XRTS as Diagnostics for Warm Dense Matter (heated by Particle Beams)

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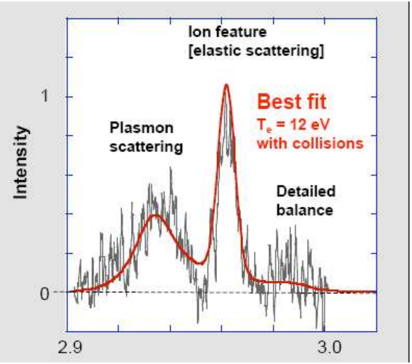
centre for fusion, space and astrophysics

THE UNIVERSITY OF WARWICK

X-Ray Scattering as a Diagnostics - Fit Data to Theory



Forward scattering geometry - small k

Glenzer et al. PRL (2007)

Information obtained

- Electron density:
  from the position of the plasmon peak
- Ionisation degree:
  from the ratio of the electron to and ion feature

Warning: experimental points have been fit to existing/simple theory and might match other theories as well!

X-Ray Scattering – Diagnostics & Theory Test Problem

Light scattered from strongly coupled, partially ionized plasmas

$$P(\theta,\omega) \sim S_{ee}^{tot}(k,\omega) = |f_i(k)+q(k)|^2 S_{ii}(k,\omega) + Z_f S_{ee}^0(k,\omega)$$
$$+Z_b \int d\omega' \, \tilde{S}^{ce}(k,\omega-\omega') S_s(k,\omega')$$

Chihara, 1987, 2000

1st term: **Ion feature** (electrons co-moving with the ions)

- Static approximation possible: $S_{ii}(k,\omega) \sim S_{ii}(k)\delta(\omega)$
- Weak coupling treatment (RPA) fails; **strong correlations** important!
- Needed:
  1. Bound electron density – ion form factor $f(k)$
  2. Electron density in the screening cloud $q(k)$
  3. Ion structure factor $S_{ii}(k)$
- Term yields: ionization degree Z, (ion) temperature T_i

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1^{st} term: **Ion feature** (electrons co-moving with the ions)

2^{nd} term: **Electron feature** (free electrons)

- Dynamic treatment needed (electron modes - plasmons)
- Weak coupling treatment (RPA) appropriate (+ weak collisions)
- Needed: response function for **degenerate** electron gas $\chi(k,\omega)$
- Term yields: electron density n_e, (electron) temperature T_e

3^{rd} term: **Inelastic Raman scattering** (unimportant for light elements)

X-Ray Scattering – Diagnostics & Theory Test Problem

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mainly described in RPA

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Chihara, 1987, 2000

1st term: **Ion feature** **S_{ii}(k), f(k) and q(k) ???**

2nd term: **Electron feature** (free electrons)

- Dynamic treatment needed (electron modes - plasmons)
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Full Quantum Simulations for the Electron/Ion Structure

The goal is to include

- **Full quantum mechanics** (diffractions/exchange) for the electrons
- **All correlations** in the target (especially ionic structure)

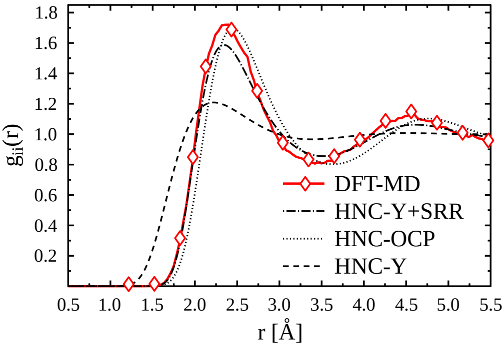
Method applied: Density Functional Theory + MD (DFT-MD)

1. Solve Kohn-Sham equations for given ion positions (effective Schrödinger equation ⇒ states and energy levels)
2. Populate energy levels according to Fermi-distribution
3. Calculate forces (i-i and i-e) on ions ⇒ Move ions; ⇒ **Start again!**
4. After initial time, equilibrium properties follow: $g_{ii}(r)$, $g_{ei}(r)$, p, E_{cor}

Problems:

- Very long run times for DFT-MD (weeks) ⇒ Switch to HNC or MC ?
- Box size and noise make Fourier transformation hard

Ionic Structure: HNC versus DFT-MD (Aluminum)



Warm Aluminium with:

$n_i = 2.7 \times 10^{22}\,\mathrm{cm}^{-3}$

$T = 1.2 \times 10^4\,\mathrm{K}$

(isochorically heated)

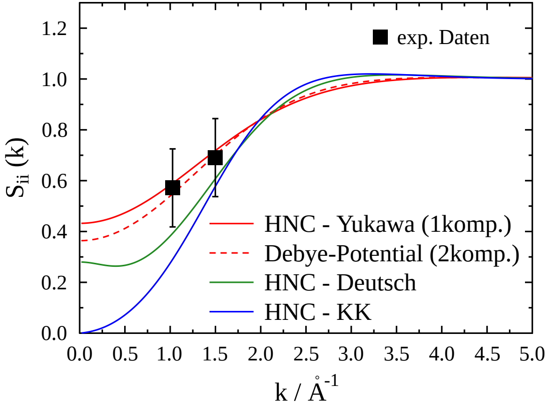
Wünsch et al., PRE (2009)

⇒ **good agreement with Yukawa+SSR model**

- Yukawa model: linearly screened interaction potential (deg. electrons)
- Full shells results additional repulsion at small distances $\sim 1/r^4$ (SRR part)
- Y-SRR Model works for heavier elements as well !

Experimental Verification: Ionic Structure in Lithium

Structure in compressed Lithium



Static structure factor for a lithium plasma with $n_i = 5.2 \times 10^{22}\,\mathrm{cm}^{-3}$, $T = 4.5\,\mathrm{eV}$, $\bar{Z} = 1.35$.

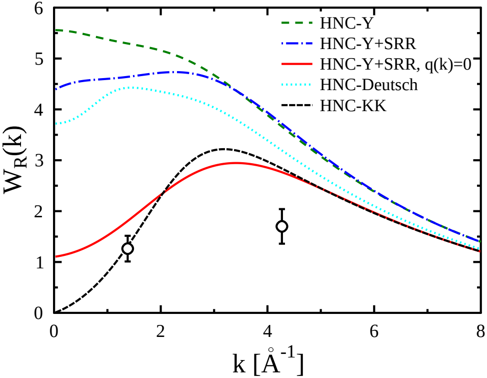
García Saiz et al., Nature Physics (2009)

Insights gained:

- Good agreement: DFT-MD simulations and experiments
- Good agreement: linearly screened HNC and experiments
- HNC with quantum potentials yields too strongly coupled ions (screening too weak)

Experimental Verification: Ionic Feature for Beryllium

Weight of the Ion Feature in Isochorically Heated Beryllium



Exp. data: Glenzer et al., PRL (2003/2007)

Ion peak using HNC

$$W_R(k) = |f_i(k) + q(k)|^2 \, S_{ii}(k)$$

plasma parameters:

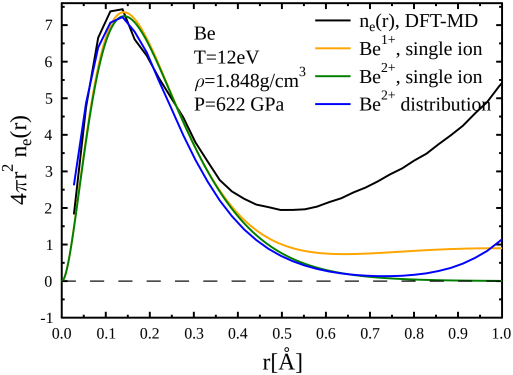
$n_i = 1.23 \times 10^{23}\,\mathrm{cm}^{-3}$,

$T = 12\,\mathrm{eV}$, $Z = 2$

$\Rightarrow$ **Agreement of KK–Exp. is mainly due to compensating errors!**

$\Rightarrow$ **Best agreement with experiments is achieved for q(k) = 0**

Bound State Structure in Beryllium from DFT-MD



Warm Beryllium with:

$n_i = 1.23 \times 10^{23}\,\mathrm{cm}^{-3}$

$T = 1.39 \times 10^{5}\,\mathrm{K}$

(isochorically heated)

⇒ **Many bands needed!**
energy cutoff $>$4000 eV

⇒ **Core structure resolved!**

⇒ **Charge state of $Z = 2$**

⇒ **Core structure yield valuable information:**

- Electron densities for small distances unchanged from isolated ions
- No hint of further ionization beyond $Z = 2$
- Screening cloud hard to diagnose as signal dominated by 1s electrons

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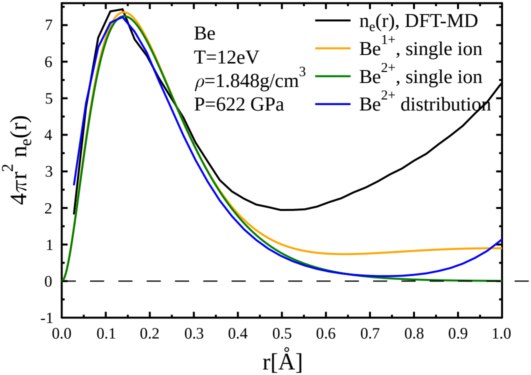

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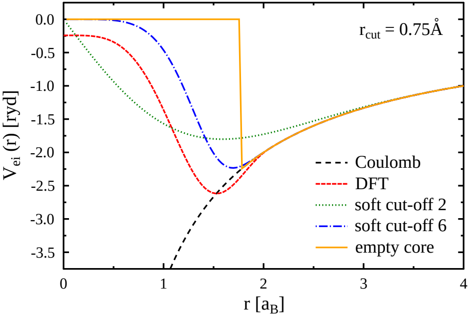
⇒ **X-ray scattering signal at small k not well described: q(k)?**

Screening Function q(k) for Partially Ionized Matter

New physics to take into account:

- Debye/Thomas-Fermi screening ignores effect of bound electrons, but uses effective charge only (Coulomb interactions on all scales!)
- Bound electrons block real space around ionic cores

⇒ Successful concept from solid state physics: **empty core potentials**



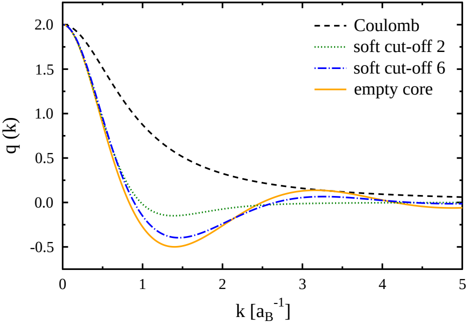
- Type 1: hard cutoff Coulomb potential
- Type 2: soft cutoffs $\sim \left[1 - e^{(r/r_c ut)^{\alpha}}\right]$
- DFT pseudo-potenial for comparison

⇒ Use these pseudo-potenials in linear response theory to obtain q(k)!

Screening Function q(k) for Partially Ionized Matter

Effect of different pseudo-potenials on the screening function:

- General solution:
  $q(k) = \chi_e^{RPA}(k)\, V_{ei}(k)$
- hard cutoff potential:
  $q(k) = Z\, \frac{\kappa_e^2}{k^2+\kappa_e^2}\, \cos(kr_{cut})$
  (κ_e inverse screening length)
- other potentials:
  numerical results only



$\Rightarrow$ Large changes due to pseudo-potenitals possible for intermediate k

$\Rightarrow$ Even negative q(k) are possible, but correct $k \to 0$ behavior

$\Rightarrow$ Effect depends strongly on value of cut-off radius r_{cut}

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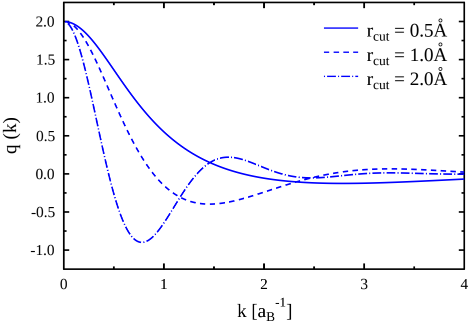

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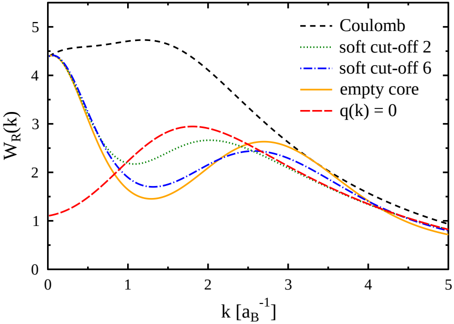
Screening Function q(k) for Partially Ionized Matter

Effect of pseudo-potenials on the weight of the Rayleigh peak:



Gericke et al. (submitted)

Rayleigh peak defined by:

$$W_R(k) = |f_i(k) + q(k)|^2 \, S_{ii}(k)$$

plasma parameters:

$n_i = 1.23 \times 10^{23}\,\text{cm}^{-3}$,

$T = 12\,\text{eV}$, $Z = 2$

⇒ Large modulations due to pseudo-potenitals for intermediate k

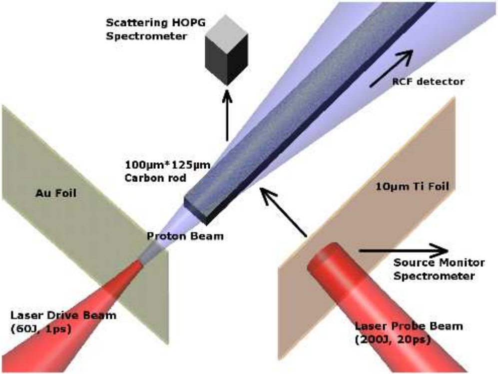
⇒ Trend towards experimental results, but no qualitative agreement

⇒ Different k-behavior than in experiments found (no linear increase);

⇒ experimental results are still best described by $q(k) = 0$ curve

Probing Melting of Carbon by X-ray Thomson Scattering

Setup of an ion beam-driven melting experiment



Probing the ion peak
+ incoherent scattering

- Heating by laser ions
- Heating is isochorically
- Melting possible, **but** carbon has no fluid phase under normal pressure

A. Pelka et al. (submitted)

⇒ **Inertial confinement of high pressure liquid**
⇒ **XRTS can be used as a probe for phase transition**

Probing Melting of Carbon by X-ray Thomson Scattering

The following 4 slides have been deliberately removed to allow for on-line posting of the talk.

Apologies for inconveniences this removal might cause.

Dirk Gericke

Thanks to many collaborators from

- University of Oxford,
- Technische Universität Darmstadt,
- Queen's University Belfast,
- Lawrence Livermore National Laboratory,
- Sandia National Laboratories,
- Goethe Universität Frankfurt,
- University of California at Los Angeles,
- University of Warwick

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Thank you!