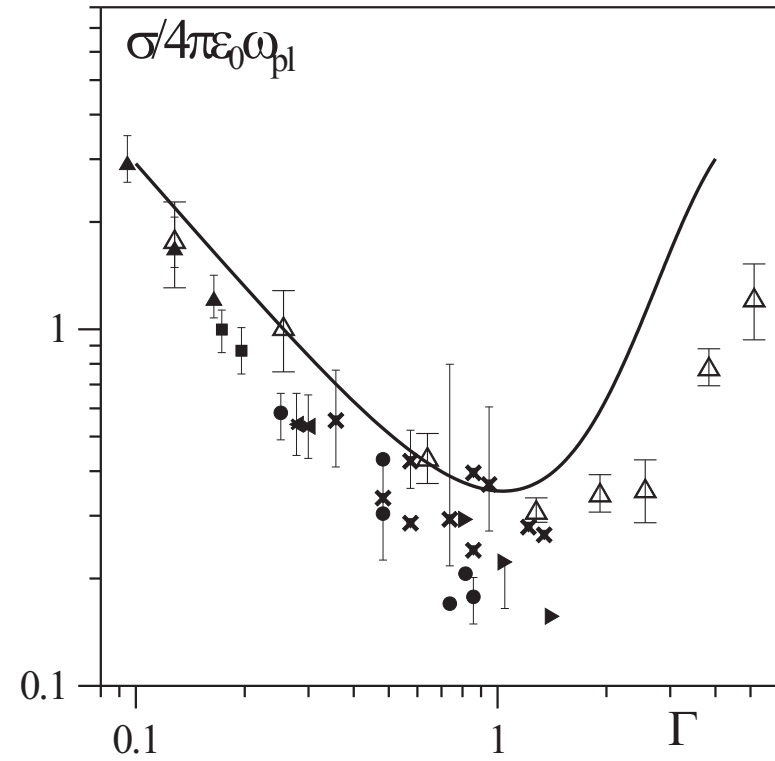
- △ — MD simulations  $T = 33000\text{K}$
- full line — interpolation formula  $T = 33000\text{K}$
- filled symbols — experimental data (Mintsev et al.)

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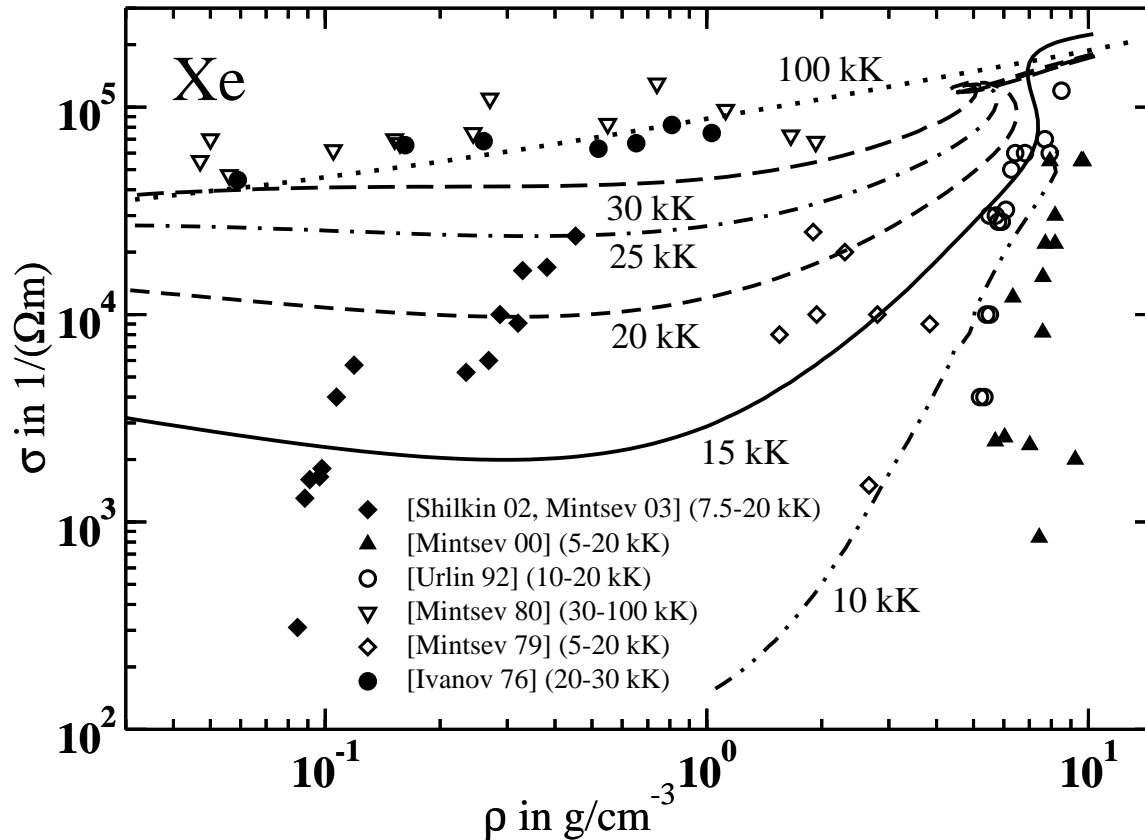
Static conductivity

$$\sigma_{dc} = \lim_{\omega \rightarrow 0} \sigma(\omega) = \frac{\epsilon_0 \omega_{pl}^2}{\nu_{dc}} = \frac{e^2 n_e}{m_e} \tau_{dc}$$

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# DC conductivity in xenon

electrical conductivity of **xenon** in comparison to experimental data



partially ionized plasma  $\Rightarrow$  bound states, depletion of free charge carriers, additional scattering mechanisms (COMPTRA04)

# Conclusions I

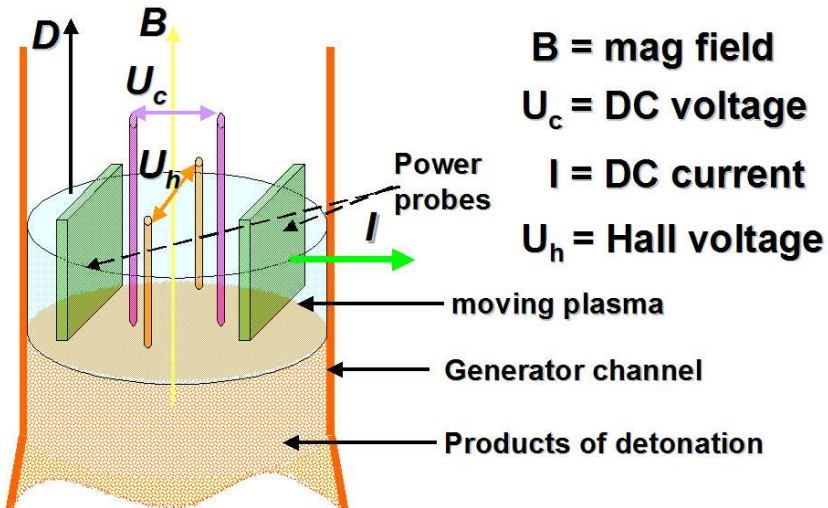
- linear response theory (**Zubarev approach**) to derive expressions for static and dynamical conductivity
- Kubo formula or force-force correlation functions
- systematic and consistent inclusion of strong collisions, dynamical screening, e-e interaction and effects in **partially ionized** systems
- results from perturbation theory, molecular dynamics simulation and experiments are consistent in weakly coupled plasmas
- high frequency behaviour of collision frequency
- quantum statistical simulations: QMD, WPMD, PIMC



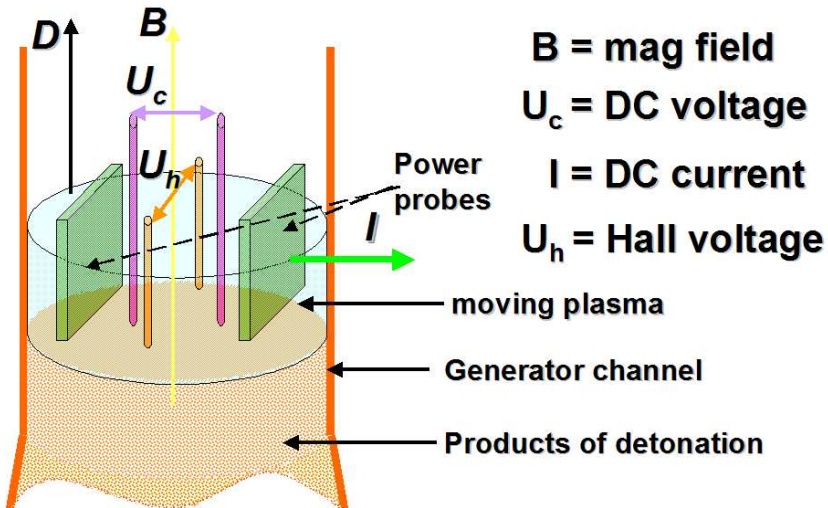
# Applications

- Hall effect
- optical properties
- reflectivity
- Thomson scattering

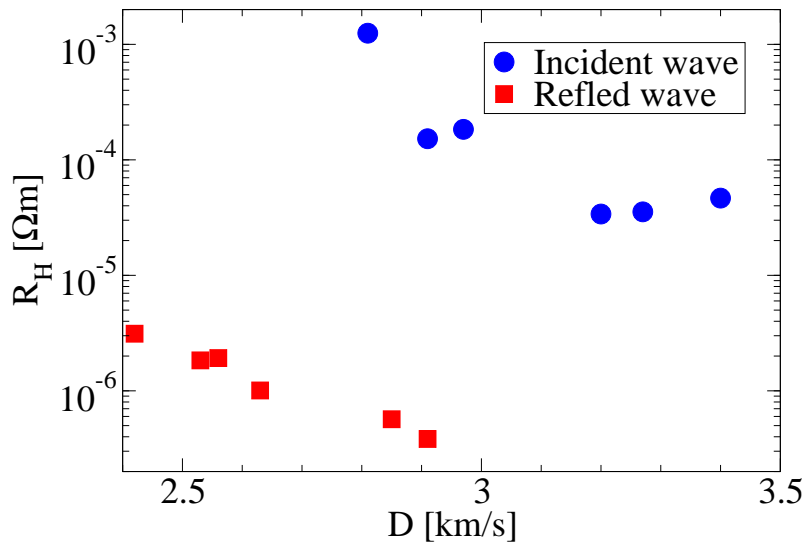
# Hall measurement



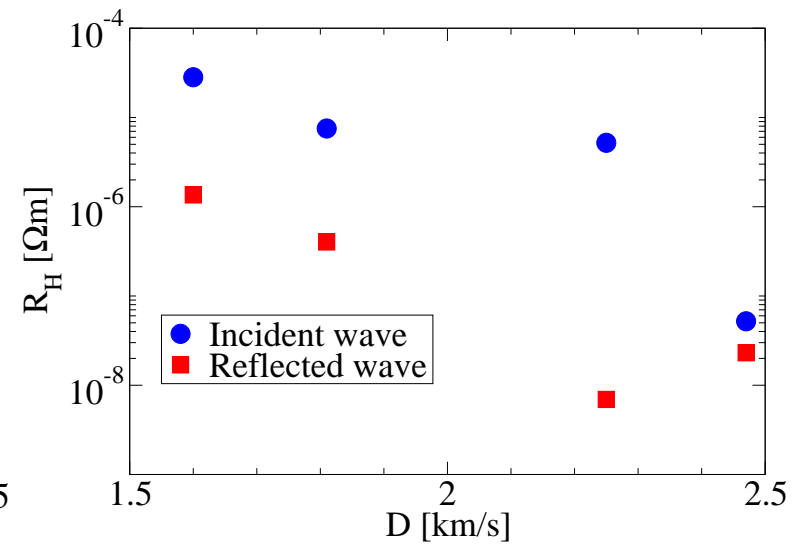
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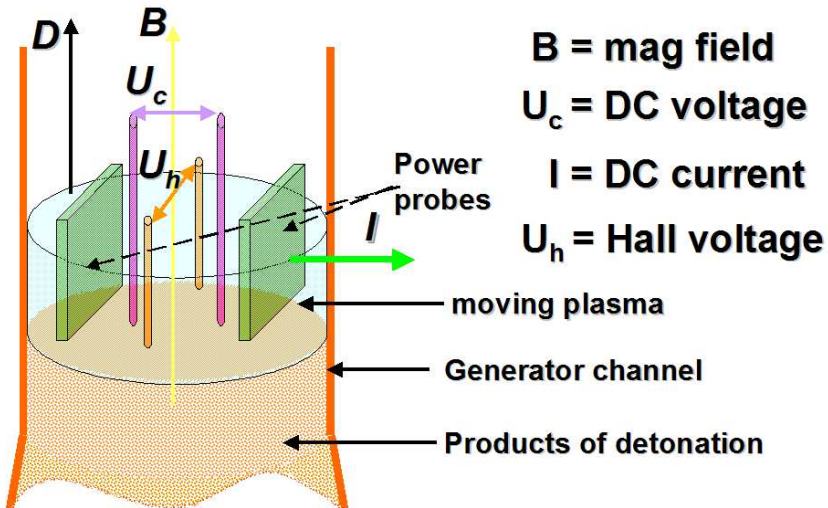
Argon



Xenon



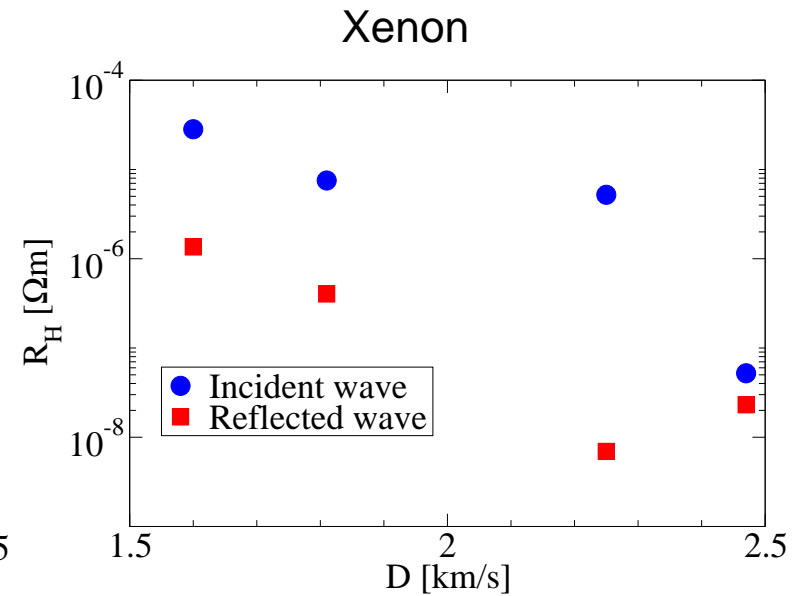
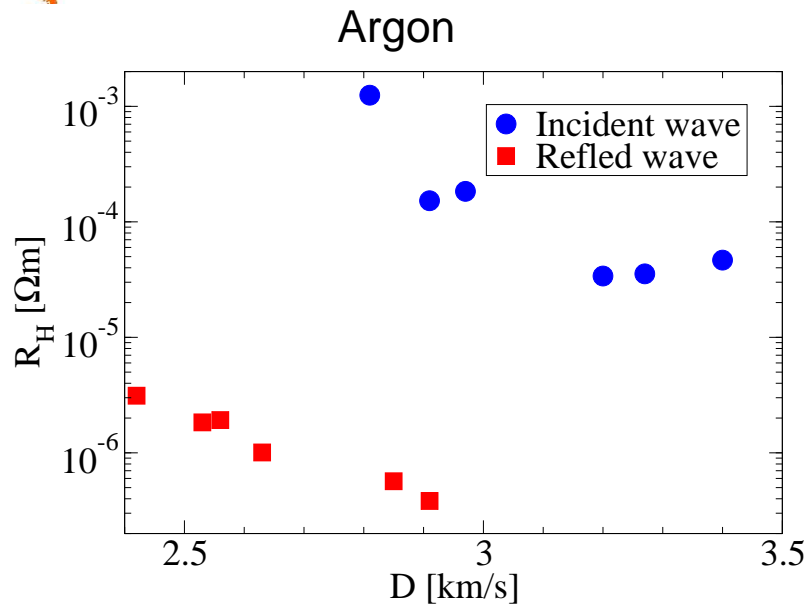
# Hall measurement



- Hall voltage  $U_h$

$$\vec{E}_h = R_h (\vec{J} \times \vec{B}) = \frac{U_h}{d}$$

- free electron densities  $n_e$  calculated from a thermodynamic model  
 $\Rightarrow R_h = r_h / (e n_e)$



# Electromagnetic transport properties

many-particle system under the influence electric field  $\vec{E}$  and magnetic field  $\vec{B}$

electric current densities:  $\vec{J} = \sigma \vec{E} + \sigma R_h \left( \vec{J}_{\text{el}} \times \vec{B} \right) = -\frac{e}{\Omega} \langle \hat{R} \rangle$

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$$m_e \dot{\hat{R}} = \hat{P} + \frac{e}{2} (\vec{B} \times \hat{R})$$

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Lorentz force

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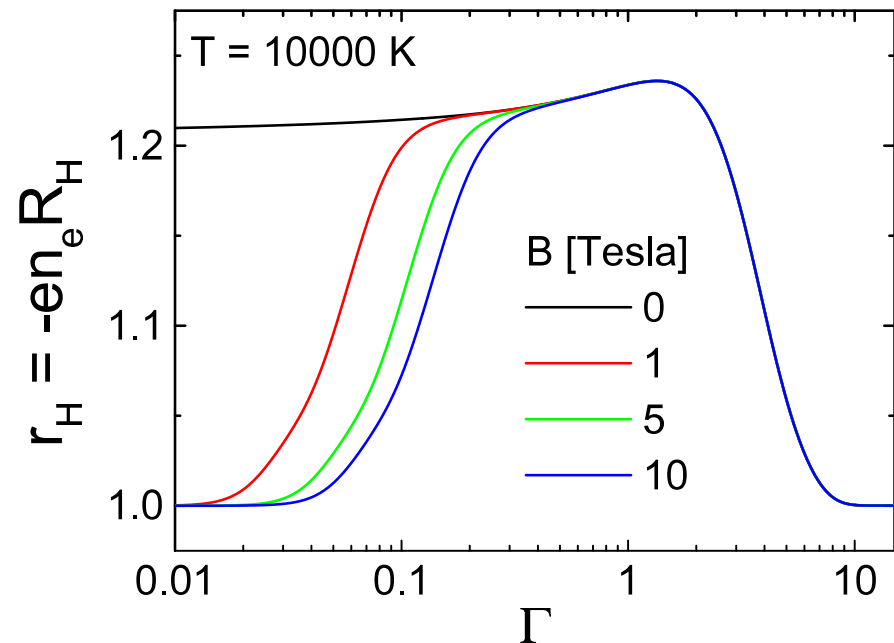
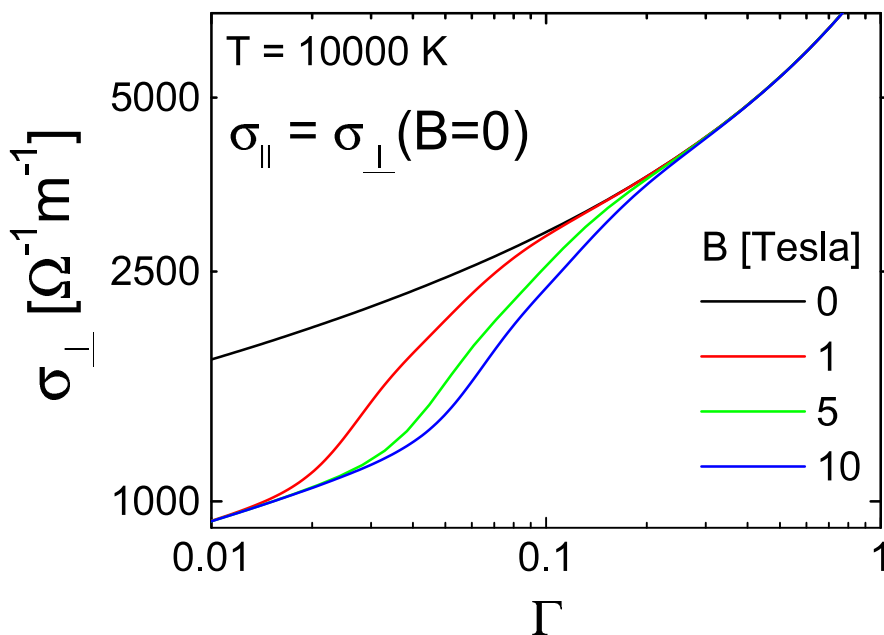
equilibrium correlation functions  $\langle \dot{\hat{P}}_m ; \dot{\hat{P}}_n \rangle + \omega_e^2 \langle \hat{P}_n ; \hat{P}_m \rangle$

with electron cyclotron frequency  $\omega_e = \frac{eB}{m_e}$



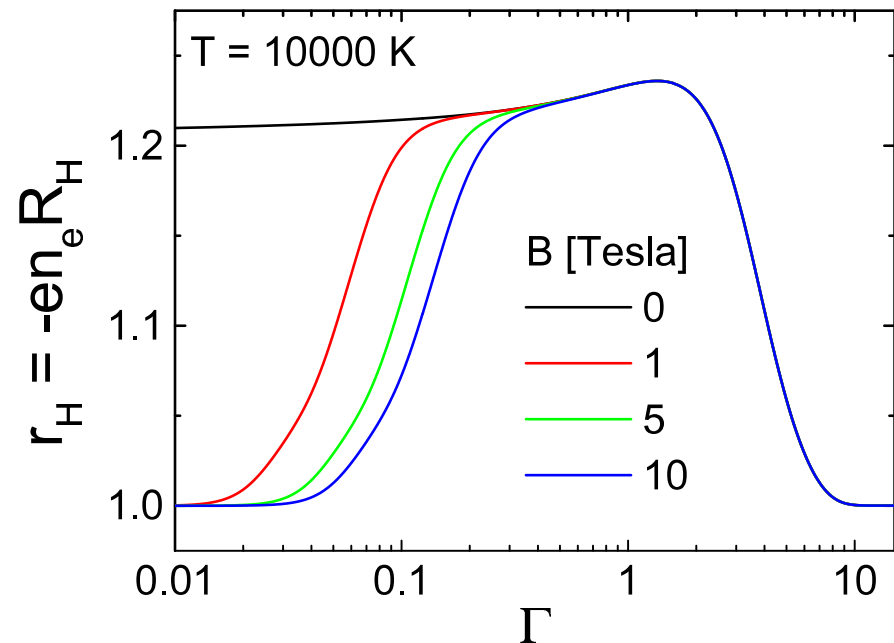
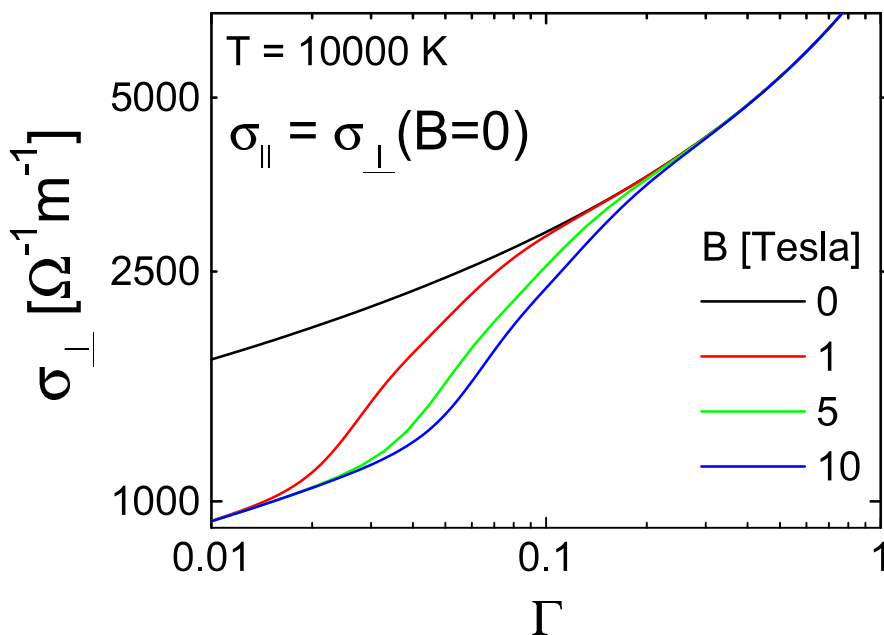
# fully ionized plasma in magnetic field

- LRT within five moment approximation
- transport cross section in Born approximation for statically screened e-i and e-e potential (Debye potential)
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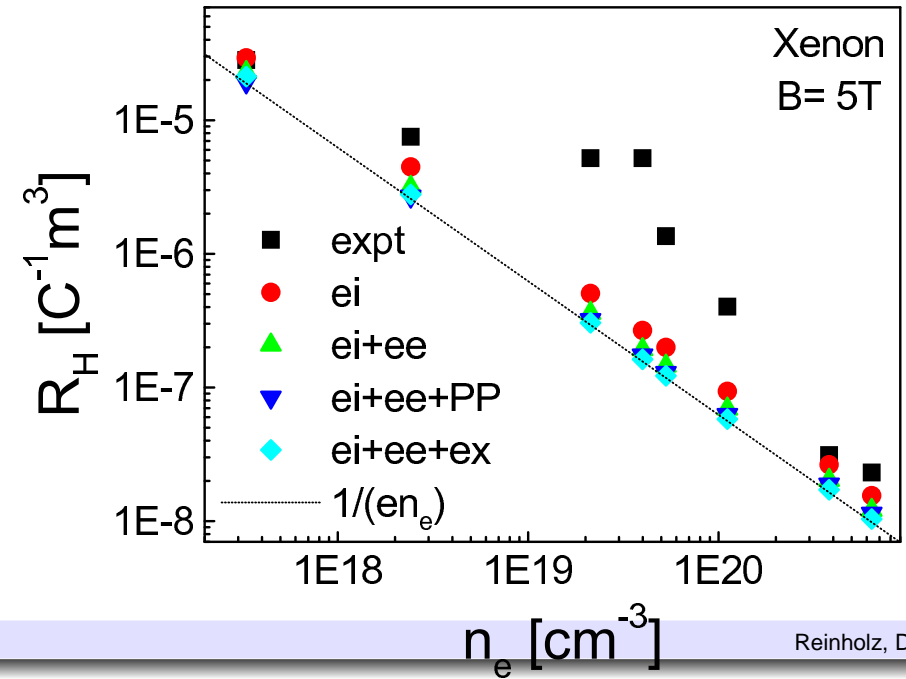
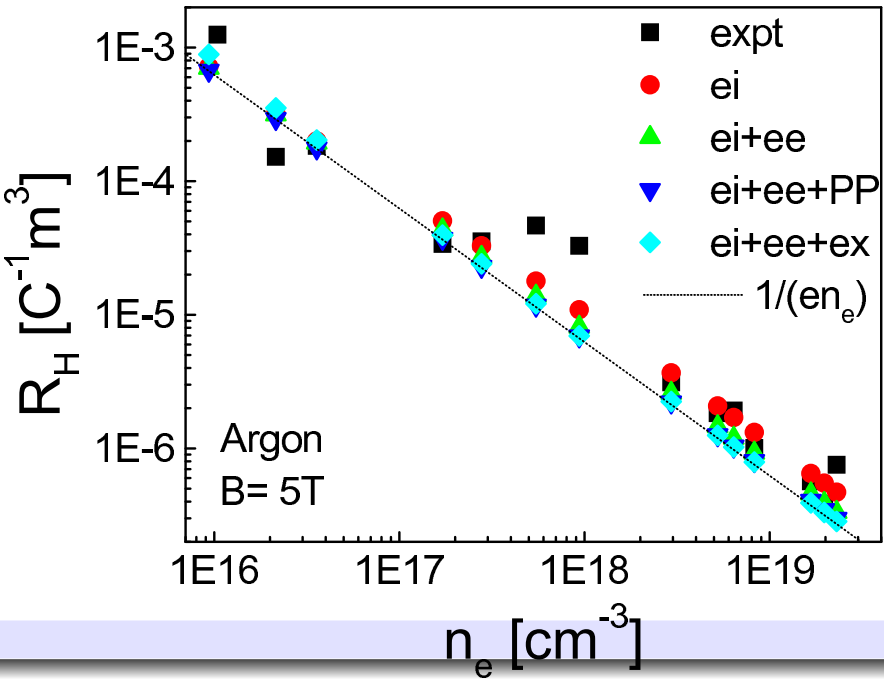


- conductivity is reduced in low density limit (higher moments are not relevant)
- maximum in Hall factor shifts to higher densities with decreasing temperature

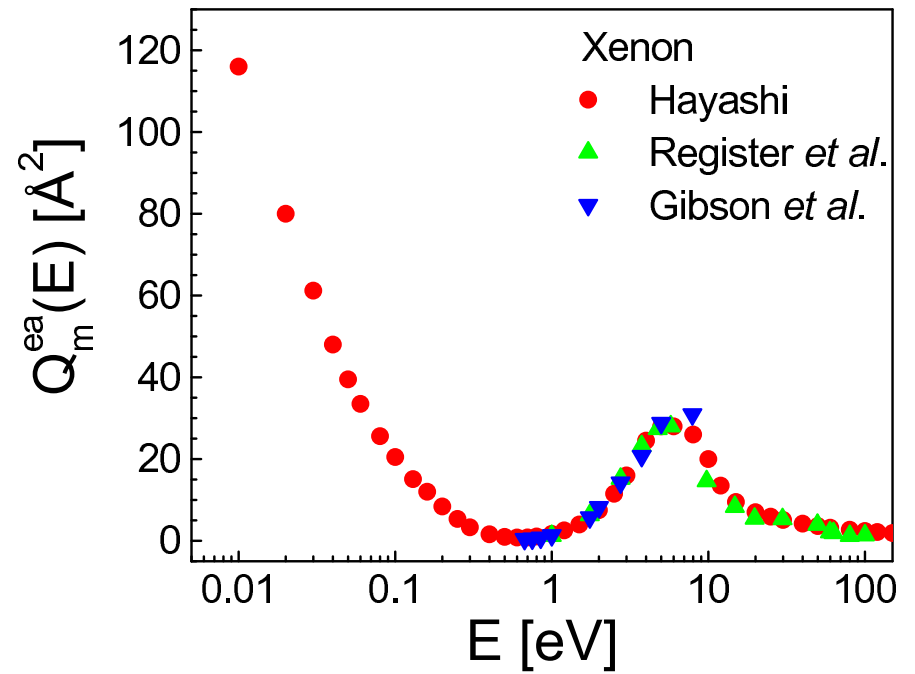
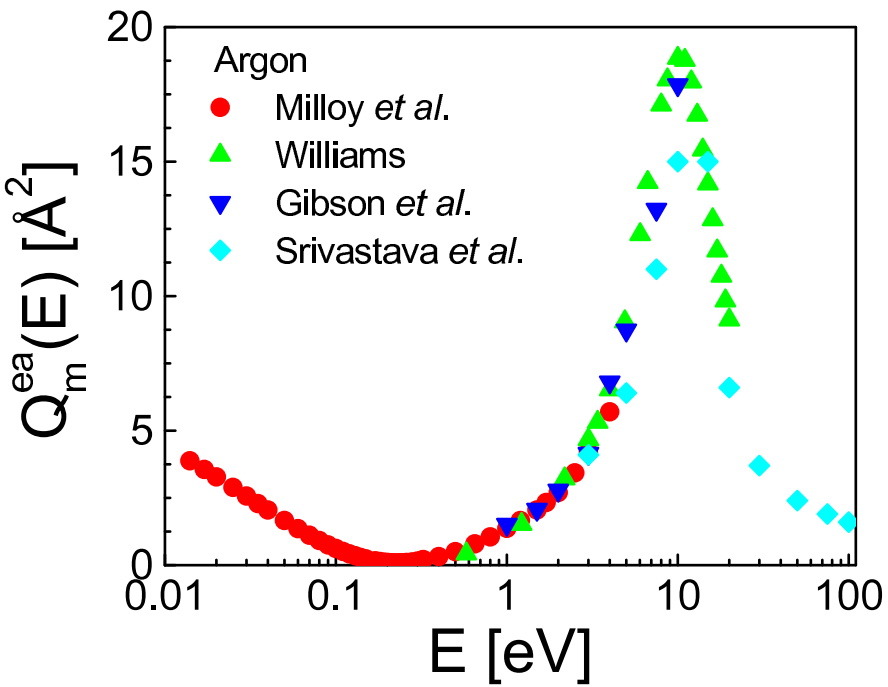
# Hall coefficient in partially ionized plasma

scattering mechanisms:

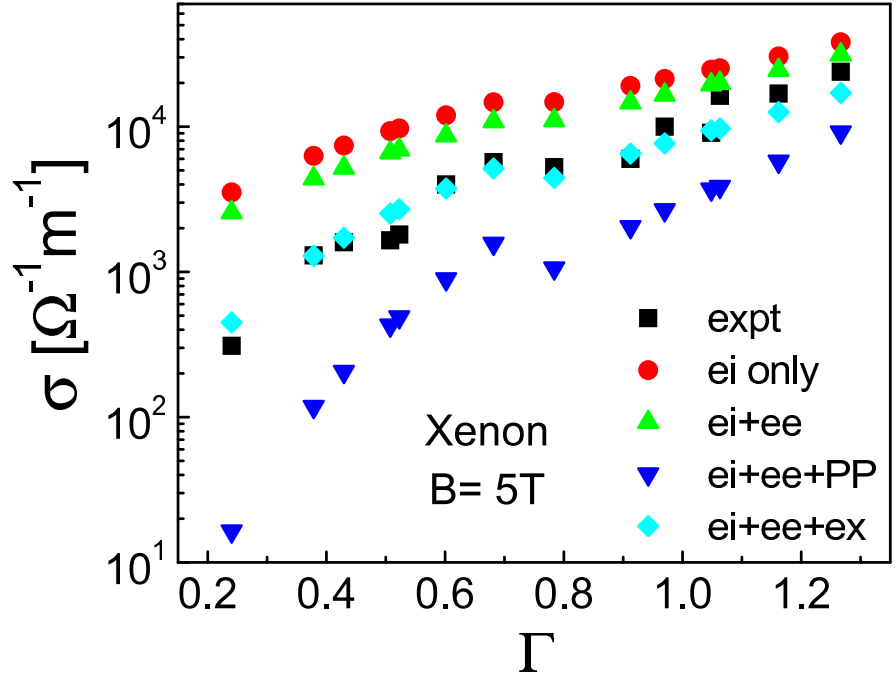
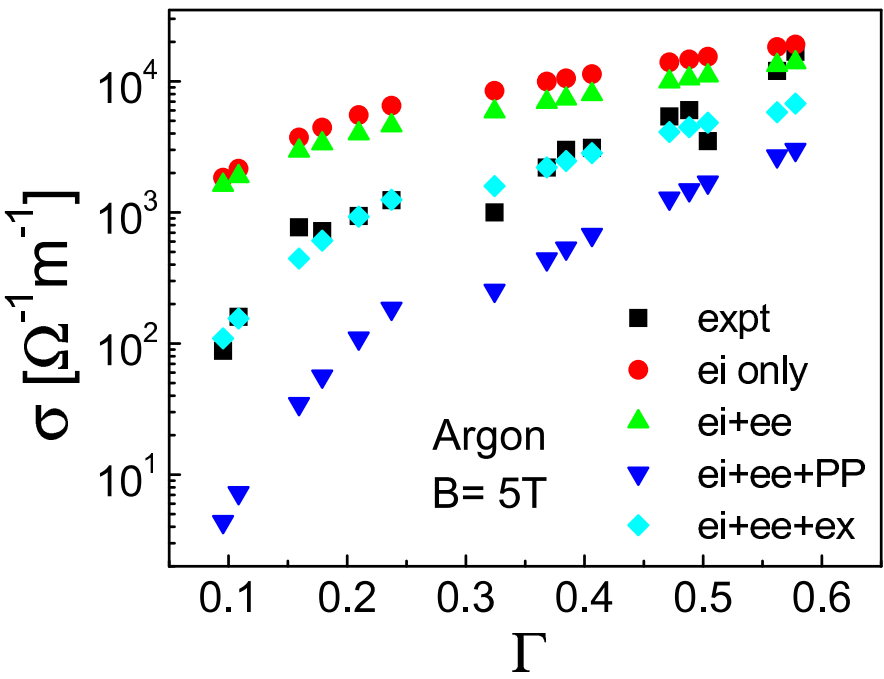
$$F = F_{ei} + F_{ee} + F_{ea}$$



# transport cross section



# conductivity in magnetic field



# Conclusions II

- extension of linear response theory to include **magnetic field** effects in order to describe **Hall effect**
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- correlations are not relevant for high magnetic fields ( $r_H=1$ ) except in a small parameter region of intermediate correlation strength
- outlook
  - more detailed calculations necessary for comparison with experiment (ionization degree, transport cross section)
  - Hall factor as **diagnostic tool** for determination of system parameters



# Dielectric and optical response

$$\epsilon(\mathbf{k}, \omega) = 1 + \frac{i}{\epsilon_0 \omega} \sigma(\mathbf{k}, \omega) = 1 - \frac{\omega_{\text{pl}}^2}{\omega(\omega - i\nu(\omega))}$$

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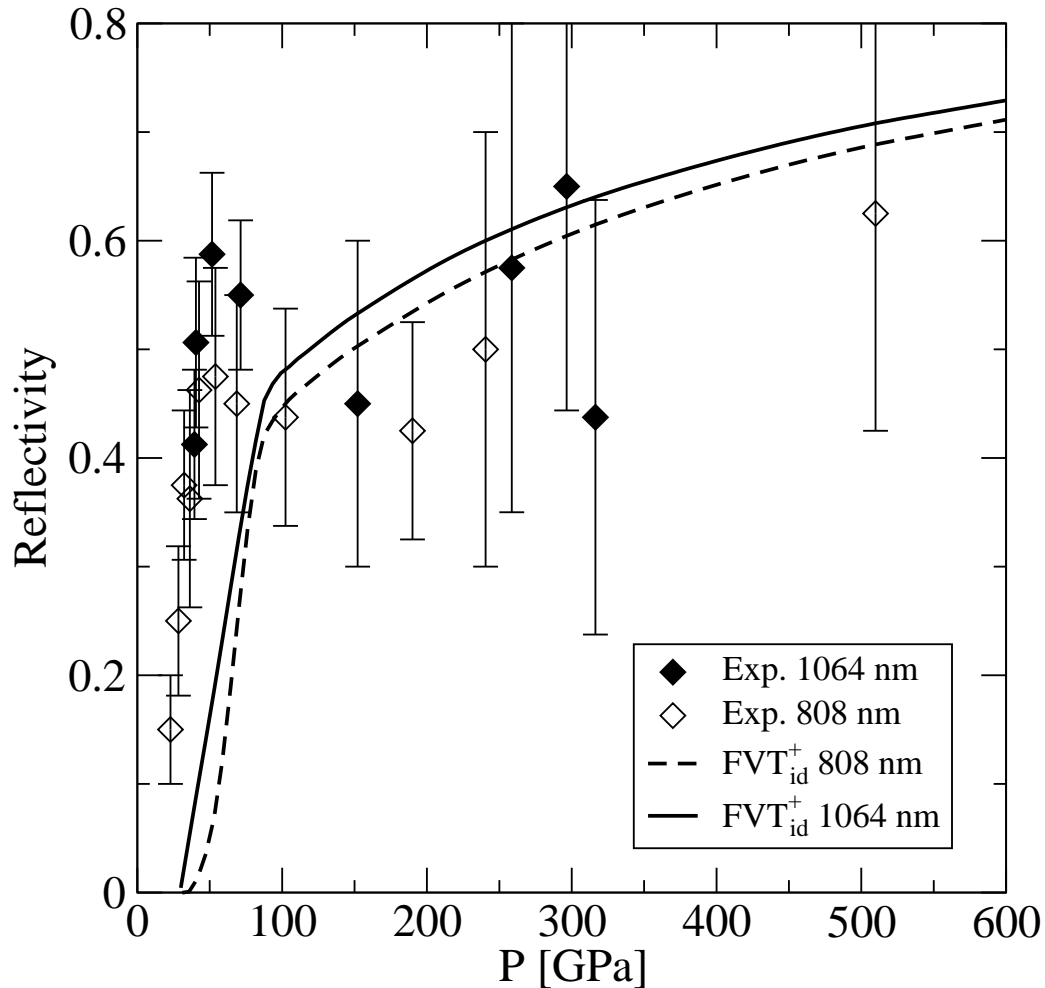
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- reflectivity at normal incidence

$$R(\omega) = \left| \frac{\sqrt{\epsilon(\omega)} - 1}{\sqrt{\epsilon(\omega)} + 1} \right|^2$$

# Reflectivity of Deuterium



- shock wave experiments along Hugoniot
- assuming step like shock wave front

$$R(\omega) = \left| \frac{\sqrt{\epsilon(\omega)} - 1}{\sqrt{\epsilon(\omega)} + 1} \right|^2$$

with

$$\text{RPA } \epsilon(\omega) = 1 - \frac{\omega_{\text{pl}}^2}{\omega^2}$$

$$\text{Drude } \epsilon(\omega) = 1 - \frac{\omega_{\text{pl}}^2}{\omega(\omega + i\nu_{dc})}$$

- insulator-plasma transition

# Reflectivity of xenon

shock compressed dense plasma:

⇒ pressure 1.6 - 20 GPa,  $T \approx 33\,000$  K, density  $0.5 - 4 \text{ g cm}^{-3}$

laser:  $\lambda = 1.06 \mu\text{m}$ ,  $0.694 \mu\text{m}$ ,  $0.532 \mu\text{m}$

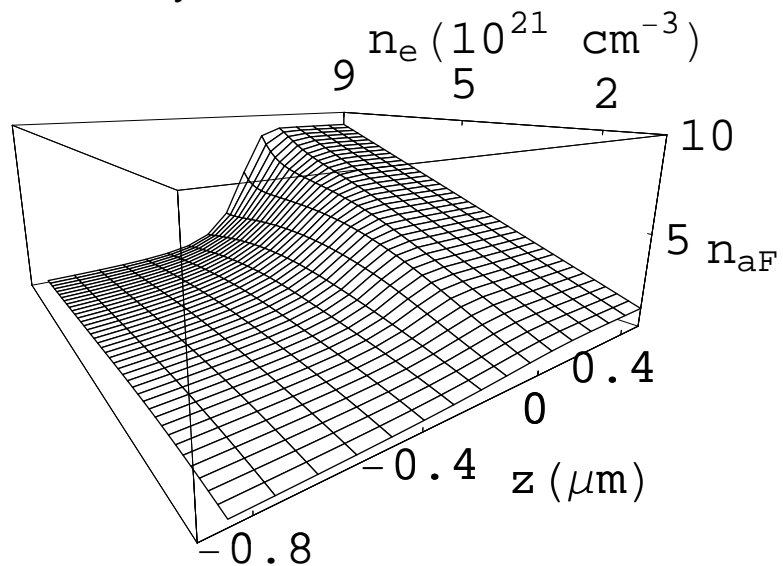
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distribution of density of free electrons  $n_e(z)$   
in shock wave front in dependence on elec-  
tron density  $n_e$



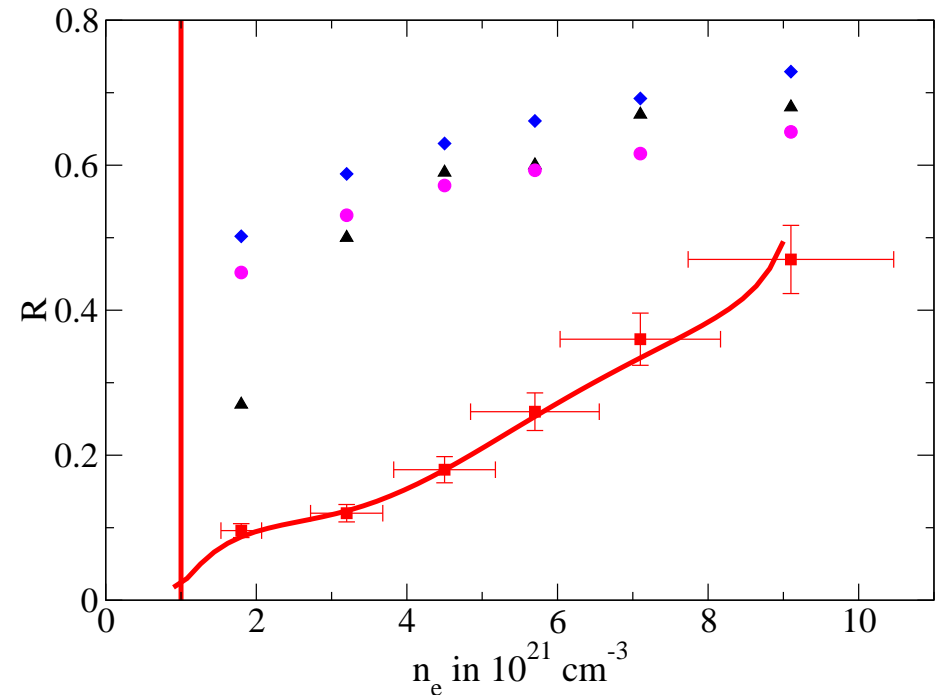
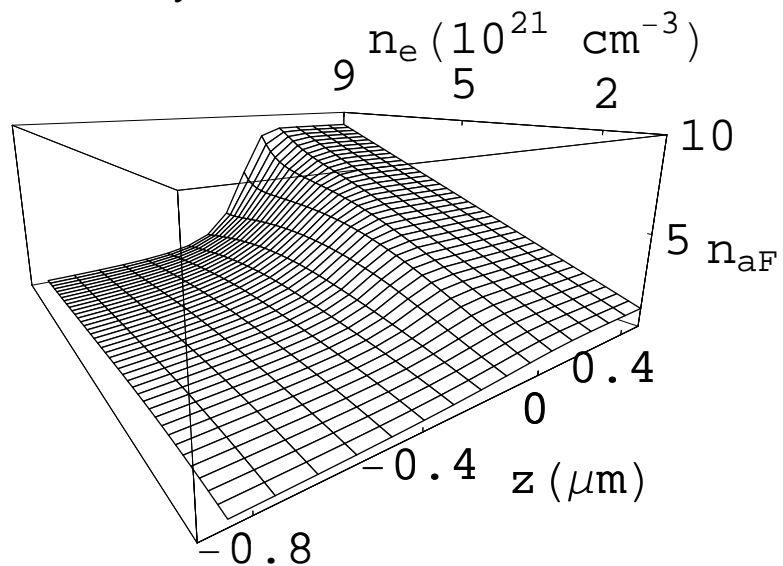
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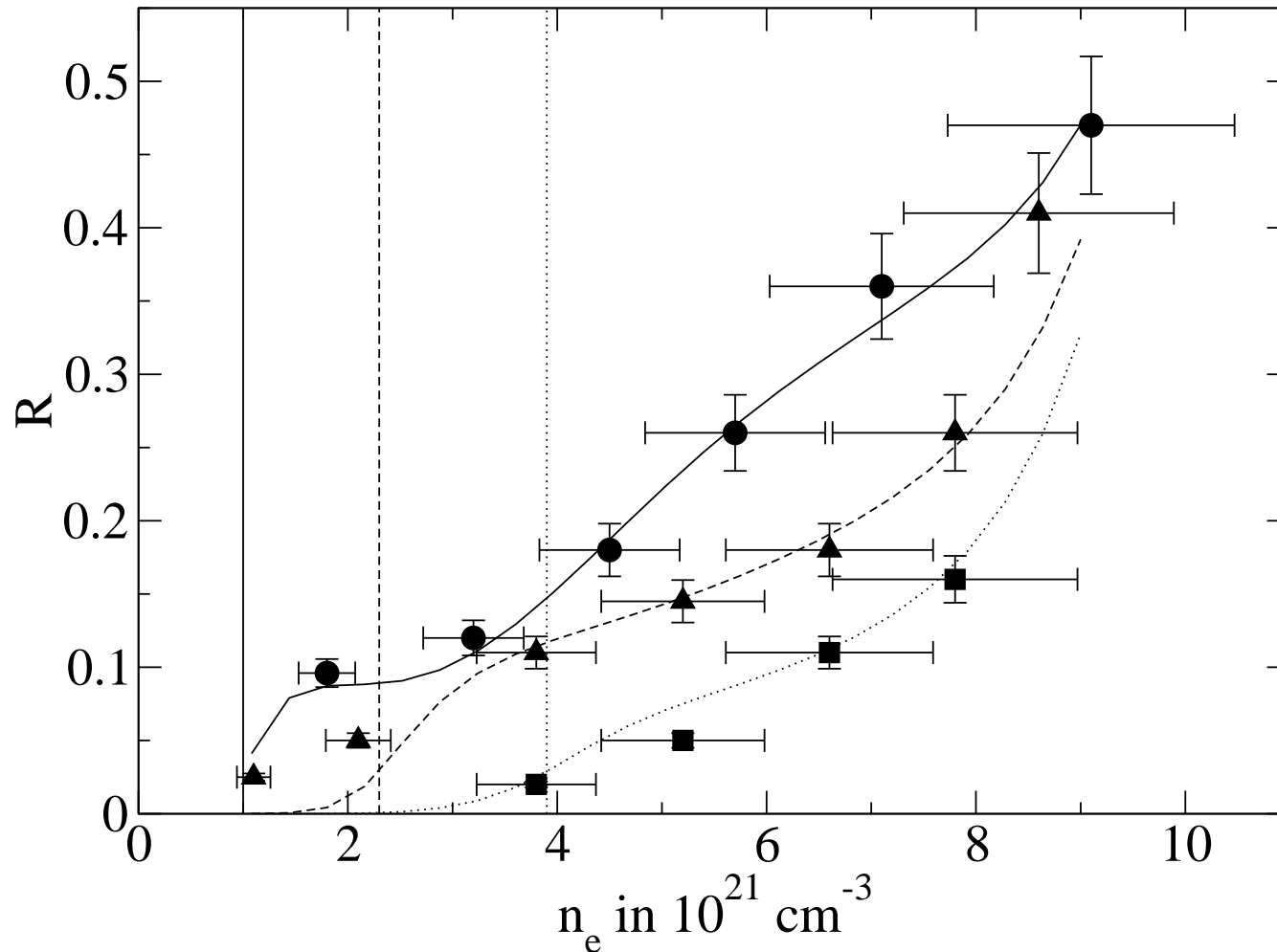
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comparison of experiment with theoretical calculations for  $1.06 \mu\text{m}$ : molecular dynamic simulation ( $\blacktriangle$ );  $ERR_{dc}$  Padé formula for  $\nu_{ei,ee}$  ( $\blacklozenge$ );  $ERR_{dc}$  incl.  $\nu_{ea}$  ( $\bullet$ ); full line - shock front profile



# Reflectivity of xenon



Reflectivity coefficient  $R$  for Xenon calculated with asymmetric Fermi profile in comparison with measurements (symbols with error bars) for laser wavelengths 1.06  $\mu\text{m}$  (solid line, ●), 0.694  $\mu\text{m}$  (dashed line, ▲), and 0.532  $\mu\text{m}$  (dotted line, ■), the corresponding critical densities  $n_e^{\text{cr}}$  are indicated with vertical lines

*Raitza et al., J. Phys. A 39 (2006) 4393*

# Thomson Scattering

scattering cross section:

$$\frac{d^2\sigma}{d\Omega d\omega} = \sigma_T \frac{k_1}{k_0} S(k, \omega)$$

$$\mathbf{k} = \mathbf{k}_0 - \mathbf{k}_1, \omega = \omega_0 - \omega_1$$

$k_0$  ( $k_1$ ): incident (scattered) wavevector

$\sigma_T$ : Thomson cross section

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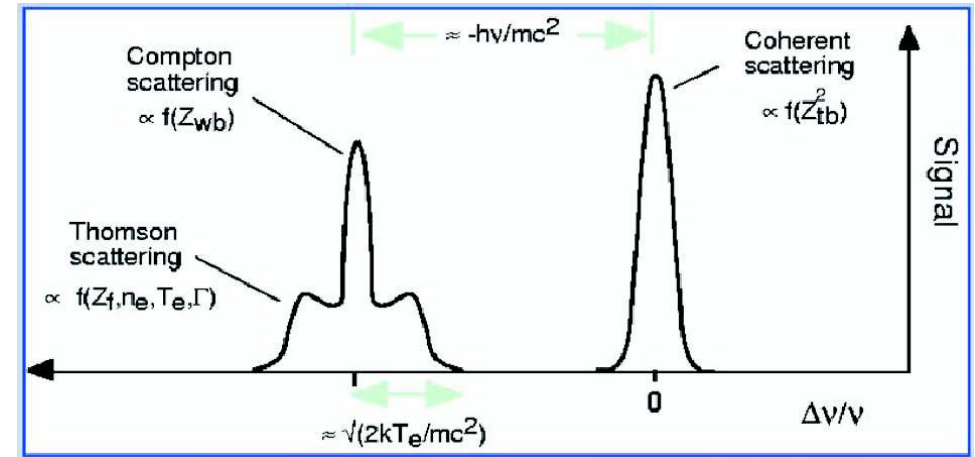
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*O.L. Landen et al., JQSRT 71 (2001) 465*

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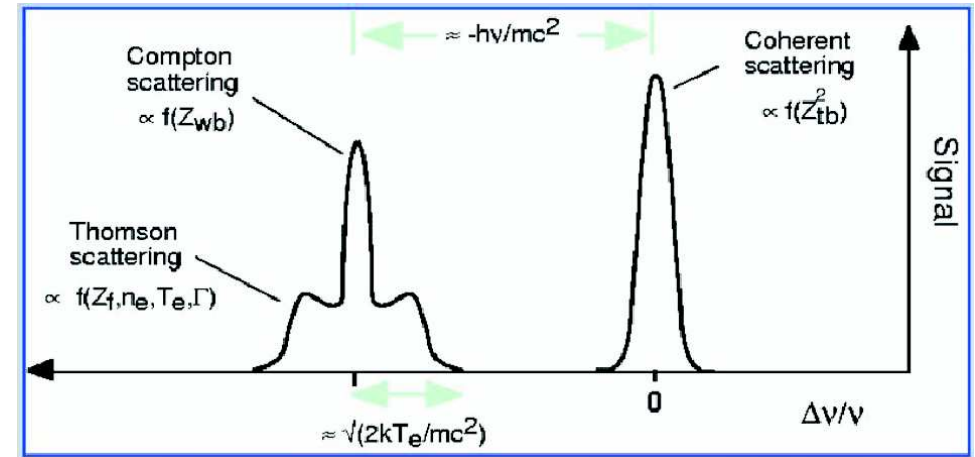
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$$S(k, \omega) = |f_I(k) + q(k)|^2 S_{ii}(k, \omega) + Z_f S_{ee}(k, \omega) + Z_C \int d\omega' \tilde{S}(k, \omega - \omega') S_s(k, \omega')$$

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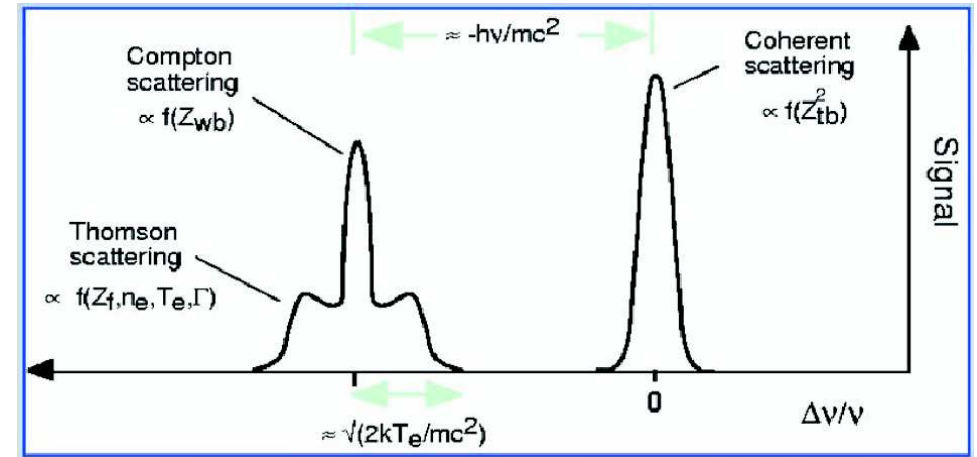
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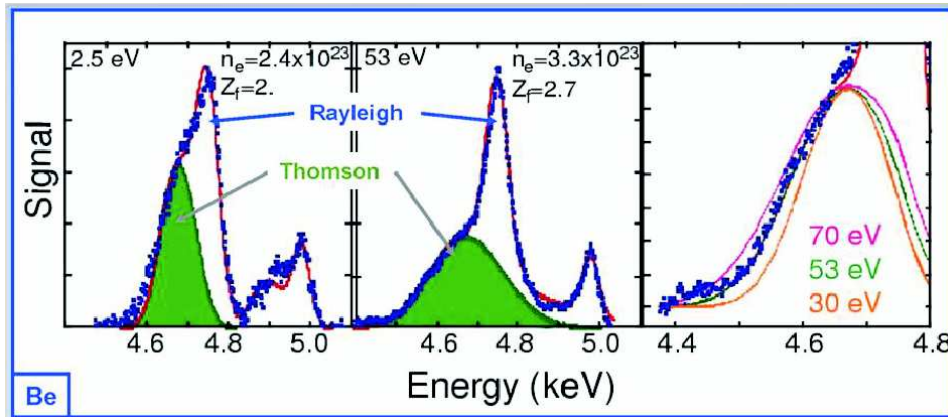
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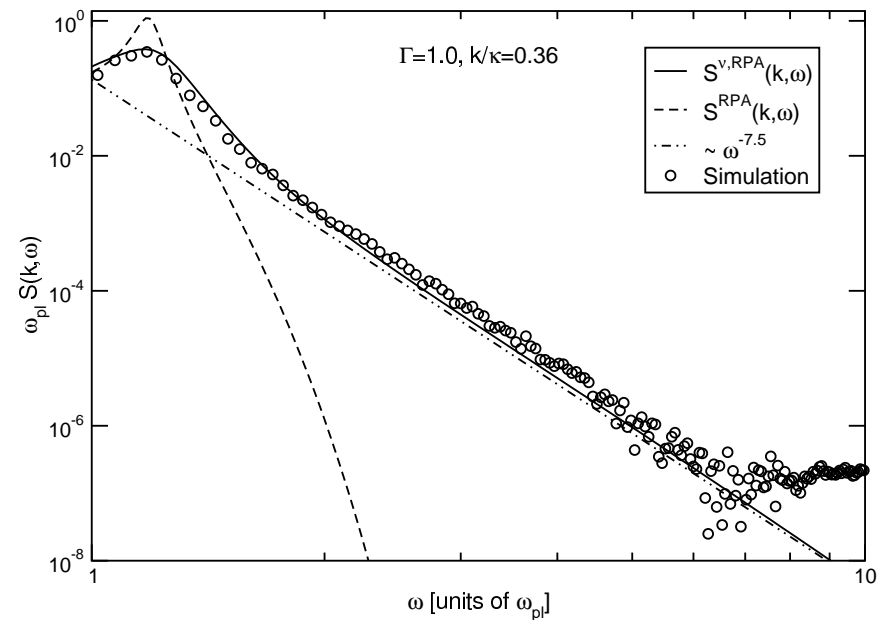
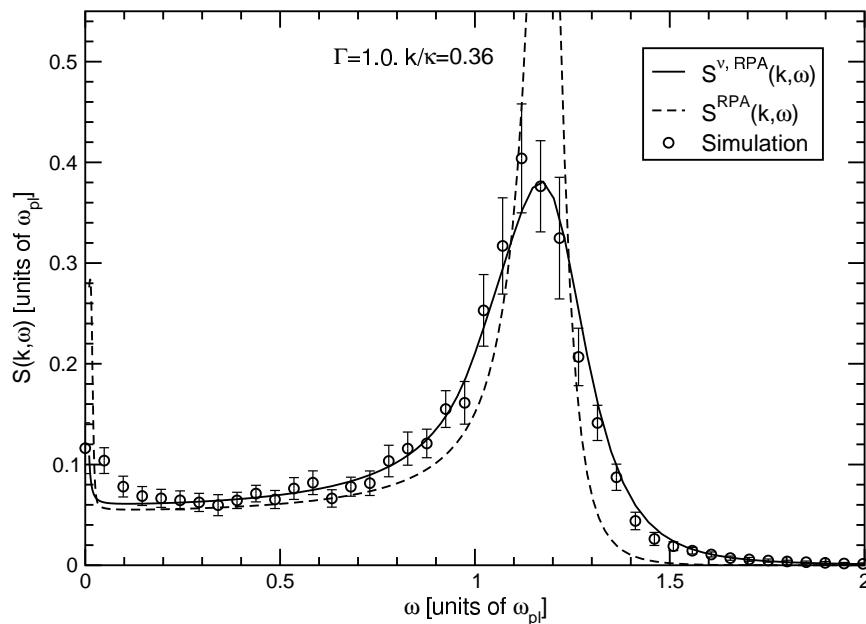


*Glenzer et al., PRL 90 (2003) 175002*

Experiment on Beryllium at 30 kJ  
 Omega laser facility in Rochester  
 heating: Rh X-ray (2.7 keV - 3.4 keV)  
 scattering source: He-like Ti  $\alpha$ -line  
 (4.75 keV)  
 scattering angle:  $\Theta_S = 125^\circ$

# Dynamic structure factor

$$S_{ee}(\mathbf{k}, \omega) = \frac{1}{\pi V(k)} \frac{1}{e^{-\beta\hbar\omega} - 1} \text{Im}\epsilon_{\text{long}}^{-1}(\mathbf{k}, \omega)$$



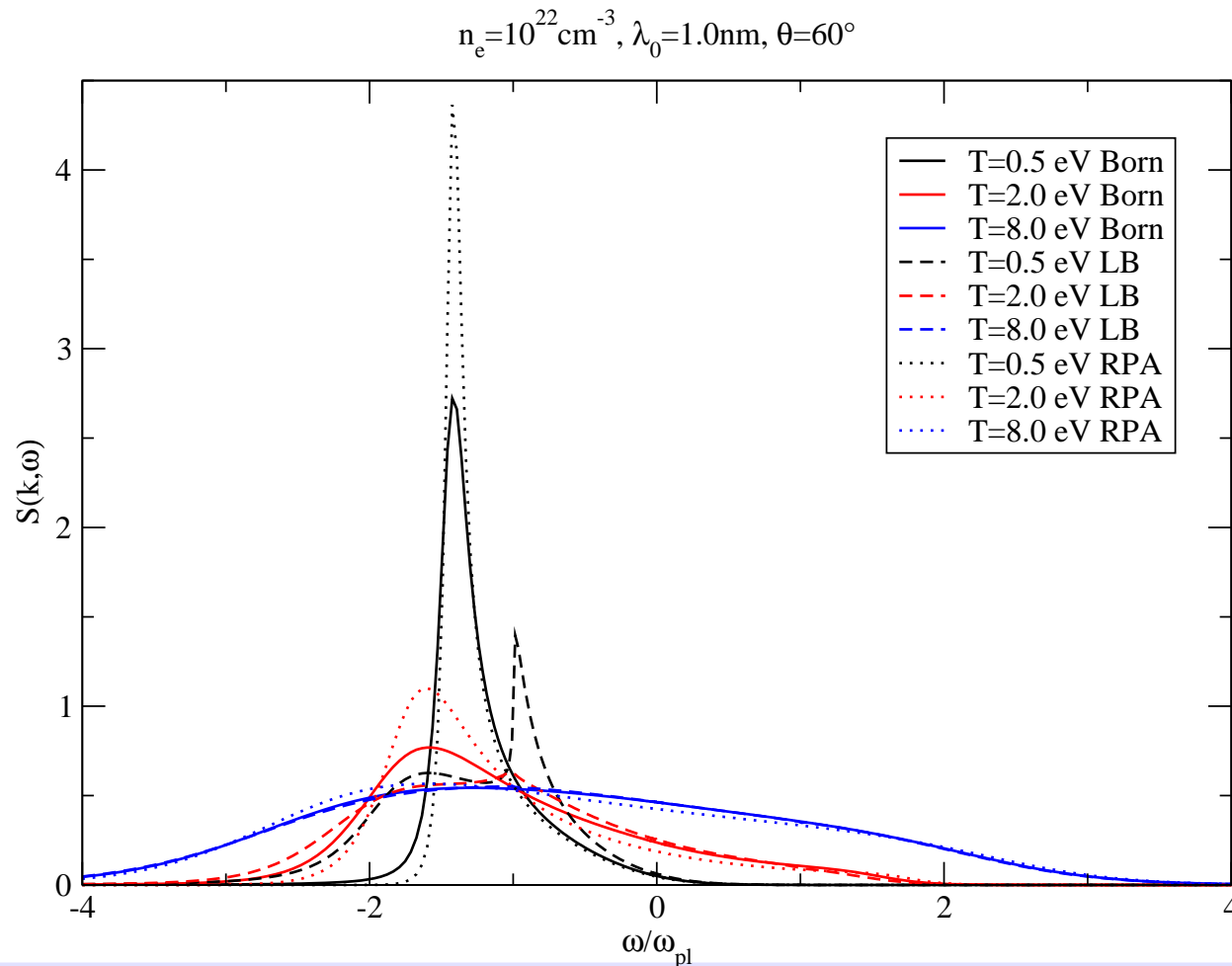
dynamic structure factor for an electron-proton model plasma with Deutsch-like effective interaction in **RPA** and in **Mermin**-like approximation which utilizes a dynamically screened collision frequency  $\nu(\omega)$

*A. Selchow et al. PRE 64 (2001) 056410*

# Thomson scattering

diagnostic tool for warm dense matter:

determination of plasma parameters using VUV and X-ray  
relevance of collision



# Determination of temperature and density

- Electron temperature  $T_e$  can be determined for all frequencies via

**detailed balance:**

$$Y = \frac{S_{ee}(k, \omega)}{S_{ee}(-k, -\omega)} = e^{-\frac{\hbar\omega}{k_B T_e}}$$

- electron density  $n_e$  is given by position of plasmon peak, related to dispersion relation  $\text{Re } \epsilon(k, \omega) = 0$

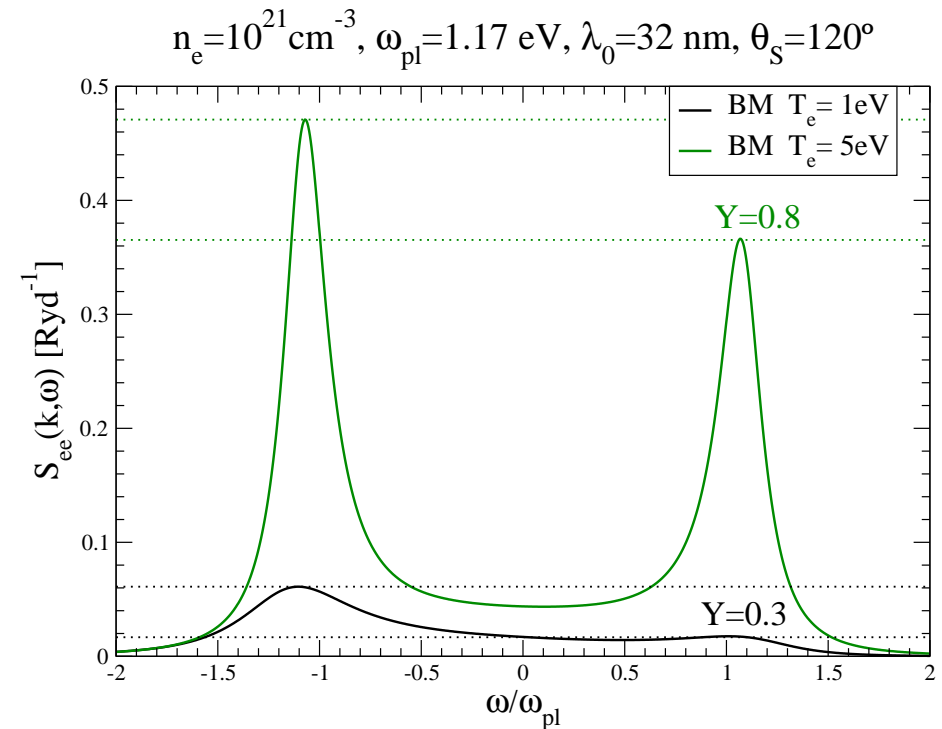
↪ in RPA: **Gross-Bohm** relation [1]:

$$\omega_R^2 \approx \omega_{pl}^2 + 3k^2 v_{th}^2$$

↪ with  $\omega_{pl} = \sqrt{\frac{e^2 n_e}{\epsilon_0 m_e}}$  and the thermal velocity  $v_{th}^2 = k_B T_e / m_e$

- Note: for warm dense matter resonance position  $\omega_R$  can be shifted by collisions

[1] Bohm, Gross, PR 75 (1949) 1851





# Conclusions III

- The **dielectric function** governs different physical properties such as the dc and optical conductivity.
- Central quantity in describing transport and optical properties is the **dynamical collision frequency**.
- Results obtained from **linear response** theory and **MD simulations** are in good agreement for dynamic structure factor as well as in long-wavelength limit.
- In order to describe experimental results
  - inclusion of **bound states** (partial ionization, polarization potential, spectral function, Mott effect)
  - **density and temperature profiles**
- **Thomson scattering** in warm dense matter and **bremsstrahlung** are of particular interest due to recent developments of experimental opportunities.

# Transport properties

many-particle system under the influence of external perturbations  $X_i$ :  
electric field  $\vec{E}$ , temperature gradient  $\nabla T$ , magnetic field  $\vec{B}$

consider electric charge and energy current densities:

$$\vec{J}_{\text{el}} = \sum_i \hat{\mathcal{L}}_{0i} \vec{X}_i = \sigma \left( \vec{E} - S \nabla T \right) + \sigma R_H \left( \vec{J}_{\text{el}} \times \vec{B} \right) + \sigma N \left( \nabla T \times \vec{B} \right)$$

$$\vec{J}_q = \sum_i \hat{\mathcal{L}}_{1i} \vec{X}_i = TS \vec{J}_{\text{el}} - K \nabla T - NT \left( \vec{J}_{\text{el}} \times \vec{B} \right) - L \left( \nabla T \times \vec{B} \right)$$

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$\sigma$  – electrical conductivity

$K$  – thermal conductivity

$S$  – thermopower

$R_H$  – Hall coefficient

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Hall voltage  $U_H$

$$\vec{E}_H = R_H \left( \vec{J}_{\text{el}} \times \vec{B} \right) = \frac{U_H}{d}$$

# Transport and Onsager coefficients

assume geometrical configuration:  $\nabla T \parallel \vec{E} \perp \vec{B}$

components parallel to  $\vec{E}$  and  $\vec{B}$  or  $\vec{B} = 0$

$$\sigma_{\parallel} = e^2 \mathcal{L}_{01}$$

$$S_{\parallel} = \frac{1}{eT} \left( h - \frac{\mathcal{L}_{11}}{\mathcal{L}_{01}} \right)$$

components perpendicular to  $\vec{B}$

$$\sigma_{\perp} = \frac{e^2 \tilde{\mathcal{L}}_{01}}{\eta}$$

$$S_{\perp} = \frac{1}{eT} \left( h - \frac{\tilde{\mathcal{L}}_{11}}{\tilde{\mathcal{L}}_{01}} \left( 1 + \omega_e^2 \frac{\tilde{\mathcal{L}}_{02} \tilde{\mathcal{L}}_{12}}{\tilde{\mathcal{L}}_{01} \tilde{\mathcal{L}}_{11}} \right) \eta \right)$$

$$R_H = - \frac{\tilde{\mathcal{L}}_{02}}{em_e \tilde{\mathcal{L}}_{01}^2} \eta$$

$h$  - enthalpy

electron cyclotron frequency  $\omega_e = \frac{eB}{m_e}$

$$\vec{J} = \text{Tr} \left\{ \hat{j} \hat{\rho} \right\}$$

$$\eta = \left( 1 + \omega_e^2 \frac{\tilde{\mathcal{L}}_{02}^2}{\tilde{\mathcal{L}}_{01}^2} \right)^{-1}$$

# Relaxation time approach

kinetic approach: solving linearized Boltzmann equation with relaxation time approach

$$\tilde{\mathcal{L}}_{ij} = \frac{n_e}{m_e} \left\langle \frac{\epsilon^i \tau^j}{1 + \omega_e^2 \tau^2} \right\rangle$$
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$$\mathcal{L}_{ij} = \frac{n_e}{m_e} \langle \epsilon^i \tau^j \rangle$$

$$\tau = \frac{1}{v_e n_i Q^{ei}}$$

$$\langle \dots \rangle = -\frac{2 m_e}{3 n_e \hbar^2} \int d^3 p \dots v^2 \frac{df_0}{d\epsilon}$$

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$$\sigma_{\perp} = \frac{e^2 n_e}{m_e} \left\langle \frac{\tau}{1 + \omega_e^2 \tau^2} \right\rangle \left( 1 + \frac{\left\langle \frac{\omega_e^2 \tau^2}{1 + \omega_e^2 \tau^2} \right\rangle^2}{\left\langle \frac{\tau}{1 + \omega_e^2 \tau^2} \right\rangle^2} \right) \Rightarrow \sigma_{\parallel} = \frac{e^2 n_e}{m_e} \langle \tau \rangle$$

$$r_H = -e n_e R_H = \frac{\left\langle \frac{\tau^2}{1 + \omega_e^2 \tau^2} \right\rangle^2}{\left\langle \frac{\tau}{1 + \omega_e^2 \tau^2} \right\rangle^2 + \left\langle \frac{\omega_e^2 \tau^2}{1 + \omega_e^2 \tau^2} \right\rangle^2} \Rightarrow r_H = \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2}$$



# Low density limit

$\{P_n\}$	$\sigma^* \ln \Lambda$		$-eS/k_B$		$r_H$	
	$ei$	$ei + ee$	$ei$	$ei + ee$	$ei$	$ei + ee$
0	0.2992	0.2992	0	0	1	1
0, 1	0.9724	0.5781	1.1538	0.8040	1.5325	1.2586
0, 1, 2	1.0145	0.5834	1.5207	0.7110	1.9786	1.2068
0, 1, 2, 3	1.0157	0.5875	1.5017	0.7139	1.9343	1.2077
0, 1, 2, 3, 4	1.0158	<b>0.5892</b>	1.5004	<b>0.7039</b>	1.9333	<b>1.2036</b>
0, 1, ..., 10	<b>1.0159</b>	...	<b>1.5000</b>	...	<b>1.9328</b>	...
Relax app	1.0159	—	1.5000	—	1.9328	—
Spitzer <sup>2</sup>	—	0.591	—	—	—	—
Arbitrary $B$	0.2992	0.2992	0	0	1	1

[1] Reinholz, Redmer and Tamme, *Contrib. Plasma Phys.* **29** (1989)

[2] Spitzer and Härm, *Phys. Rev.* **89** (1953)