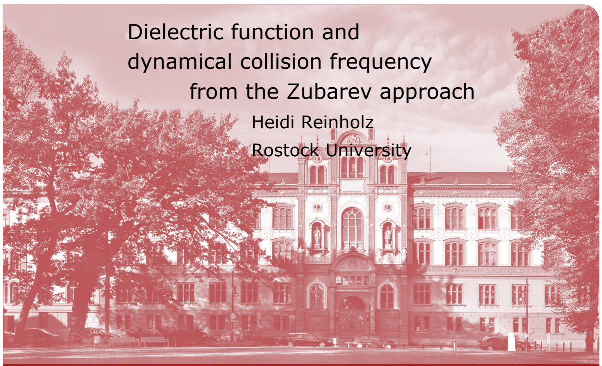


Dielectric function and dynamical collision frequency from the Zubarev approach

Heidi Reinholz
Rostock University

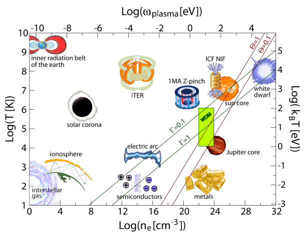
Colloquium Zubarev-100, Dubna 18./19.4.2018

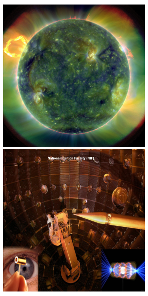
Outline

- Motivation
- Diagnostics – some examples
- Theory - generalized Zubarev formalism
- Diagnostics – more on examples
- Outlook

Motivation

- Dense plasma & warm dense matter



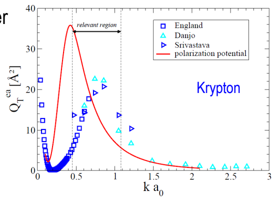


ICF @ NIF, Livermore

Diagnostics

- Dense plasma & warm dense matter
- Diagnostics – some examples
  - ✓ Inert gases (dc conductivity)

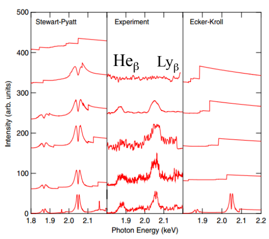
electron-atom-interaction



Diagnostics

- Dense plasma & warm dense matter
- Diagnostics – some examples
  - ✓ Inert gases (dc conductivity)
  - ✓ K_α fluorescence (IPD)

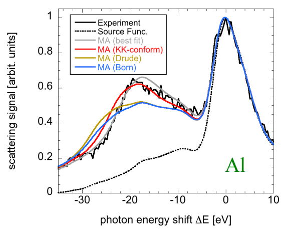
ionization potential depression



shock compressed aluminum
D.J. Hoarty et al., PRL **110**, 265003 (2013)

Diagnostics

- Dense plasma & warm dense matter
- Diagnostics – some examples
  - ✓ Inert gases (dc conductivity)
  - ✓ K_α fluorescence (IPD)
  - ✓ Thomson scattering in Al



Outline

- Dense plasma & warm dense matter
- Diagnostics – some examples
  - ✓ Inert gases (dc conductivity)
  - ✓ K_α fluorescence (IPD)
  - ✓ Thomson scattering in Al
- Theory - generalized Zubarev formalism

Tschernogolovka/Russia
shock waves

FLASH (XUV)
@ DESY Hamburg

Dielectric function

$$\epsilon(\vec{k},\omega) = 1 + \frac{i}{\epsilon_0\omega}\sigma(\vec{k},\omega)$$

✓ Sum rules, Kramers-Kronig relation

➤ dynamical structurfactor $S(\vec{k},\omega) = \frac{1}{\pi\, V(k)}\,\frac{1}{\mathrm{e}^{-\beta\hbar\omega}-1}\,\mathrm{Im}\epsilon_l^{-1}(\vec{k},\omega)$

➤ optical information: reflection, absorption

$$\lim_{k\to 0}\epsilon_t(\vec{k},\omega) = \left(n(\omega) + \frac{ic}{2\omega}\alpha(\omega)\right)^2$$

! dynamical conductivity ←→ statical conductivity

Drude formula $\sigma(\omega) = \frac{\omega_{\rm pl}^2}{i\omega + 1/\tau}$ with relaxation time $\tau = \frac{1}{\nu} = \frac{\sigma_{\rm dc}}{\epsilon_0\omega_{\rm pl}^2}$

Dense plasma

correlated Coulomb systems
- collisions
- medium effects: dynamical screening, collective excitations
- bound states, continuums correlations

$$\hat{H} = \sum_p E_p \hat{a}_p^\dagger \hat{a}_p + \sum_{pq} V_{\rm ei}(q)\hat{a}_{p+q}^\dagger \hat{a}_p + \frac{1}{2}\sum_{p_1p_2q} V_{\rm ee}(q)\hat{a}_{p_1+q}^\dagger \hat{a}_{p_2-q}^\dagger \hat{a}_{p_2}\hat{a}_{p_1}$$

many particle theories
- (linear) response theory $\hat{\rho}(t)$
- kinetic equations $f(\vec{p},t) = \mathrm{Tr}\,\{\hat{\rho}(t)\,\delta\hat{n}_p\}$

$$\vec{j}(t) = \frac{e}{m\Omega_0}\sum_p \hbar\vec{p} f(\vec{p},t) = \frac{e}{m\Omega_0}\vec{P}_1(t) = \frac{e}{m\Omega_0}\mathrm{Tr}\,\{\hbar\vec{p}\delta\hat{n}_p\}$$

$\tilde{j}(\omega) = \sigma(\omega)\tilde{E}$ relaxation time approximation,
Kubo versus Drude formula

Generalized Zubarev formalism

- extended von-Neumann equation

$$\frac{\partial\rho(t)}{\partial t} + \frac{i}{\hbar}[\mathcal{H}^t,\rho(t)] = -\lim_{\epsilon\to 0}\epsilon\,\{\rho(t) - \rho_{\rm rel}(t)\}$$

- no time reversal symmetry due to source term on r.h.s.
- initial conditions/correlations expressed via relevant statistical operator $\rho_{\rm rel}$
- formal solution

$$\rho(t) = \lim_{t_0\to-\infty}\frac{1}{t-t_0}\int_{t_0}^{t}\mathrm{d}t'\mathrm{e}^{-i\mathcal{H}(t-t')/\hbar}\rho_{\rm rel}(t')\mathrm{e}^{-i\mathcal{H}(t-t')/\hbar}$$

- non-equilibrium statistical averages

$$\langle A\rangle^t = \mathrm{Tr}\,\{\rho(t)A\}$$

Bogoliubov 1946, Zubarev 1974, Röpke: Nonequilibrium Stat. Phys. 2013
Zubarev, Morozov, Röpke: Stat. Mech. of Non-Equilibrium Processes, Berlin 1996

Relevant statistical operator

- generalized grand canonical ensemble with respect to a set of relevant observables $\{B_n\}$

$$\hat{\rho}_{\rm rel}(t) = \frac{1}{Z_{\rm rel}}\mathrm{e}^{-\beta(\hat{\mathcal{H}}-\mu\hat{N}) - \sum_n F_n(t)\hat{B}_n} \qquad \hat{\mathcal{H}} = \hat{\mathcal{H}}_0 - \sum_c e_c\hat{\vec{R}}_c\vec{E}_c$$

- from principle of maximum of the entropy

$$S(t) = -k_{\rm B}\mathrm{Tr}\,\{\hat{\rho}_{\rm rel}(t)\ln\hat{\rho}_{\rm rel}(t)\}$$

- self-consistent condition for response parameters F_n

$$\mathrm{Tr}\left\{\hat{\rho}(t)\hat{B}_n\right\} = \mathrm{Tr}\left\{\hat{\rho}_{\rm rel}(t)\hat{B}_n\right\} \quad \text{with} \quad \rho = \rho_{\rm rel} + \rho_{\rm irrel}$$

Linear response

$$\hat{\rho}_{\rm rel}(t) \approx \hat{\rho}_0 + \int_0^1 \sum_n F_n(t)\hat{B}_n(i\lambda\beta\hbar)\hat{\rho}_0\mathrm{d}\lambda$$

generalized Boltzman equation follows from $\mathrm{Tr}\left\{\hat{\rho}_{\rm irrel}(t)\hat{B}_n\right\} = 0$

$$\langle B_m;\dot{\vec{R}}_c\rangle_z e_c\vec{E} = \sum_n\left\{\langle B_m;\dot{B}_n\rangle_z - i\omega\langle B_m;B_n\rangle_z F_n\right\}$$

$$\mathrm{Tr}\,\{\rho B_m\} = \sum_n (B_m;B_n)\,F_n$$

with Kubo scalar product (A;B) and its Laplace transform <A;B>$_z$ – equilibrium correlation function

Relevant observables B_m

$$\langle B_m; \dot{\vec{R}}_c \rangle_z e_c \vec{E} = \sum_n \left\{ \langle B_m; \dot{B}_n \rangle_z - i\omega \langle B_m; B_n \rangle_z \right\} F_n$$

$$\mathrm{Tr}\,\{\rho B_m\} = \sum_n (B_m; B_n)\, F_n$$

$$\frac{\mathrm{d}S(t)}{\mathrm{d}t} = \sum_n F_n(t) \mathrm{Tr}\left\{ \rho_{\mathrm{irrel}}(t) \dot{B}_n \right\}$$

choice of relevant observables is arbitary but determines

- which initial conditions/correlations are taken into account
- dynamical build up of remaining correlations
- explicit solutions after specific approximations (variational principle, perturbation theory, Green function techniques)

Relevant observables B_m

$$\langle B_m; \dot{\vec{R}}_c \rangle_z e_c \vec{E} = \sum_n \left\{ \langle B_m; \dot{B}_n \rangle_z - i\omega \langle B_m; B_n \rangle_z \right\} F_n$$

$$\mathrm{Tr}\,\{\rho B_m\} = \sum_n (B_m; B_n)\, F_n$$

$$\frac{\mathrm{d}S(t)}{\mathrm{d}t} = \sum_n F_n(t) \mathrm{Tr}\left\{ \rho_{\mathrm{irrel}}(t) \dot{B}_n \right\}$$

- ✓ Kubo: $\rho_{rel}=\rho_0$ (curent-current correlations functions) $\sigma(\omega) \propto \langle \vec{j}; \vec{j} \rangle_{\omega+i\eta}$
- ✓ B_n: linear momentum -> force-force correlation function $\nu = \frac{1}{\tau} \propto \langle \vec{F}; \vec{F} \rangle_{i\eta}$

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

- ✓ B_n: one-particle distribution function -> kinetic theory
- ✓ B_n: two-particle distribution function -> bound states
- ✓ B_n: fluctuations $\{\delta n_p\}$ of single-particle occupation number -> kinetic equation

Kinetic equation

- choose fluctuations $\{\delta n_p\}$ of single-particle occupation number as relevant observables $\{B_n\}$ and introduce response parameters $F_p(t)$

$$\delta f(\vec{p}, t) = \sum_{p'} (\delta \hat{n}_p, \delta \hat{n}_{p'})\, F_{p'}(t)$$

$$\delta S(t) = -k_B \sum_p F_p(t)\; \delta f(\vec{p}, t) \leq 0$$

- terms in kinetic equation can be identified

$$\frac{\partial}{\partial t} f(\vec{p}, t) = \mathrm{D}\,[f(\vec{p}, t)] + \mathrm{C}\,[f(\vec{p}, t)]$$

$$-i\omega \delta \tilde{f}(\vec{p}, \omega) = \frac{e\hbar}{m} \beta \tilde{\vec{E}}(\omega) \cdot \vec{p}\, f_p (1 - f_p) + \mathrm{C}\left[\delta \tilde{f}(\vec{p}, \omega) \right]$$

- generalized Kohler variational principle for arbitrary frequency: internal entropy production as functional of an arbitrary function G_p - is a maximum if $G_p=F_p$ is solution of the linear Boltzmann equation [HR, Röpke, PRE (2012)]

Relaxation time vs Drude

- collision term in Boltzmann equation $\mathrm{C}\left[\delta \tilde{f}(\vec{p}, \omega) \right]$
- for relaxation time approximation, taken from static case $C = - \delta f\,(p) / \tau_p$ for Lorentz plasma leading to dynamical conductivity (isotropic system)

$$\sigma_{\mathrm{KT}}(\omega) = \frac{2}{3} \frac{e^2 \hbar^2 \beta}{m^2} \int \frac{d^3\vec{p}}{(2\pi)^3} \frac{p^2 f_p (1 - f_p)}{-i\omega + 1/\tau_p}$$

  - ➢ energy dependent static collision time
  - ➢ Drude type expression is not obtained, no e-e collisions, sum rules not fulfilled

- from linear response theory: generalized Drude expression with collision frequency $\nu(\omega)=1/\tau(\omega)$

$$\mathrm{C}_p[\delta \tilde{f}(\vec{p}, \omega)] = - \sum_{p'} \mathcal{L}_{pp'}(\omega) \tilde{F}_{p'}$$

$$\mathcal{L}_{pp'}(\omega) = \mathcal{L}^{\mathrm{ei}}_{pp'}(\omega) + \mathcal{L}^{\mathrm{ee}}_{pp'}(\omega)$$

$$\sigma_{\mathrm{LRT}}(\omega) = \frac{\epsilon_0 \omega_{\mathrm{pl}}^2}{-i\omega + \nu(\omega)}$$

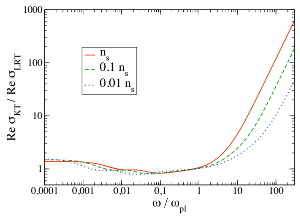
Landau,Lifshitz X; HR, Röpke PRE 2012

Relaxation time vs Drude

$$\nu_{\mathrm{LRT}}(\omega) = r^{(2)}(\omega) \frac{\beta}{m\, n\, \Omega_0} \langle \hat{\dot{P}}_1; \hat{\dot{P}}_1 \rangle_{\omega+i\epsilon}$$

solar core conditions
T=573eV
n_s=1.5 10^{25} cm^{-3}

HR, Röpke PRE 2012



Correction factor $r^{(2)}(\omega)$ due to higher moments, including e-e-correlations, for static case see *S. Rosmej PhD thesis 2018, CPP 56 (2016) 327*

Outline

- Dense plasma & warm dense matter
- Diagnostics – some examples
- Theory - generalized Zubarev formalism
  - ✓ Dielectric function
  - ✓ Non-equilibrium statistical operator
  - ✓ Dynamical collision frequency vs. Relaxation time approximation
- Diagnostics – more on examples
  - ✓ Thomson scattering in Al

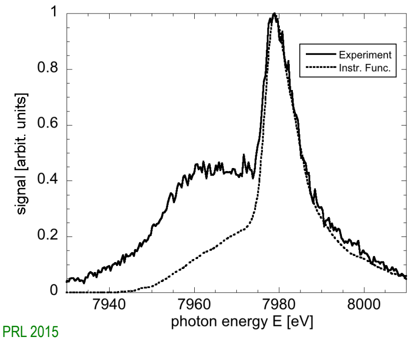
Tschernogolovka/Russia shock waves

FLASH (XUV) @ DESY Hamburg

Thomson scattering from Al foil

n_e= 1.8 10^{22} cm^{-3}
laser @ 7.98 keV
1 μm focal spot

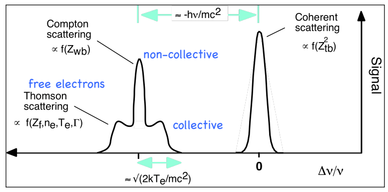
Θ = 24^0 scattering angle



Sperling, HR, Röpke et al. PRL 2015

Thomson scattering

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



interested in:
- free electron density n_e (Z_f)
- temperature T_e

Z_{wb} weakly bound electrons
Z_{tb} bound electrons

intensity I of signal from free electrons determined by Thomson scattering cross section σ_T and strukturfactor S

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

Dynamical structure factor

$$S(\vec{k},\omega) = \frac{1}{\pi\, V(k)} \frac{1}{e^{-\beta\hbar\omega}-1} \,\mathrm{Im}\,\epsilon_l^{-1}(\vec{k},\omega)$$

$$\epsilon(\vec{k},\omega) = 1 - \frac{1}{\epsilon_0 k^2}\,\Pi(\vec{k},\omega)$$

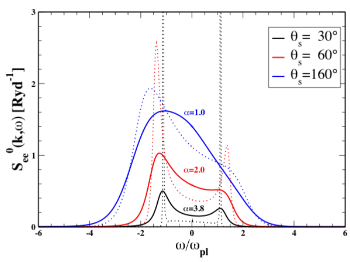
collisonless plasma ➔ RPA approximation

Thomson signal via Mermin approach for (nearly) free electrons @ small wavevectors

$$\epsilon^{\mathrm{Mermin}}(k,\omega) = 1 + \frac{1}{\epsilon_0 k^2} \frac{\Pi^{\mathrm{RPA}}(k,\omega+i\nu(\omega))}{1 - \frac{1}{1-i\omega/\nu(\omega)}\left[1 - \frac{\Pi^{\mathrm{RPA}}(k,\omega+i\nu(\omega))}{\Pi^{\mathrm{RPA}}(k,0)}\right]}$$

dynamical collision frequency $\nu(\omega)$ from generalized Drude type expression

Thomson scattering



R. Thiele et al, PRE 2007

hydrogen:
n_e = 10^{21} cm^{-3}
T = 2 eV
λ_L = 4.13 nm

•••••• ideal plasma
(RPA – random phase approximation)

—— plasma with collisions
(Born-Mermin approximation)

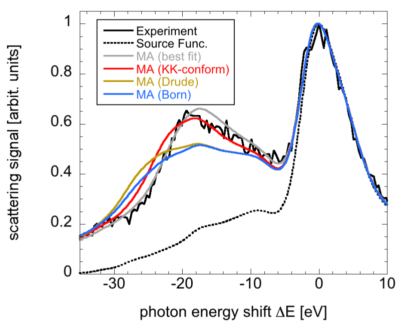
scattering parameter: $\alpha(n_e, T, \lambda_L, \Theta_s)$ > 1 collective scattering on plasmons

Thomson scattering from Al foil

N_e= 1.8 10^{22} cm^{-3}
laser @ 7.98 keV
10 μm focal spot, T=0.5eV
Θ = 24^0 scattering angle

temperature via
- SCFLY simulation code
- detailed balance

KK – Kramers-Kronig relation
(sum rule)



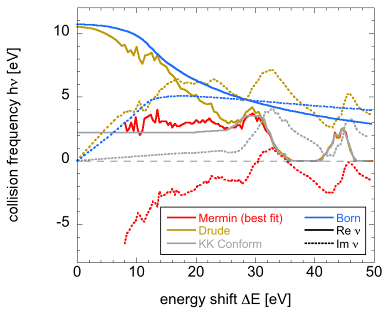
Sperling, Rosmej et al.
PRL 2015, JPB 50 (2017)

Dynamical Collision Frequency

T_e= 0.5 eV
$\hbar\omega_{pl}$=15.75 eV
n_e= 1.8 10^{22} cm^{-3}

conductivity via generalized Drude

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

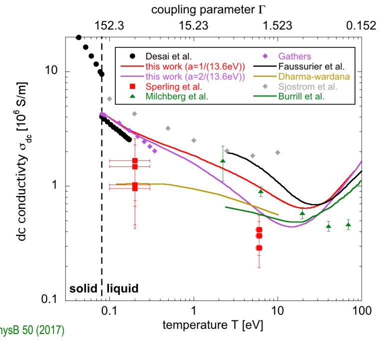


Sperling, HR, Röpke et al. PRL 2015

DC Conductivity in warm dense Al

T_e= 6 eV & 0.5 eV
n_e= 1.8 10^{22} cm^{-3}
Z_{eff} = 3

this work:
- Born approximation
- ionic structure factor: PY with fitted parameters (CHNC)
- pseudopotential with temp. dep. Pauli repulsion (a) and screening



Sperling, Rosmej et al. PRL 2015, JPhysB 50 (2017)

Outlook

Diagnostics of dense plasmas/ warm dense matter

- Consistent treatment of transport and optical properties via Zubarev approach to statistical operator
- Generalized Drude formula for collision frequency in Coulomb systems
  (strong collisions -> t-matrix,
  e-e-collisions -> renormalization factor
  partial ionization -> polarization potential, optical potential)
- dynamical structure factor beyond Born-Mermin

Thank you for your attention

Collaboraters

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