New Perspectives for the *ab-initio* Simulation and Diagnostics of Warm-dense Matter

T. Dornheim[1,2], J. Vorberger[2], Zh. Moldabekov[1,2], M. Böhme[1,2,3], K. Ramakrishna[1,2,3], M. Bonitz[4], D. Kraus[5,2], T. Döppner[6], T. Preston[7], P. Tolias[8]

[1]CASUS | [2]HZDR | [3]TU Dresden | [4]Kiel University | [5]Rostock University | [6]LLNL | [7]European XFEL | [8]KTH Stockholm

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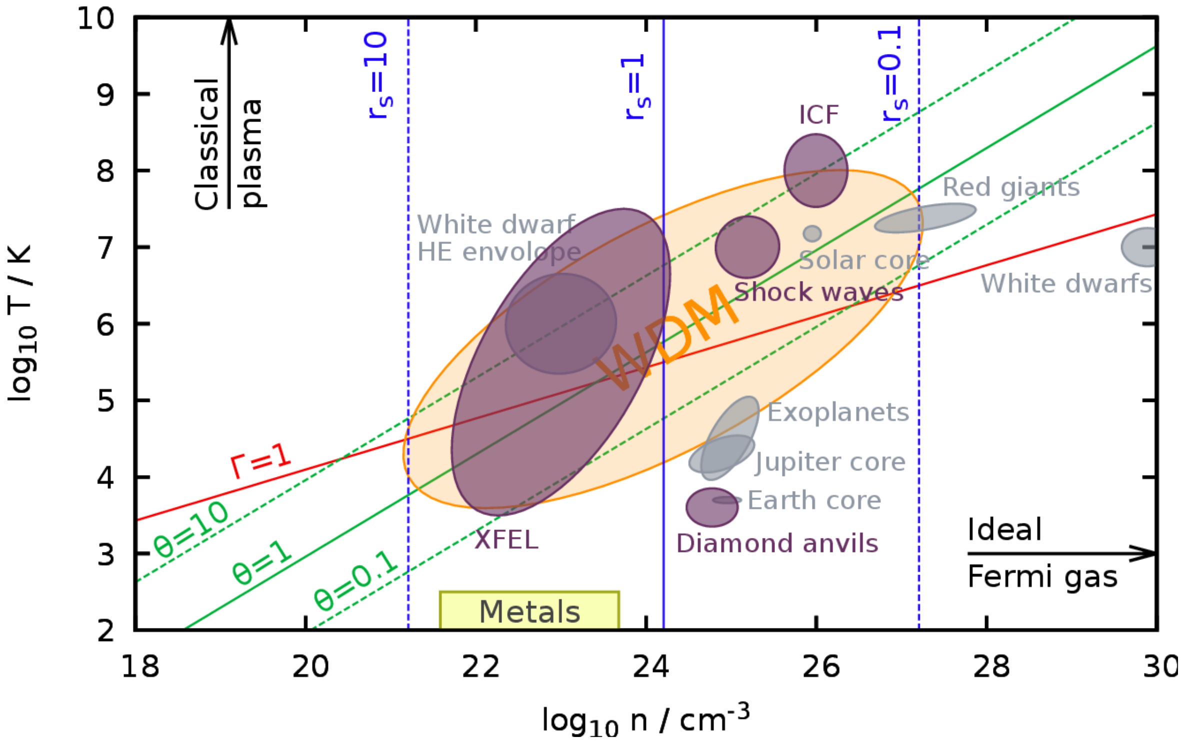
Introduction

Warm Dense Matter (WDM)

- Matter under extreme density / temperature ubiquitous throughout our universe

$r_s \sim \theta \sim \Gamma \sim 1$

→ $r_S = d/a_B$, density parameter, $\theta = k_B T/E_F$, $\Gamma = W/E_{kin}$



Taken from: **T. Dornheim**, S. Groth, and M. Bonitz, *Phys. Rep.* **744**, 1-86 (2018)

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- Examples: giant planet interiors, brown dwarfs

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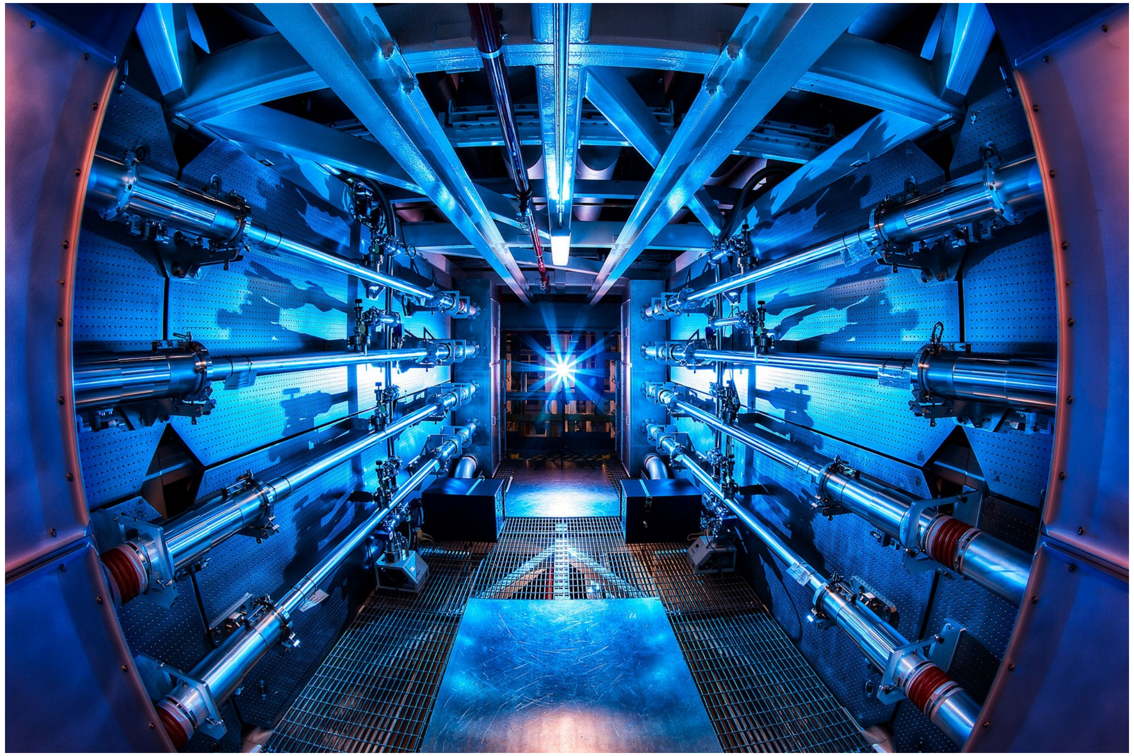
- WDM highly important for technological applications:

→ Inertial confinement fusion, etc.

National Ignition Facility (NIF)



Taken from: Lawrence Livermore National Laboratory

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WDM routinely realized in large research facilities around the globe!

- WDM highly important for technological applications:

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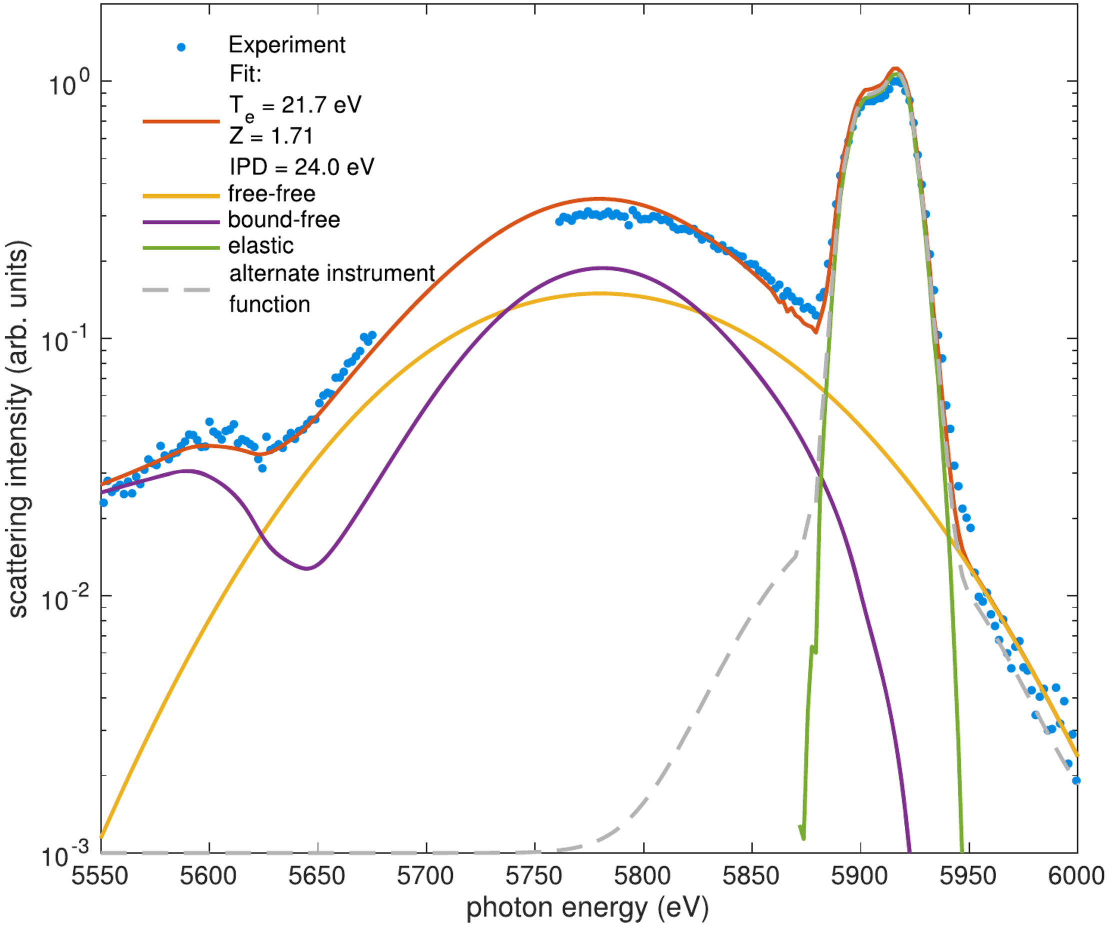
But: Rigorous WDM theory indispensable

• Diagnostics: parameters like T, n, Z, etc. cannot be measured and have to be inferred from theory

→ X-ray Thomson scattering (XRTS)

Isochorically heated graphite at LCLS (Stanford)



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- **WDM theory notoriously challenging**

$$r_s \sim \theta \sim \Gamma \sim 1$$

→ intricate interplay of:

1) Coulomb coupling

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How to achieve a real *ab initio* description of WDM?

Can we do XRTS diagnostics of WDM without models / approximations?

Ab-initio Quantum Monte Carlo (QMC) simulations

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Problem:

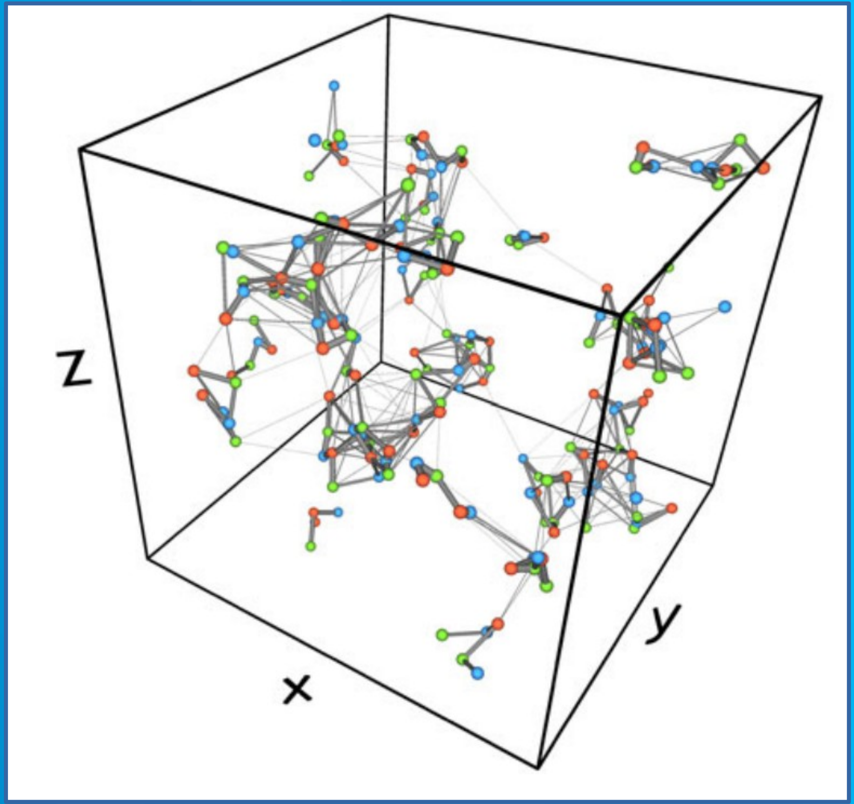
- **Density functional theory (DFT)** etc. require external input about XC-effects

→ finite *T*: XC-free energy f_{xc}

Solution:

- **Quantum Monte Carlo** methods in principle allow for exact solution of quantum many-body problems without any empirical input

- Finite *T*: **Path Integral Monte Carlo (PIMC)**



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Previous result: XC-free energy of UEG

S. Groth, T. Dornheim, T. Sjostrom, F.D. Malone, W.M.C. Foulkes, and M. Bonitz, PRL 119, 135001 (2017)

Impact on thermal DFT simulation of warm dense hydrogen

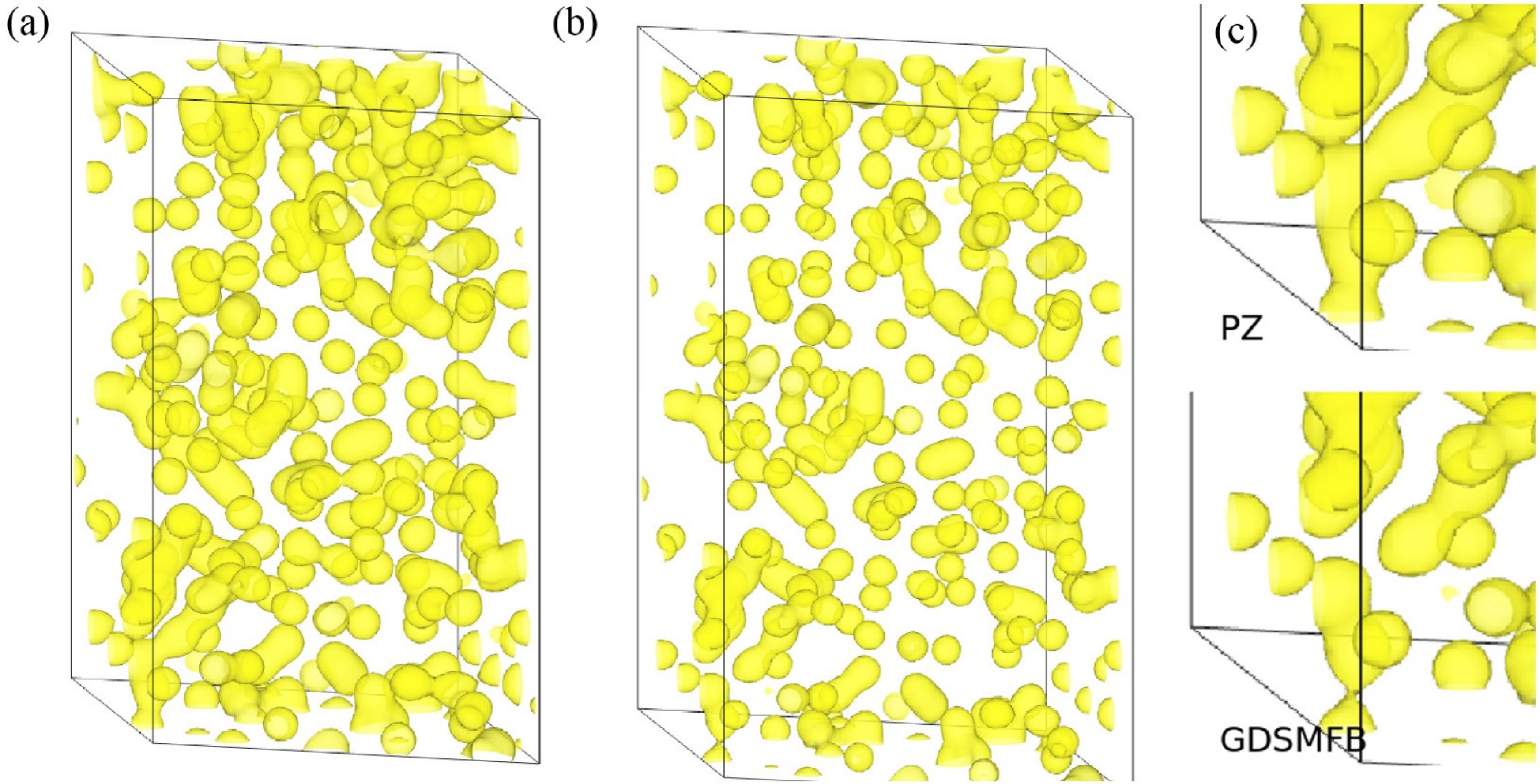
Example:

Hydrogen at T=65,000K

$r_s = 2$

(a) Ground-state LDA by Perdew And Zunger, PRB (1980) [PZ]

(b) our thermal LDA [GDSMFB]



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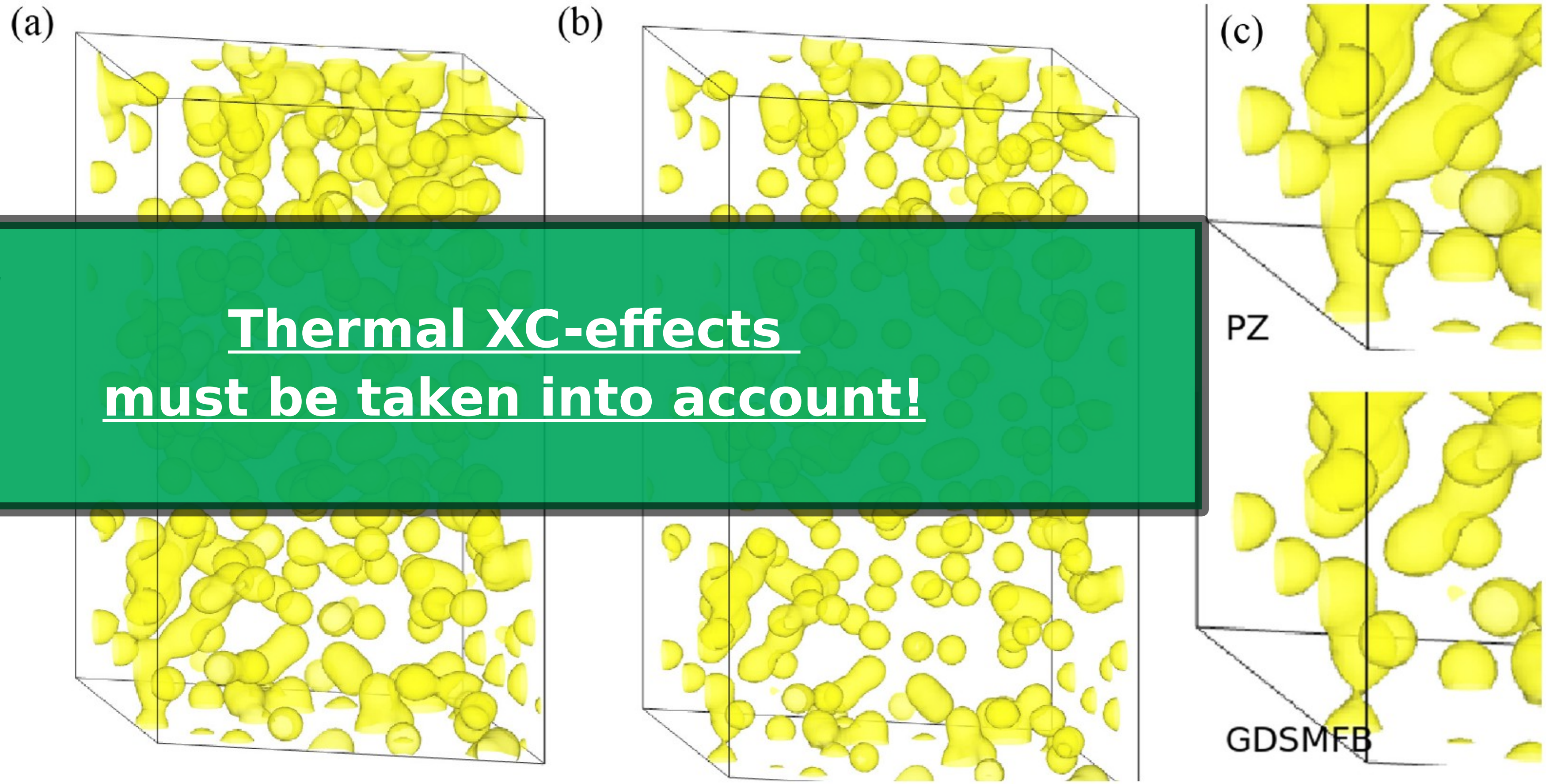

Thermal XC-effects must be taken into account!

Taken from: K. Ramakrishna, **T. Dornheim**, and J. Vorberger, *Phys. Rev. B* **101**, 195129 (2020)

Density response functions, local field correction

- Dynamic density response function

$$\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - \frac{4\pi}{q^2}\left[1 - G(q,\omega)\right]\chi_0(q,\omega)}$$

→ $\chi_0(q,\omega)$ ideal density response function

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Important input for many applications:

→ Advanced nonlocal XC-functionals for DFT

→ Stopping power, electronic friction, …

→ Effective potentials

→ Electrical/thermal conductivity

→ Interpretation of XRTS experiments

→ …

Part II: Static density response of WDM

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Imaginary time $\tau\in[0,\beta]$

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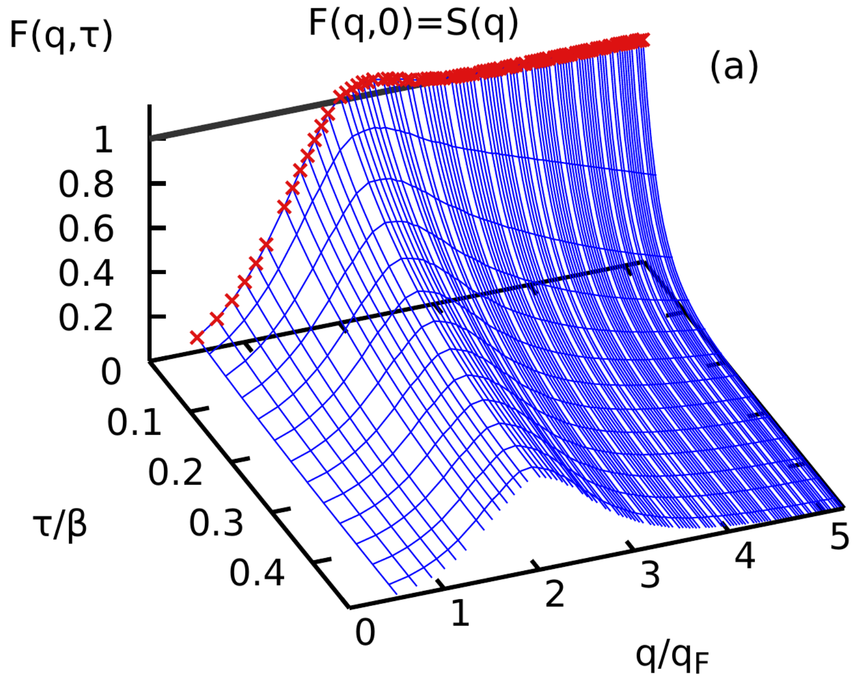

Taken from: **T. Dornheim**, T. Sjostrom, S. Tanaka, and J. Vorberger, Phys. Rev. B **101**, 045129 (2020)

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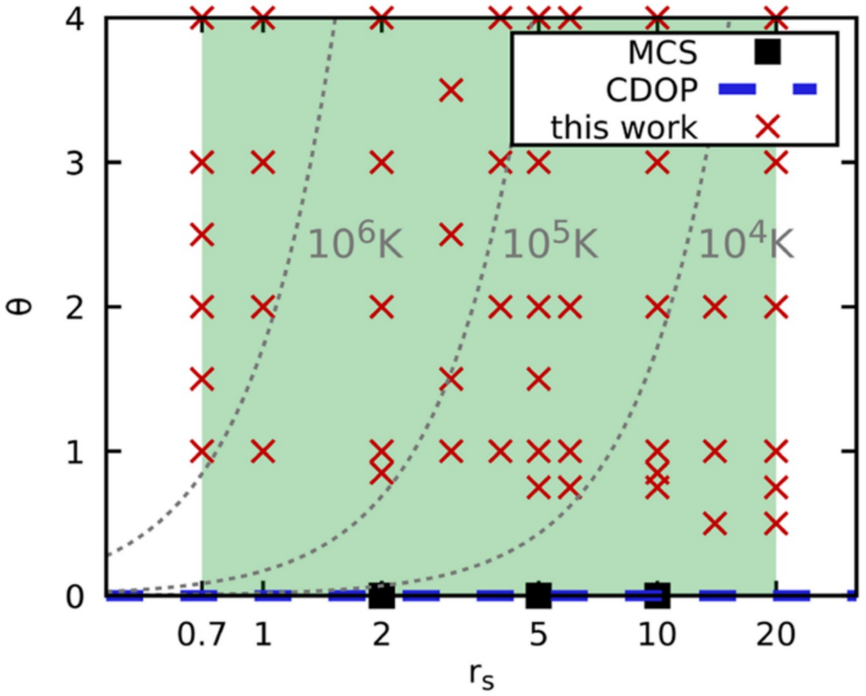

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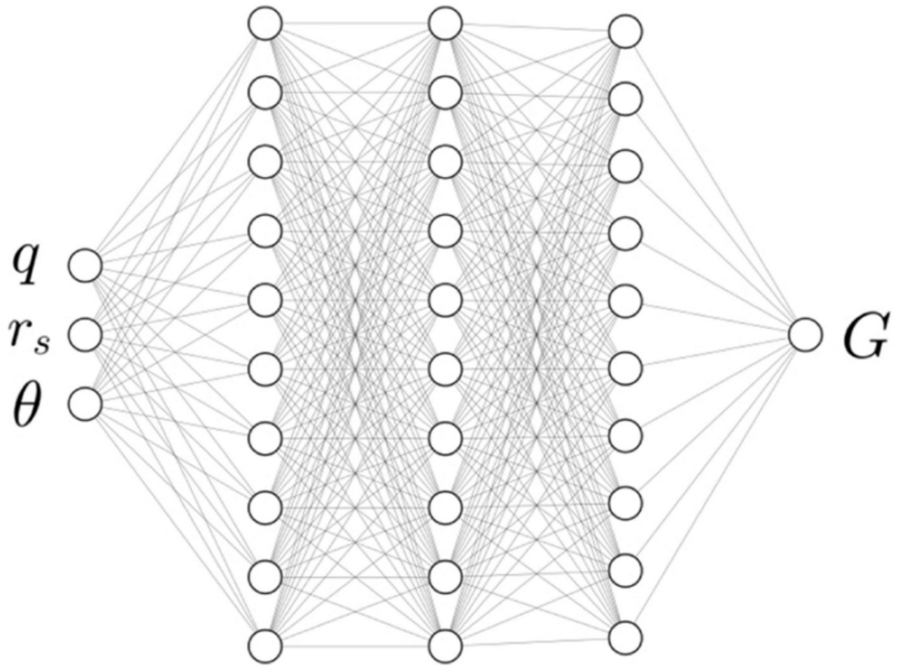
Neural net representation covering full WDM regime.



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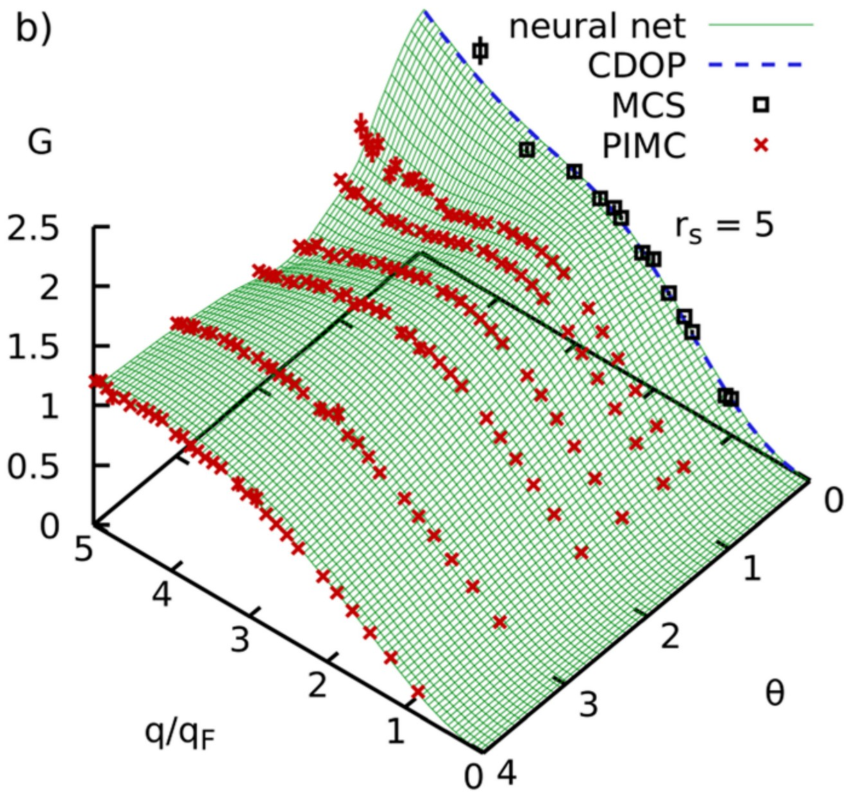

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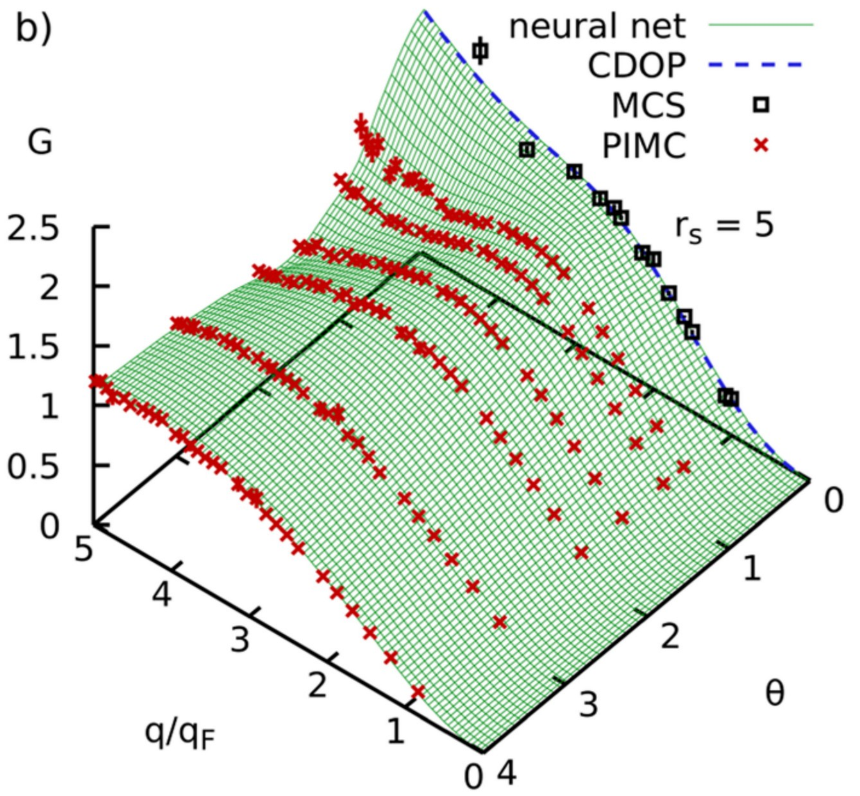

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First results for XC-kernel of hydrogen:

M. Böhme, Zh. Moldabekov, J. Vorberger, and **T. Dornheim**, *Phys. Rev. Lett.* **129**, 066402 (2022)

Part II: Static density response of WDM

Density response of warm dense hydrogen

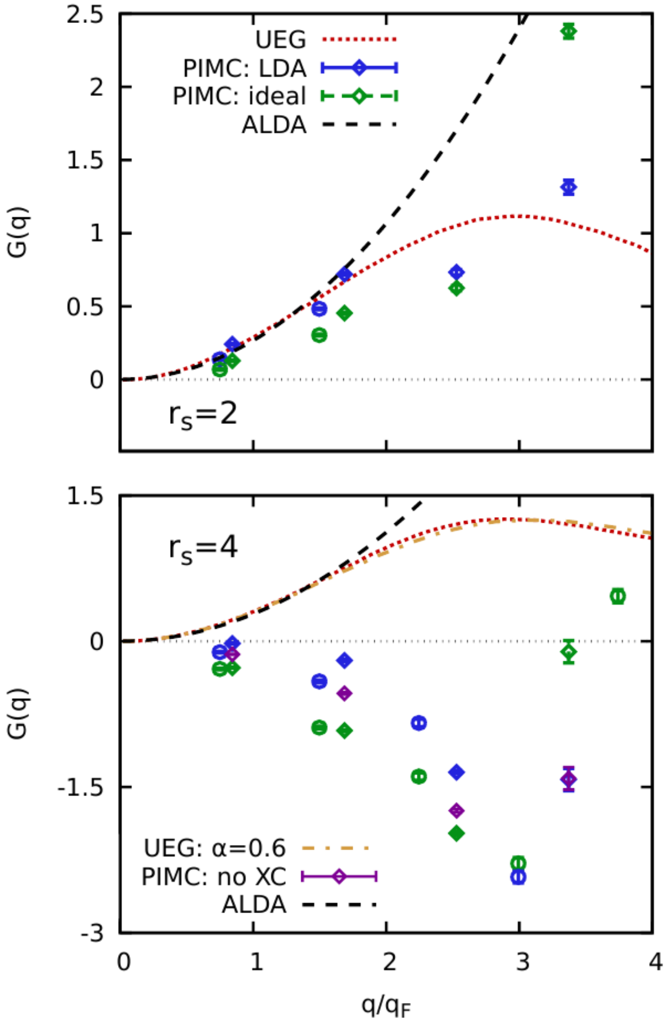
- **Exact exchange-correlation kernel of hydrogen (PIMC)**
  → Benchmark Adiabatic LDA (ALDA) etc
  → Influence of partial localization around ions?
  → …

- **UEG models break down at low density**

- **Future works:**
  → input for time-dependent DFT, etc
  → development of new XC-functionals
  → predict NIF experiments
  → …

Exchange—correlation kernel of warm dense hydrogen

Taken from: M. Böhme, Zh. Moldabekov, J. Vorberger, and **T. Dornheim**, *Phys. Rev. Lett.* **129**, 066402 (2022)



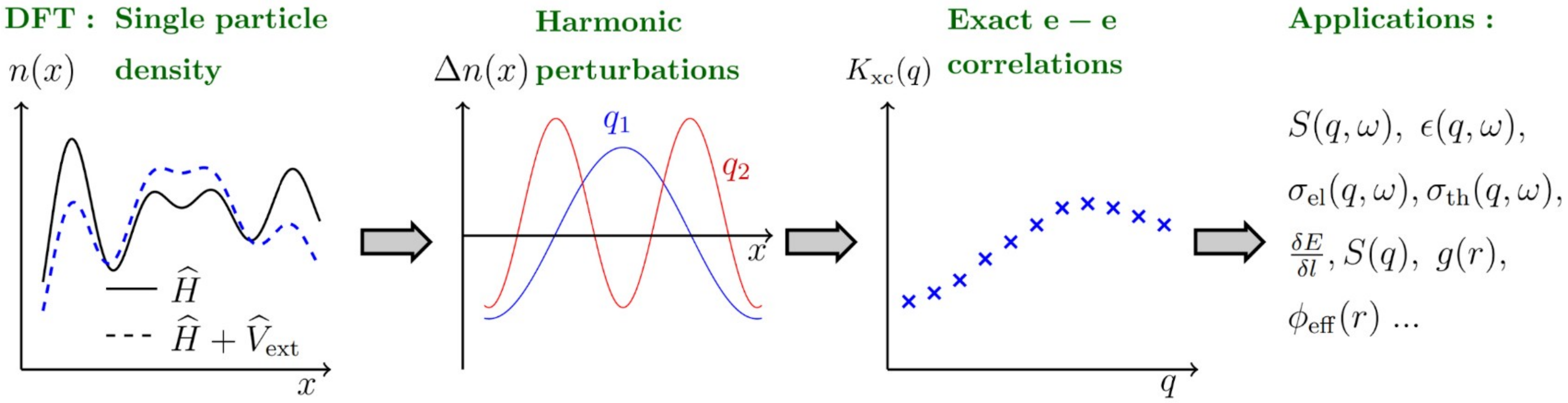
Part II: Static density response of WDM

Density response of real materials

- **Compute exchange—correlation kernel from DFT simulations**
  → Problem: DFT limited to singe-electron density
  → Solution: Perturb system, compute density response

→ **DFT gives access to exchange—correlation kernel**

Taken from: Zh. Moldabekov, M. Böhme, J. Vorberger, D. Blaschke, and **T. Dornheim**, arXiv:2209.00928



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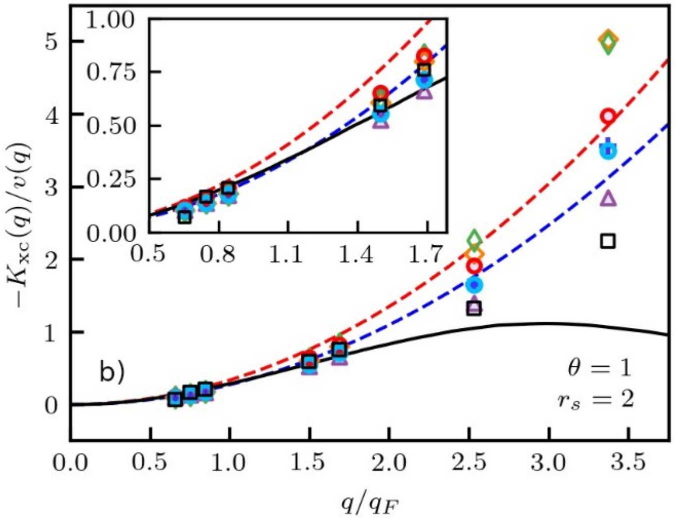
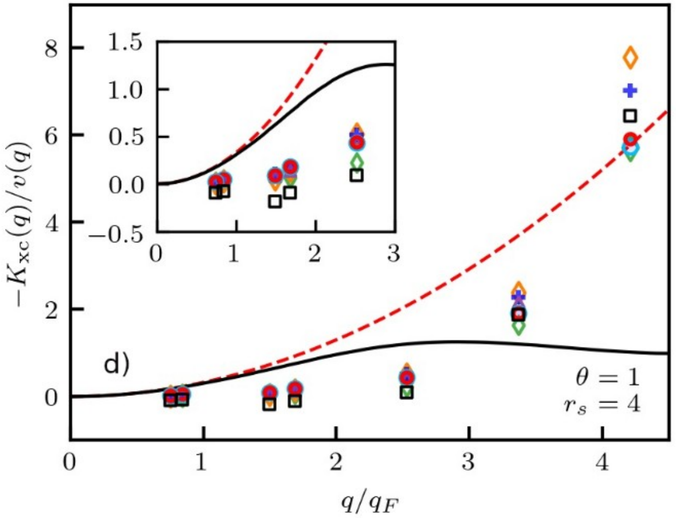
- **DFT capable to generate electronic XC-effects**
  → insights into performance of XC-functionals
  → XC-effects of real materials
  → …





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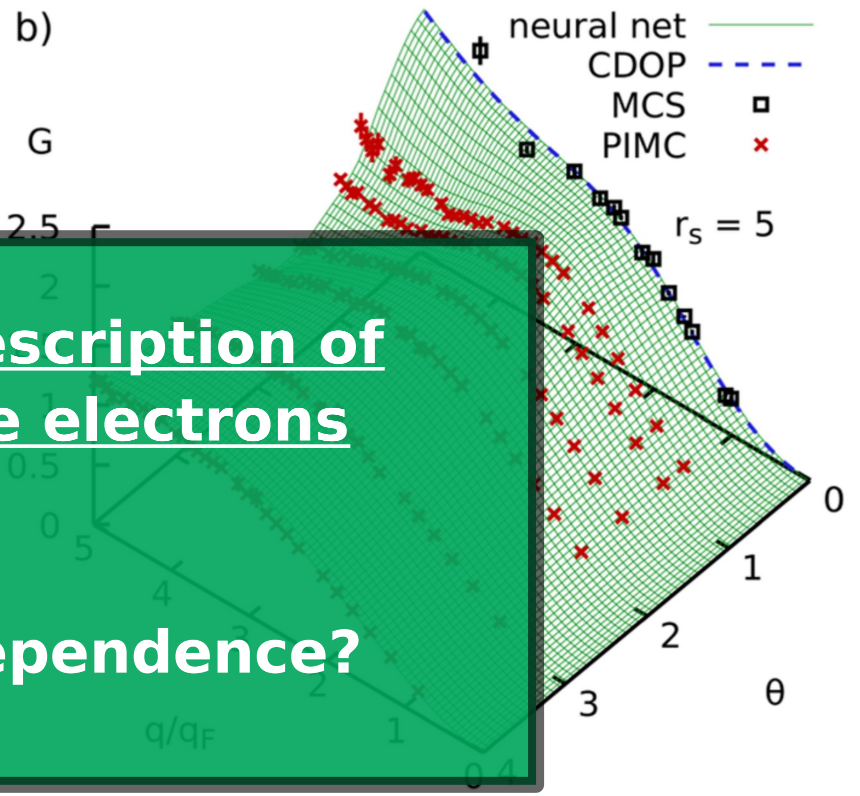
Wave-number resolved description of XC-effects of warm dense electrons

What about frequency-dependence?



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Part II: Dynamic density response of WDM

Need for dynamic properties of WDM

- **WDM Diagnostics:** obtain plasma parameters from XRTS experiments

→ Dynamic structure factor

$$F(q,t) = \frac{1}{N}\langle \rho(q,t)\rho(-q,0)\rangle$$

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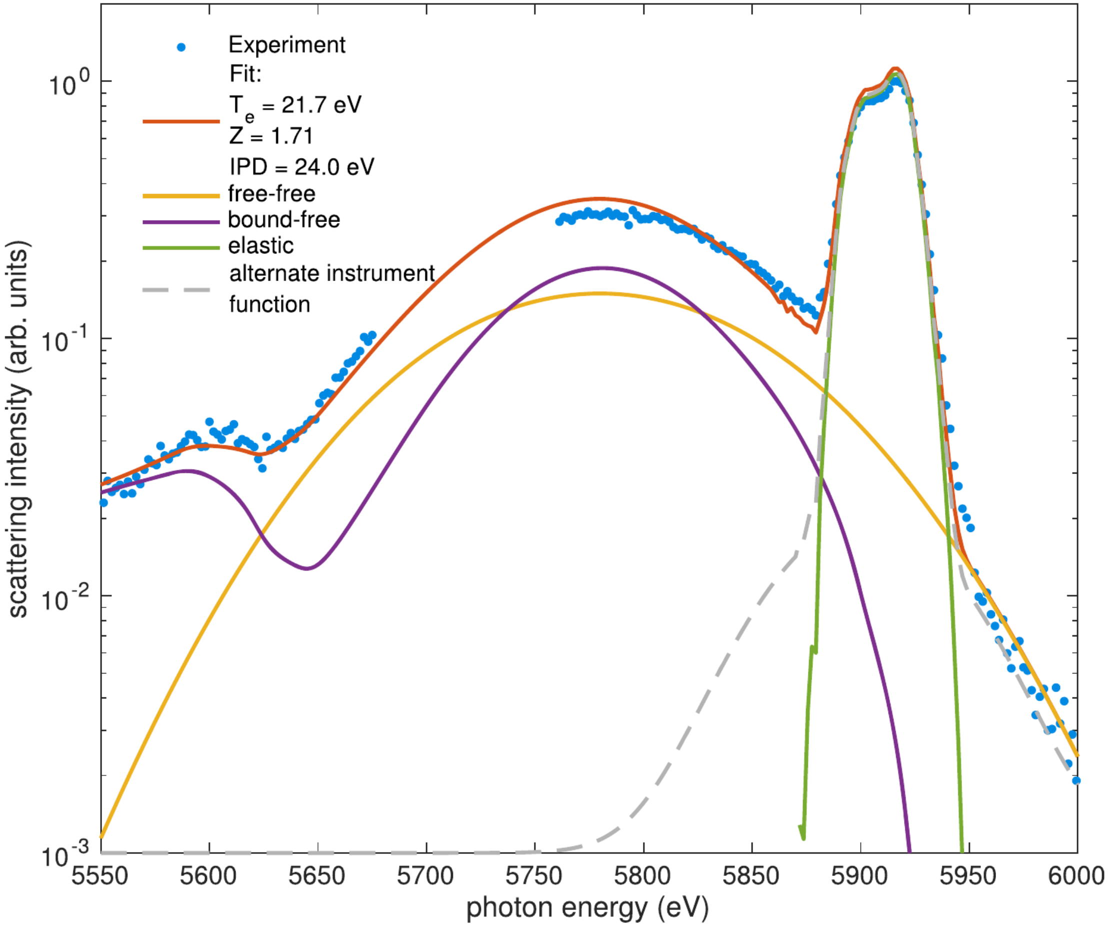

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• **Rigorous description of dynamic properties even more challenging then TD equilibrium**

→ TD-DFT: adiabatic approximation, no XC-kernel

→ Green functions: approximation in coupling

→ PIMC: Imaginary time, **analytic continuation possible for UEG!**

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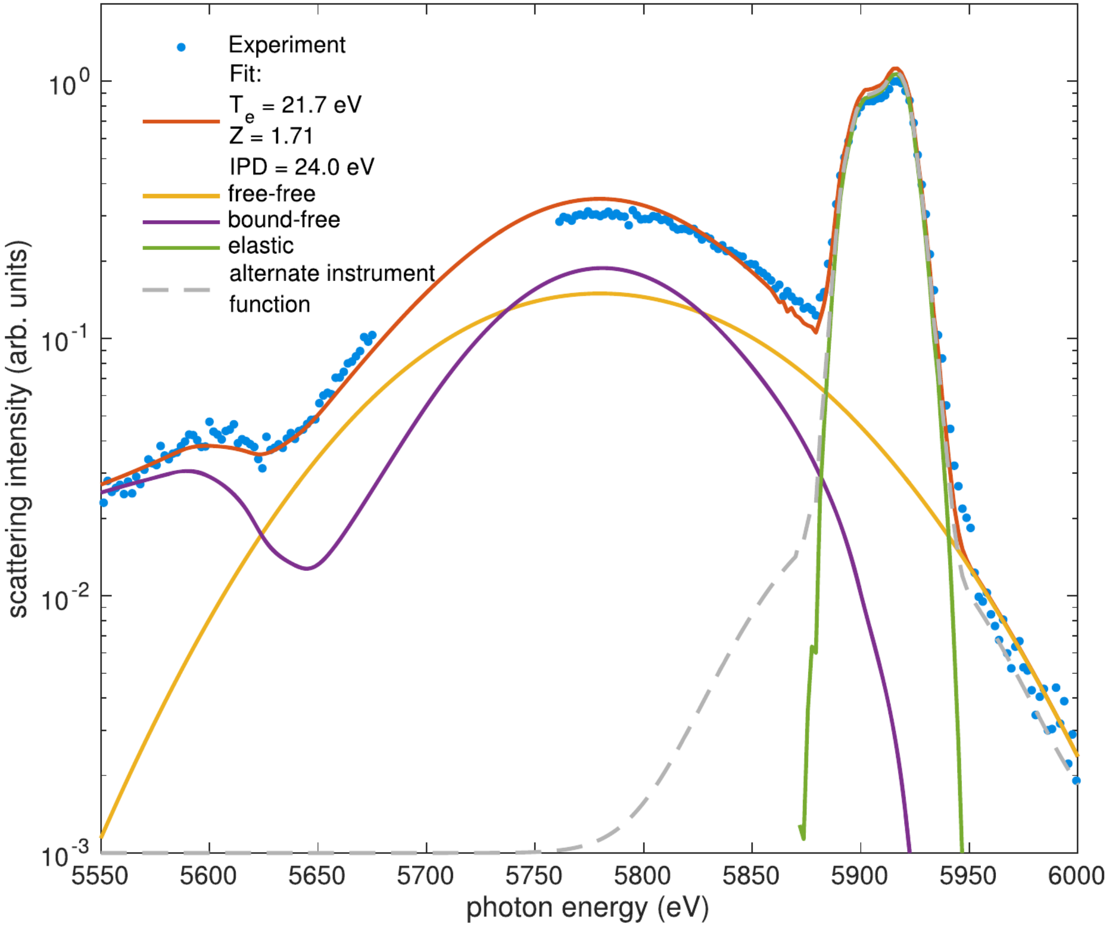

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First *ab-initio* results for dynamic structure factor of UEG

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RPA: G(**q**,ω)=0

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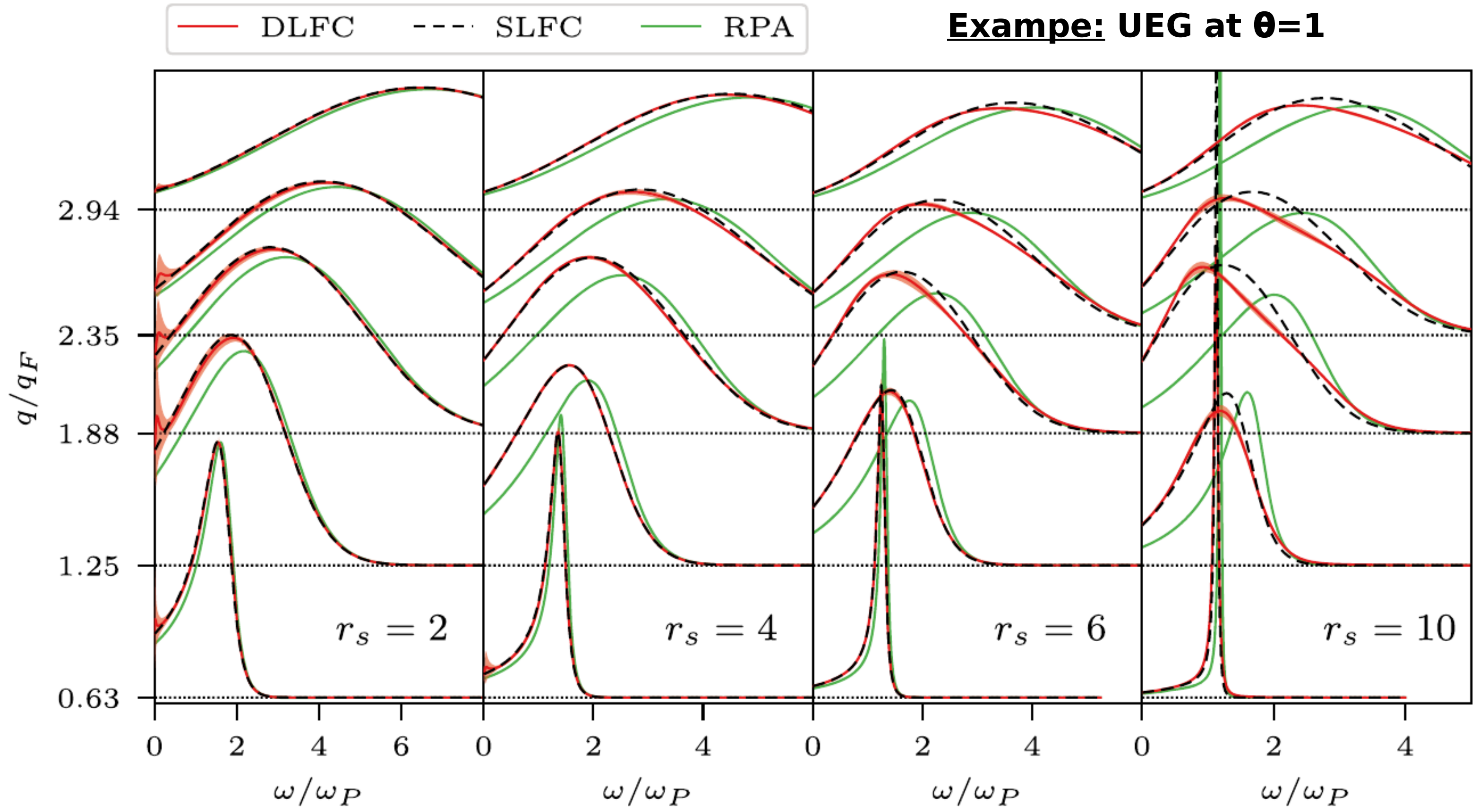
→ static approximation

Exampe: UEG at **θ=1**



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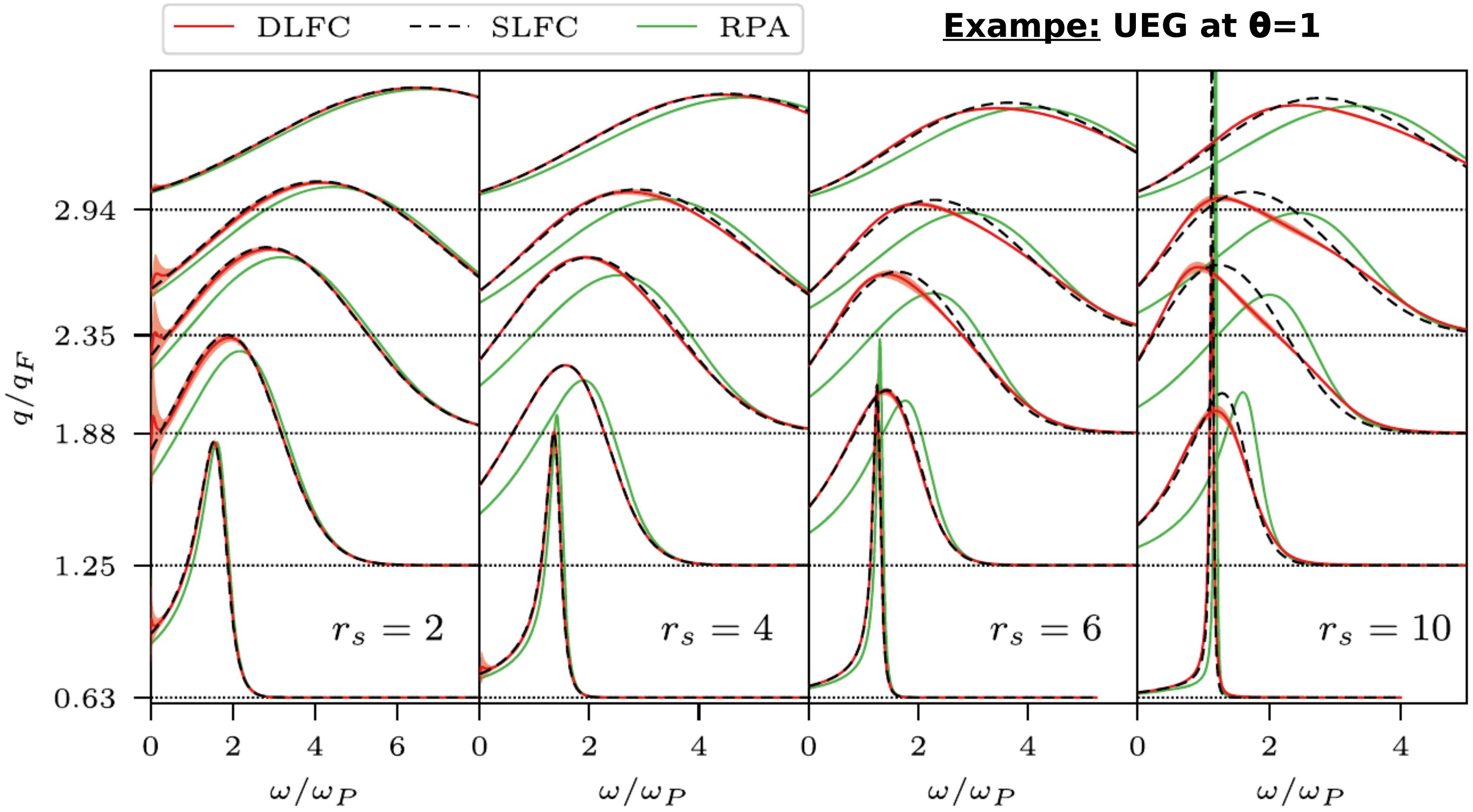

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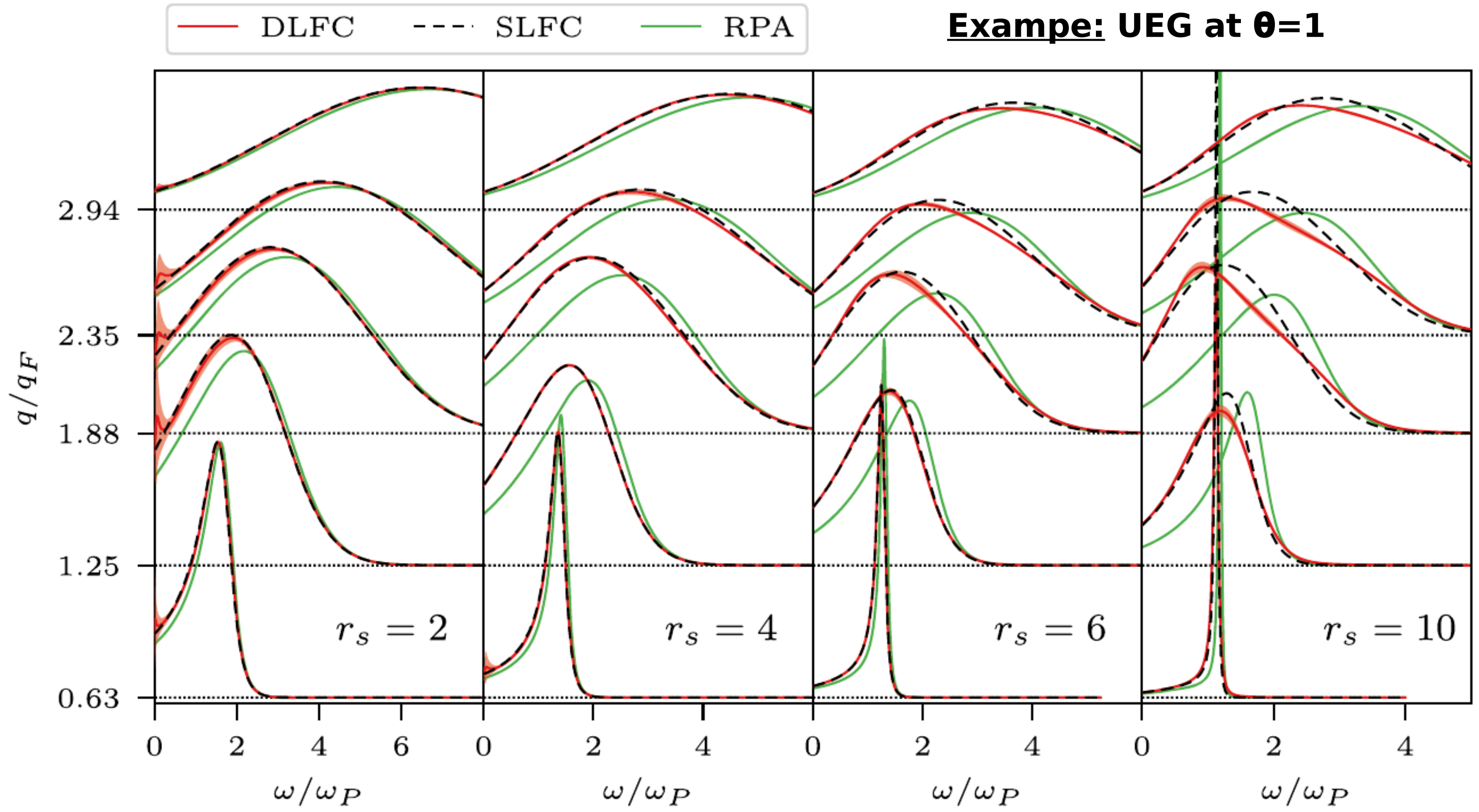

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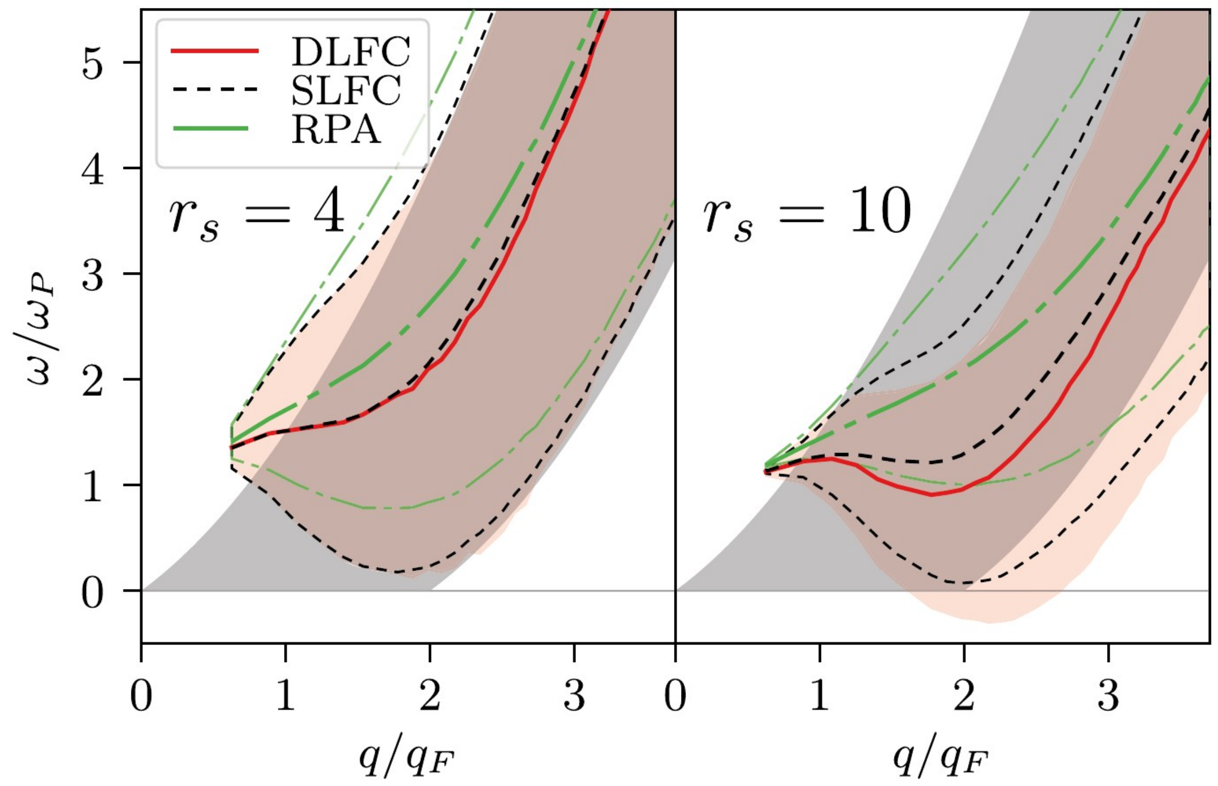

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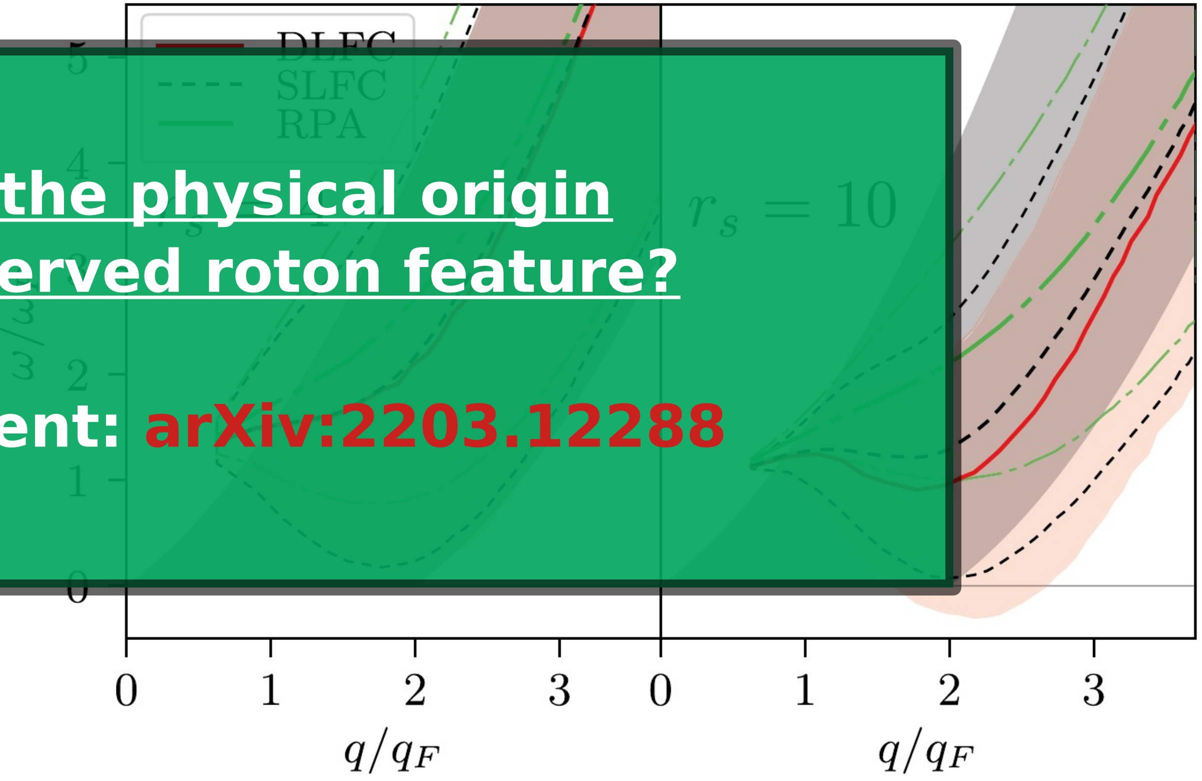


What is the physical origin of the observed roton feature?

Pair alignment: arXiv:2203.12288

Taken from: **T. Dornheim**, S. Groth, J. Vorberger, and M. Bonitz, *Phys. Rev. Lett.* **121**, 255001 (2018)

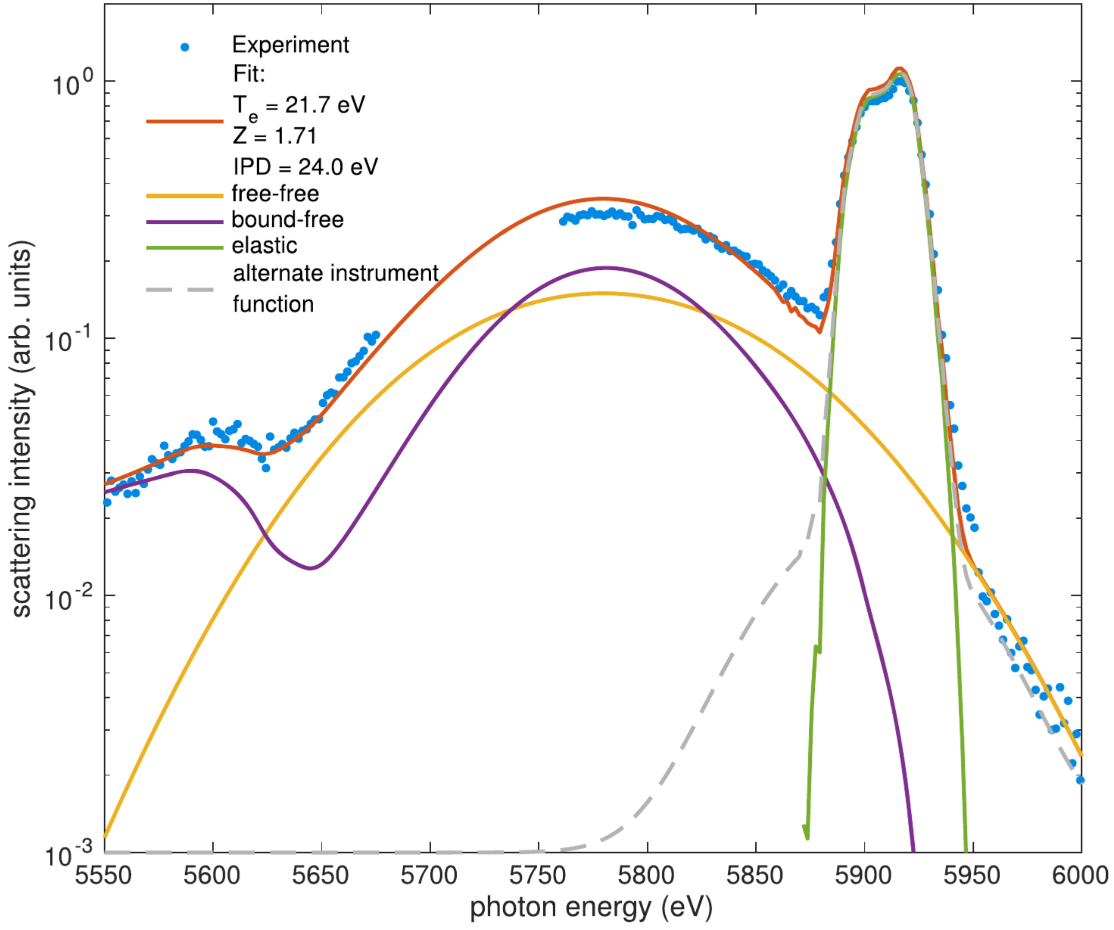
Part III: Dynamic properties in the imaginary time

X-ray Thomson scattering (XRTS)

- Standard way: construct a model for S(q,ω), convolve with instrument function R(ω), fit to XRTS signal I(q,ω)

$$I(\mathbf{q},\omega) = S(\mathbf{q},\omega) \circledast R(\omega)$$

Isochorically heated graphite at LCLS (Stanford)



Taken from: D. Kraus *et al.*, *Plasma Phys. Control. Fusion* **61**, 014015 (2019)

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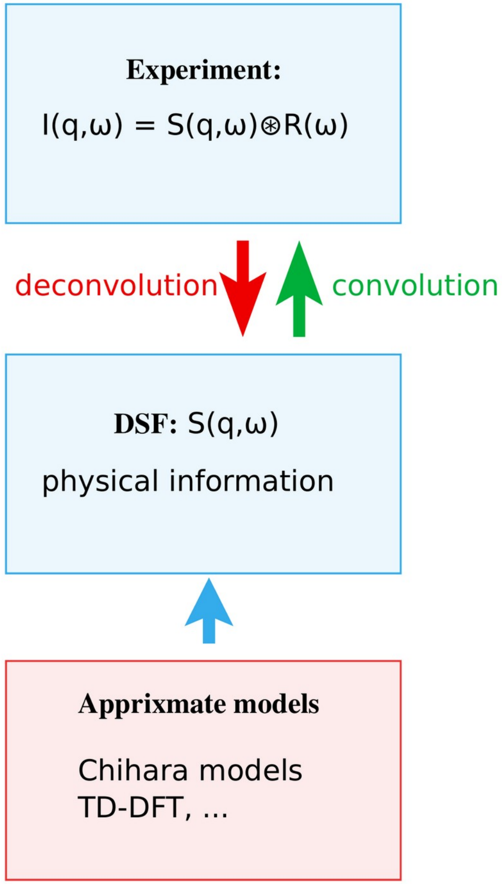
→ no direct access to physical information

→ approximate theoretical models



Taken from: **T. Dornheim**, Zh. Moldabekov, P. Tolias, M. Böhme, and J. Vorberger, arXiv:2209.02254 (submitted)

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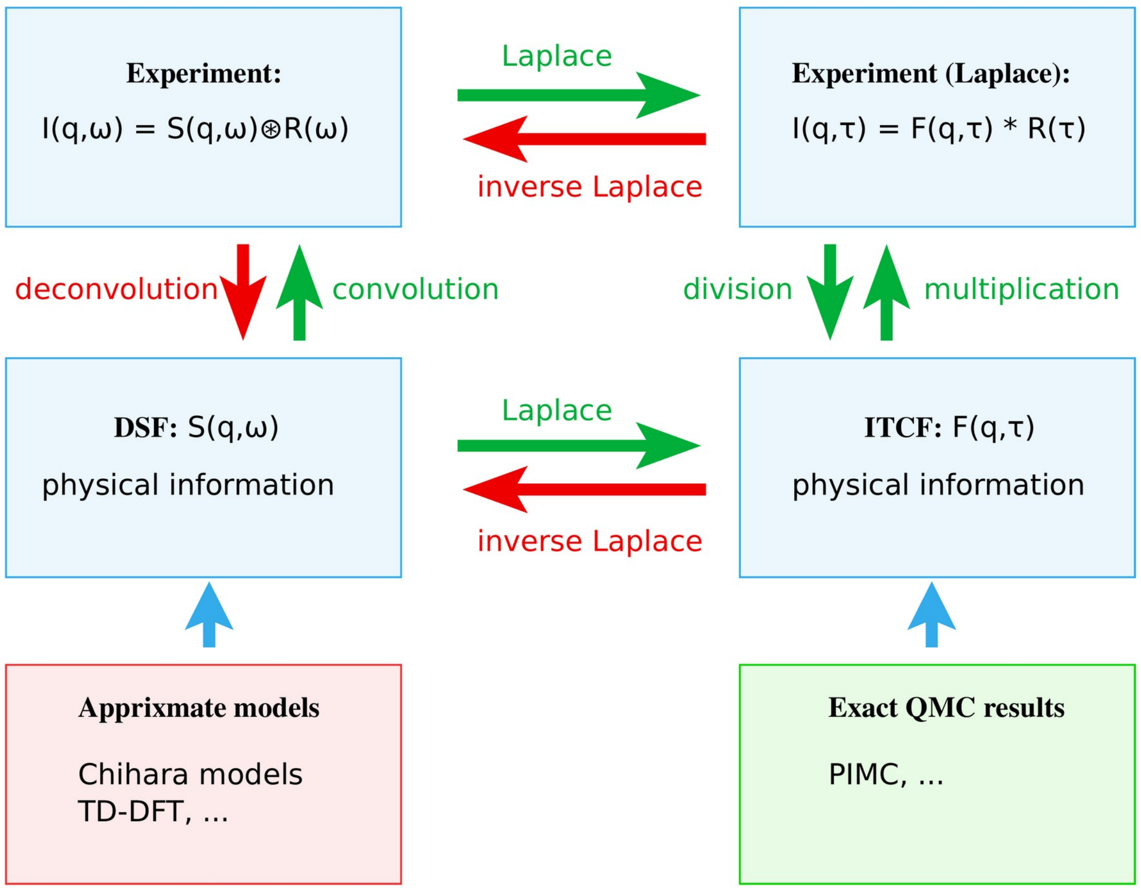

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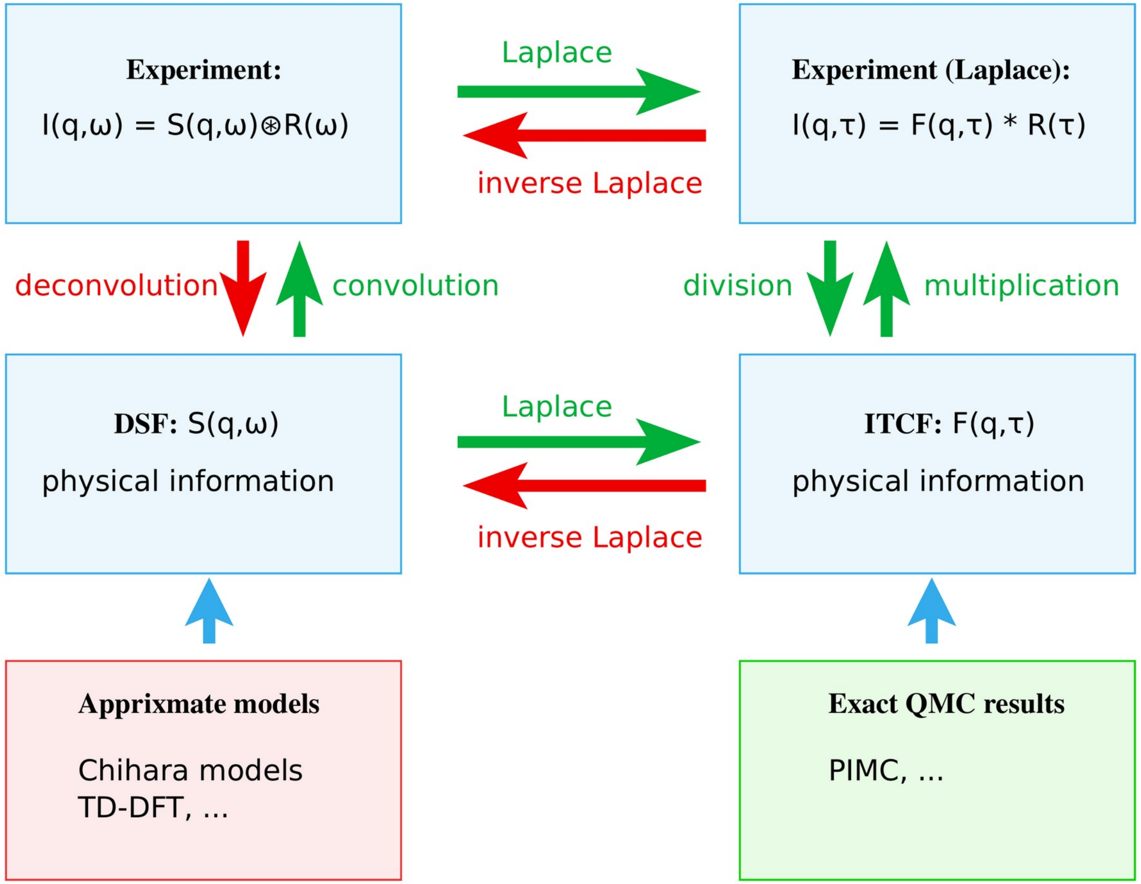

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Part III: Dynamic properties in the imaginary time

Model-free temperature from XRTS experiments:

$$S(\mathbf{q},-\omega) = S(\mathbf{q},\omega)e^{-\beta\omega}$$

- **Detailed balance in the τ-domain:**

→ works for all wave numbers

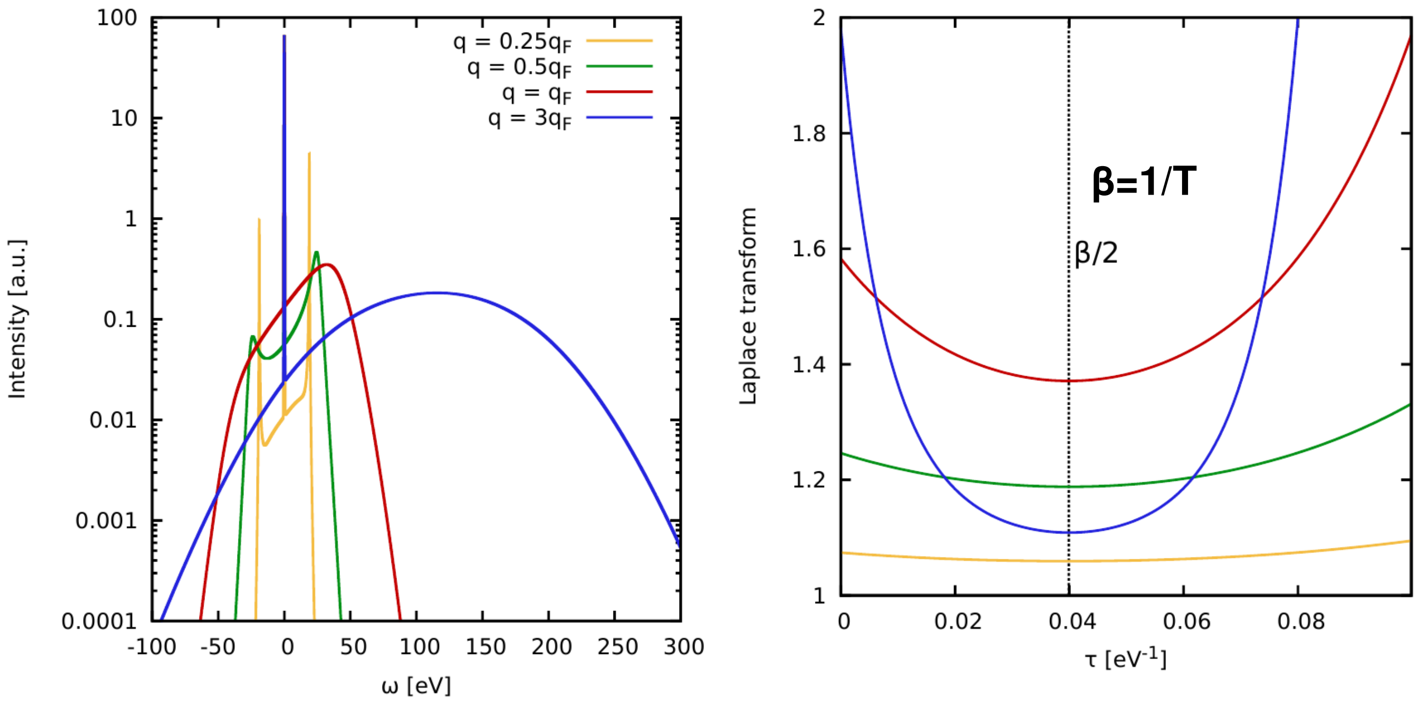
→ no explicit resolution of plasmon required

Laplace transform:

$$\mathcal{L}\left[S(\mathbf{q},\omega)\right] = \int_{-\infty}^{\infty} \mathrm{d}\omega\ e^{-\tau\omega}\ S(\mathbf{q},\omega)$$

→ **symmetry around $\tau=(2T)^{-1}$**

Left: S(q,ω) **Right:** Laplace transform



Taken from: **T. Dornheim** *et al.*, in preparation

Part III: Dynamic properties in the imaginary time

Model-free temperature from XRTS experiments:

- **Detailed balance in the τ-domain:**

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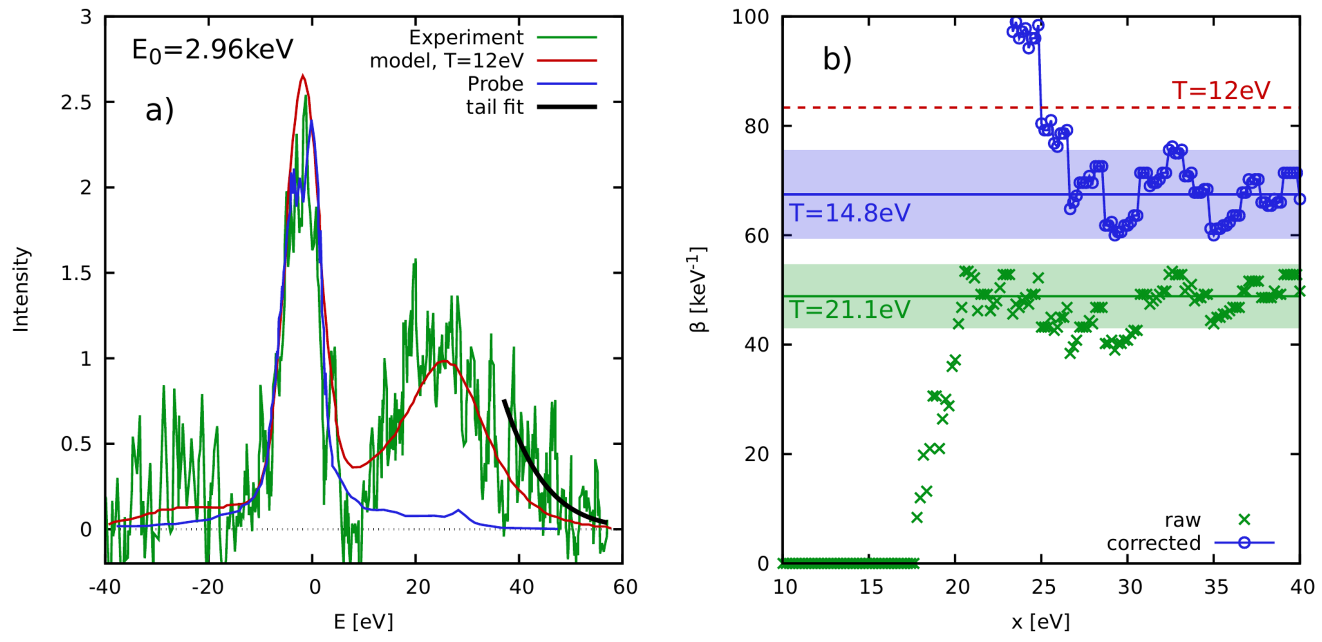
→ no explicit resolution of plasmon required

→ finite ω-range, check convergence with x

$$\mathcal{L}_x\left[S(\mathbf{q},\omega) \circledast R(\omega)\right] = \int_{-x}^{x} \mathrm{d}\omega\ e^{-\tau\omega} \left\{S(\mathbf{q},\omega) \circledast R(\omega)\right\}$$

$$\mathcal{L}\left[S(\mathbf{q},\omega)\right] = \frac{\mathcal{L}\left[S(\mathbf{q},\omega) \circledast R(\omega)\right]}{\mathcal{L}\left[R(\omega)\right]}$$

Temperature of warm dense Be [Glenzer (2007)]



Taken from: **T. Dornheim**, M. Böhme, D. Kraus, T. Döppner, T. Preston, Zh. Moldabekov, and J. Vorberger, arXiv:2206.12805

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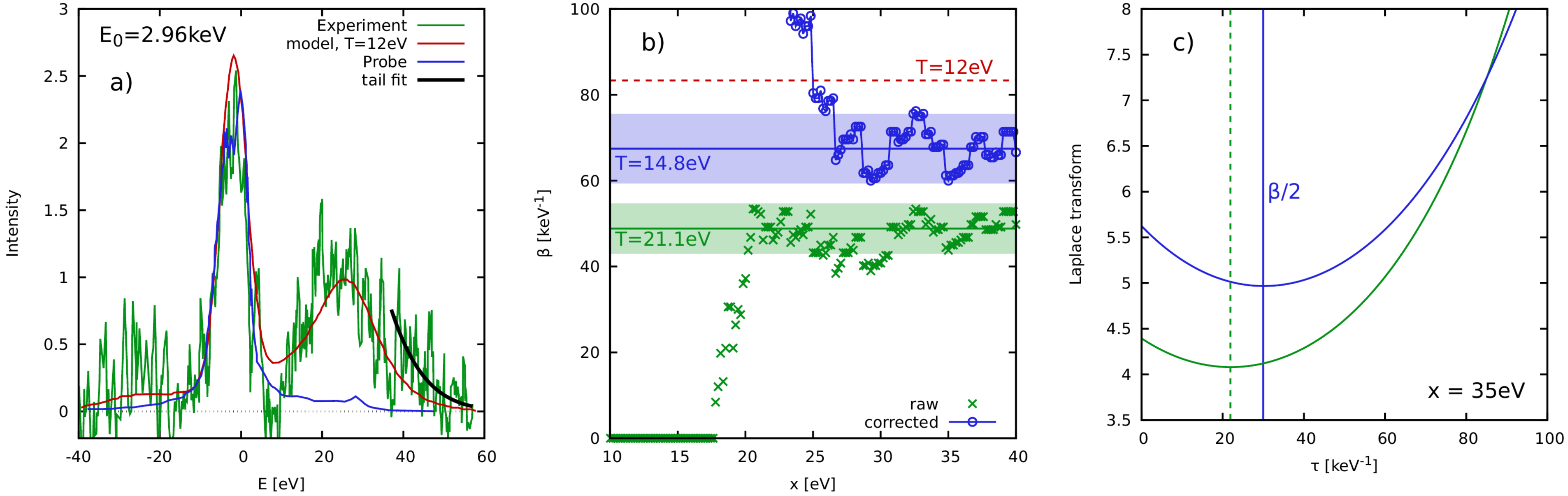

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XRTS gives direct access to T, etc

→ model-free EOS measurements

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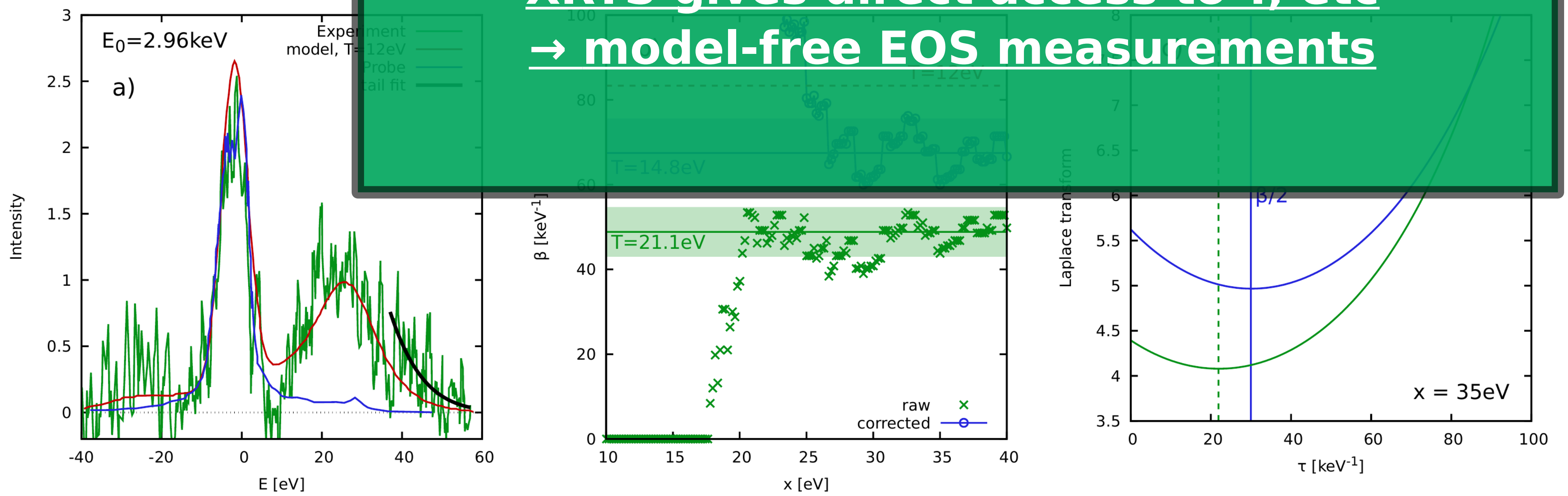

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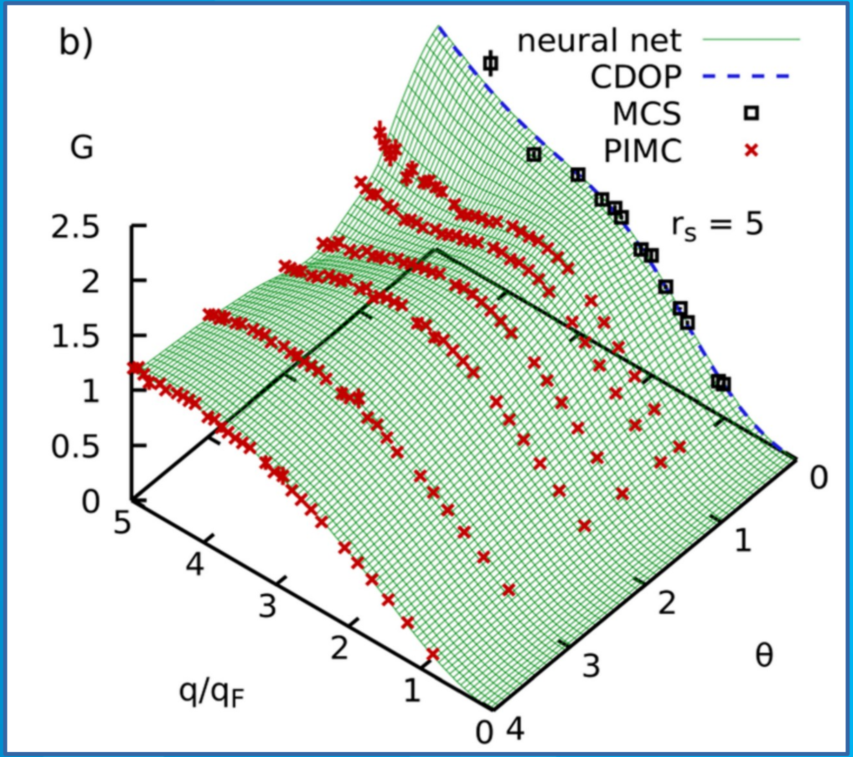
Summary and Outlook

***Ab initio* theory of WDM**

- need for finite-T XC functionals based on PIMC results
- static density response: PIMC + neural net
- PIMC results for warm dense hydrogen
- DFT framework for the study of XC-effects
- dynamic density response: PIMC + analytic continuation

Key pre-print:

arXiv:2209.00928



Taken from: **T. Dornheim**, J. Vorberger, S. Groth, N. Hoffmann, Zh. Moldabekov, and M. Bonitz, JCP **151**, 194104 (2019)

Summary and Outlook

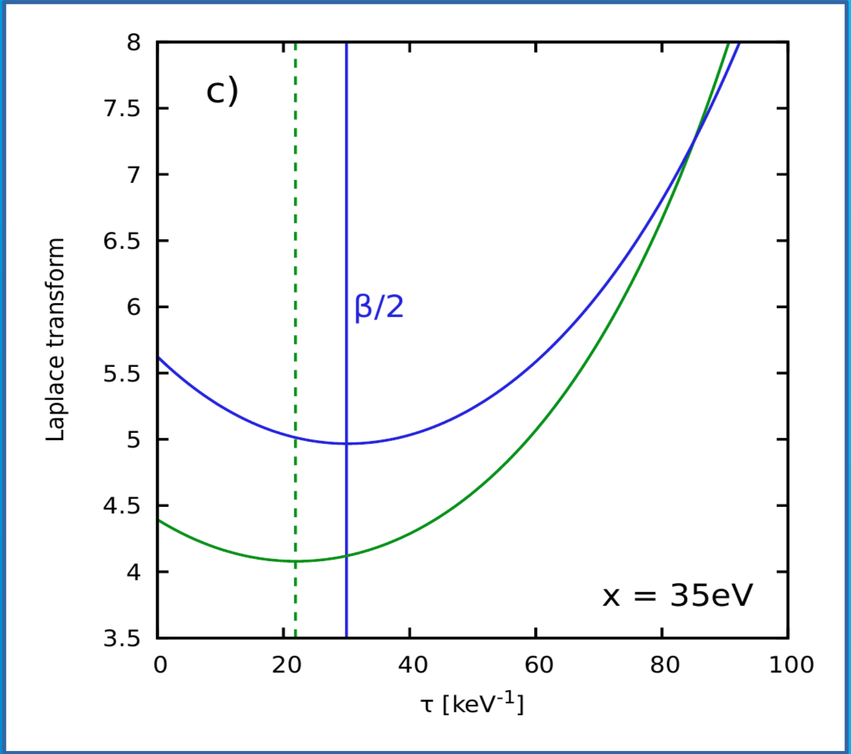
Physics in the imaginary time

- Usual ω-representation equivalent to τ-domain
- **Model-free T-diagnostics** etc.
- Future works: physical insights form the τ-domain

Key pre-prints:

arXiv:2206.12805

arXiv:2209.02254



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