Understanding warm dense matter from first principles

Tobias Dornheim et al.

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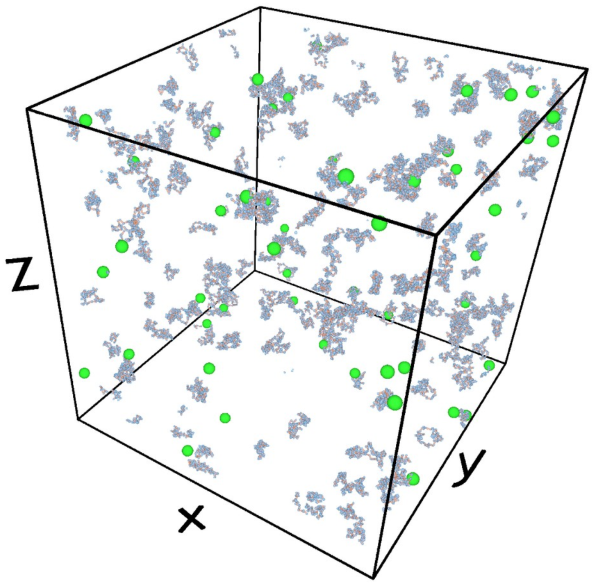
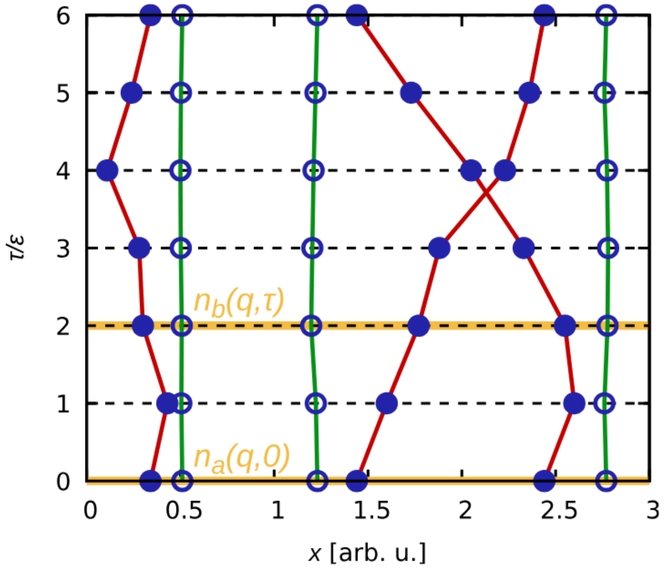
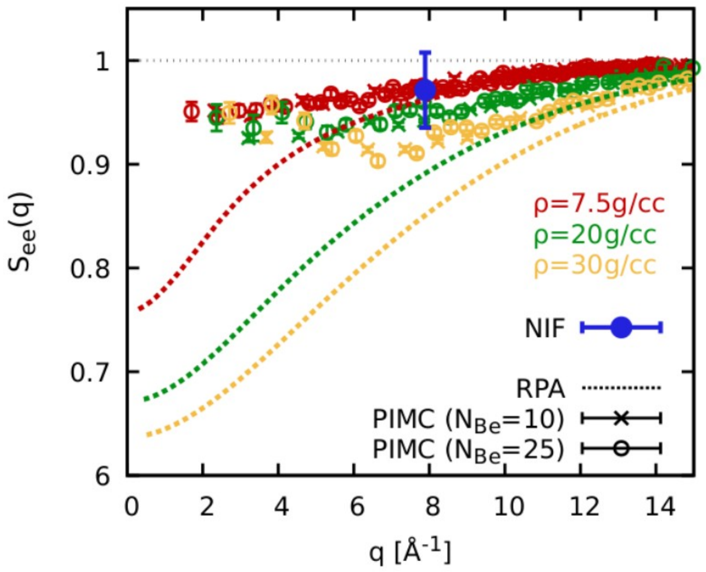
Supported by ERC Starting Grant agreement No. 101076233, “PREXTREME"







In collaboration with:

European XFEL · Lawrence Livermore National Laboratory · Universität Rostock (Traditio et Innovatio) · KTH · Institut Polytechnique de Paris · Christian-Albrechts-Universität zu Kiel

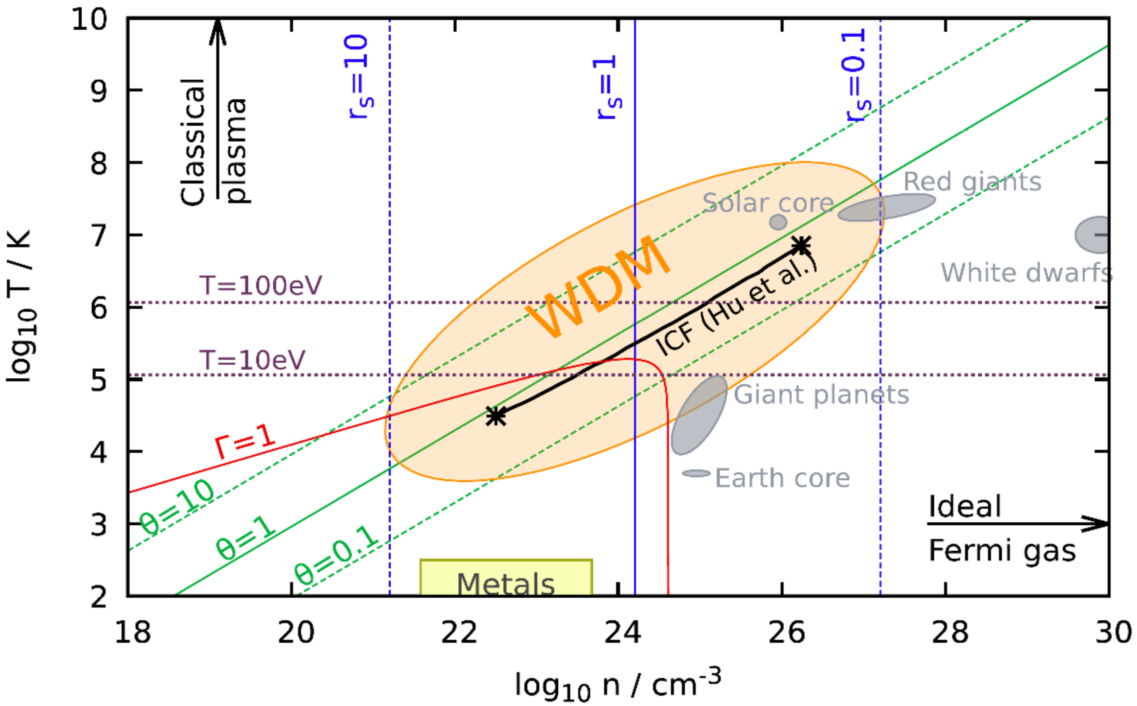
Introduction

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**, Zh. Moldabekov, K. Ramakrishna, P. Tolias, A. Baczewski, D. Kraus, Th. Preston, D. Chapman et al, Phys. Plasmas **30**, 032705 (2023)

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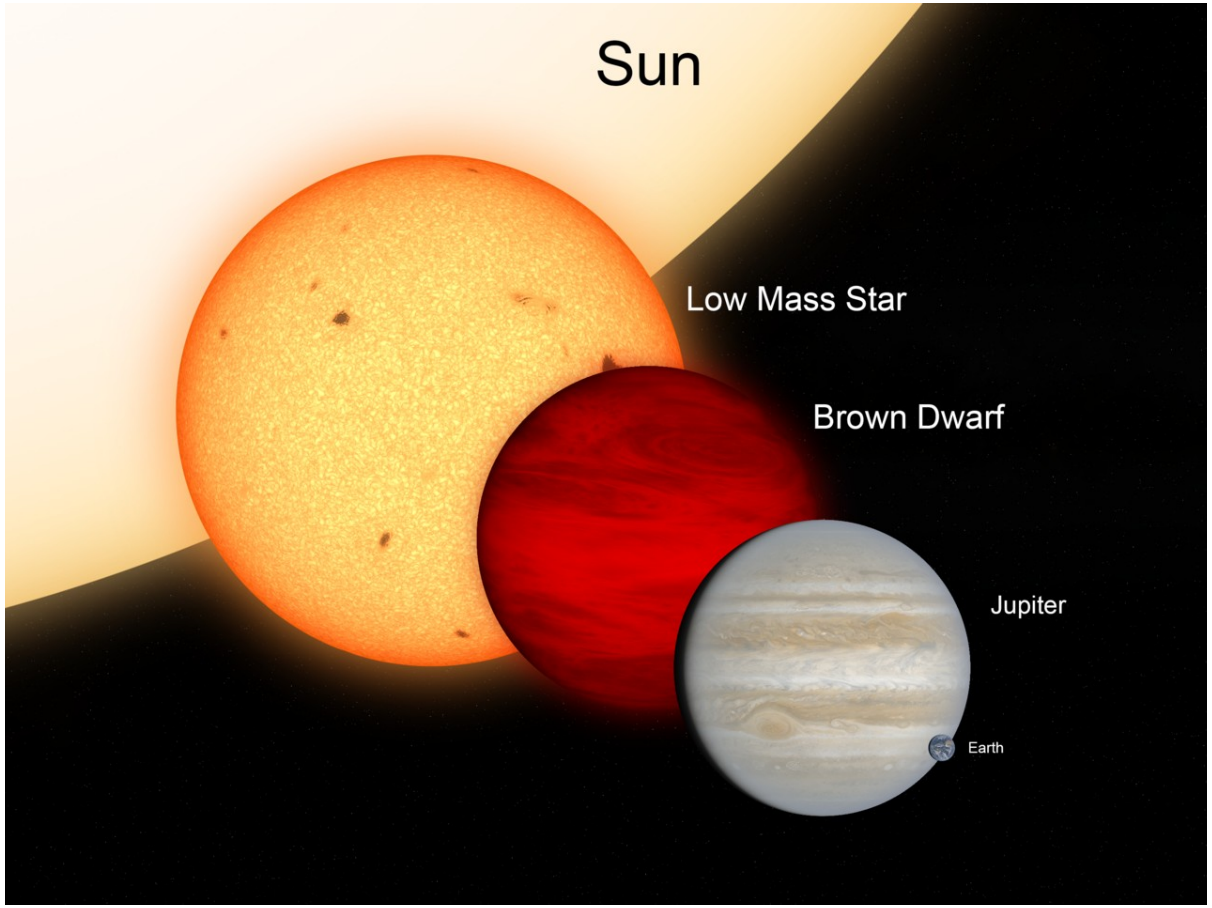
• Examples: giant planet interiors, brown dwarfs



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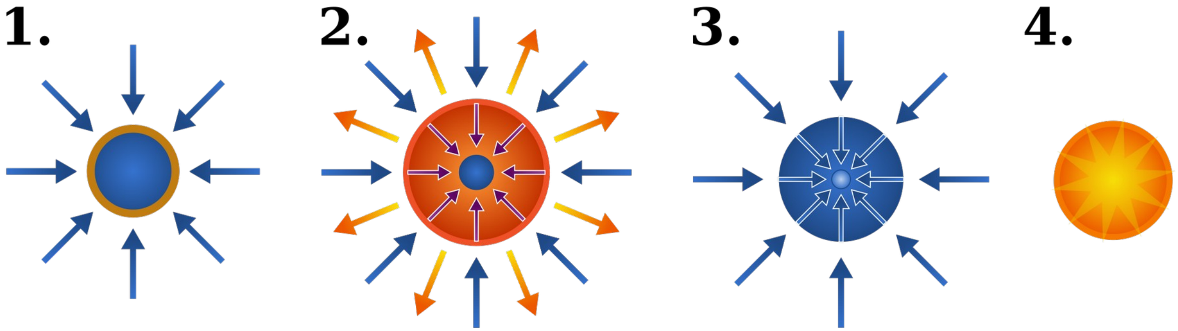
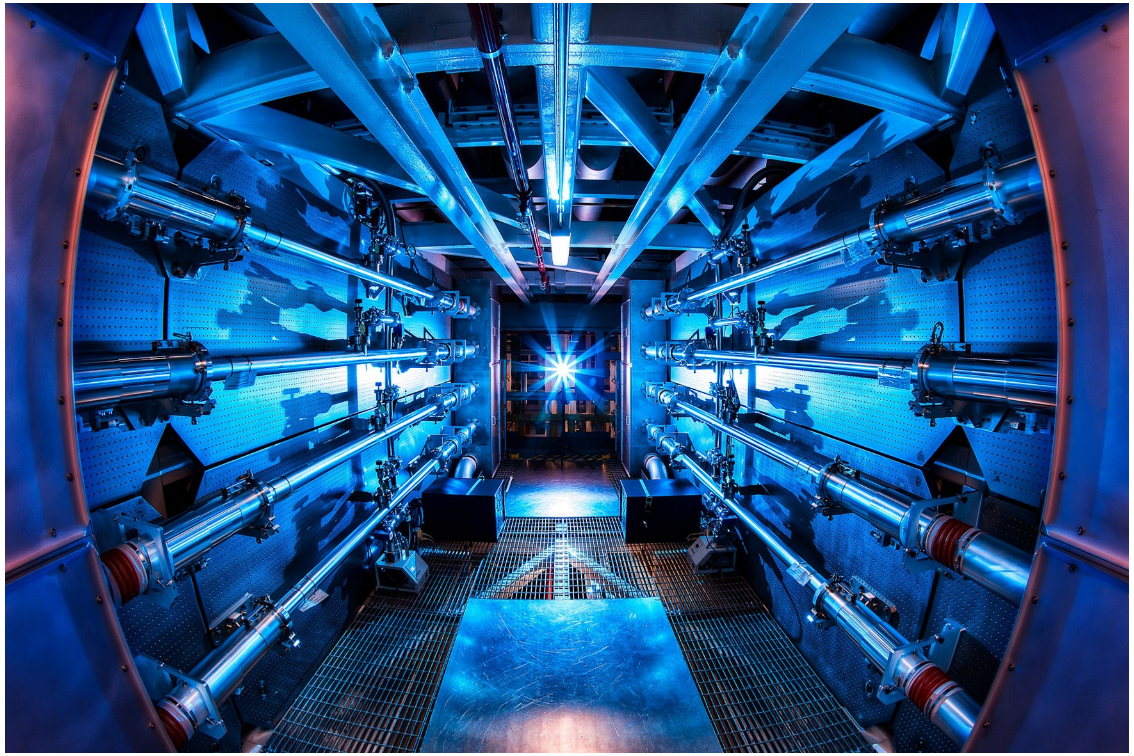
• WDM highly important for technological applications:

→ Inertial confinement fusion, etc.



National Ignition Facility (NIF)



Taken from: Lawrence Livermore National Laboratory; Wikimedia Commons

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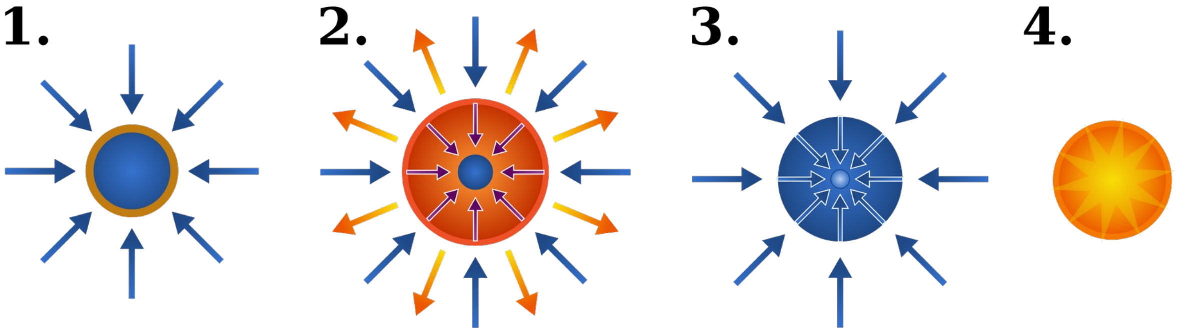
→ Inertial confinement fusion, etc.

WDM routinely realized in large research facilities around the globe!



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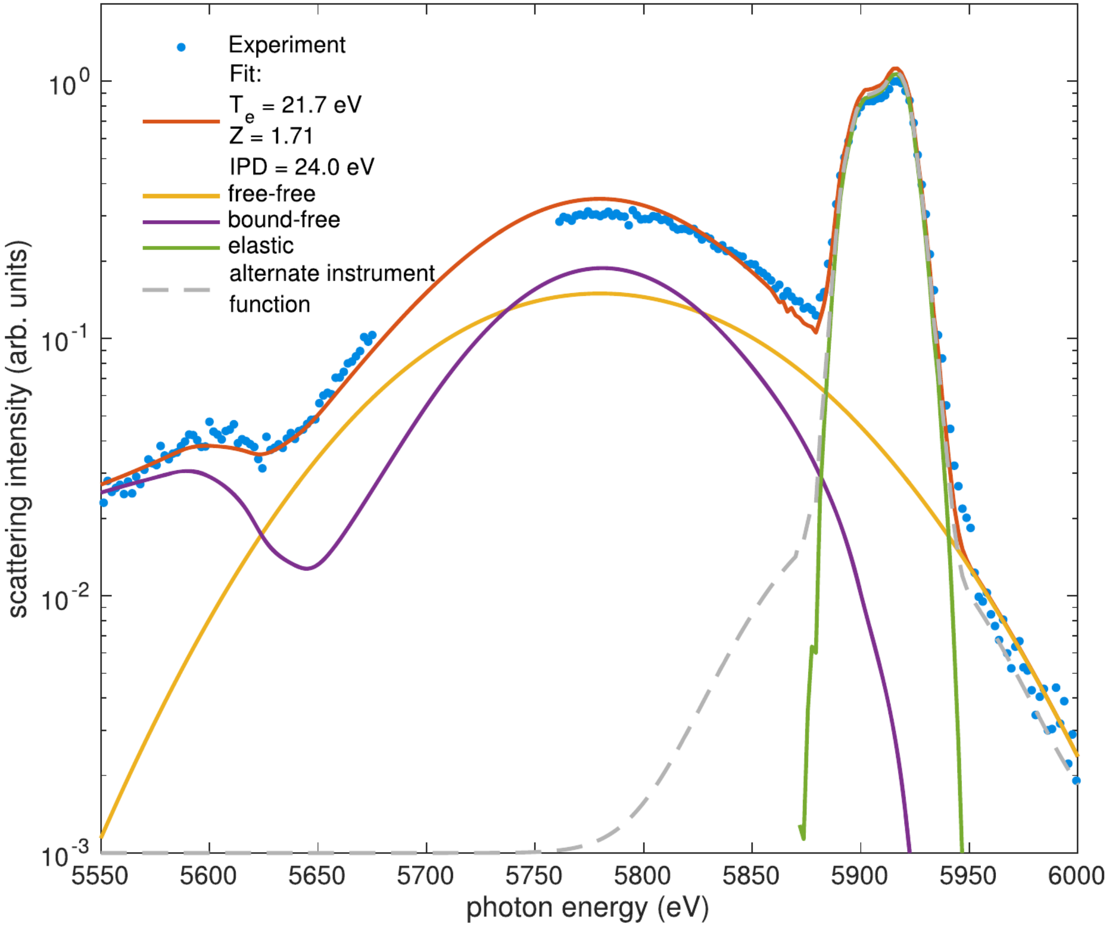
Part I: Introduction

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)



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

Part I: Introduction

But: Rigorous WDM theory indispensable

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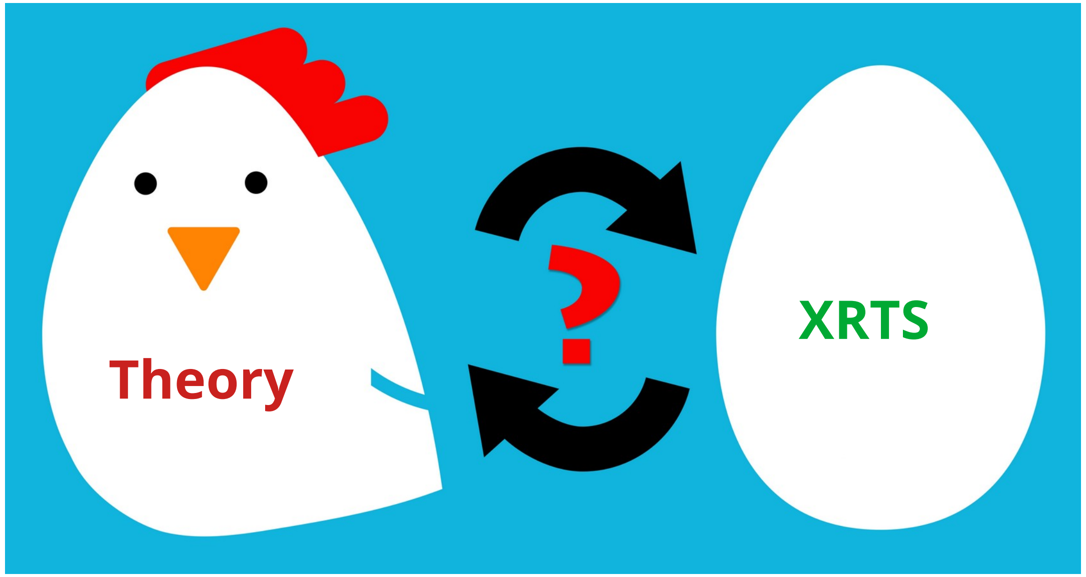
→ X-ray Thomson scattering (XRTS)

But there is a problem: Interpretation of XRTS signals model-dependent!



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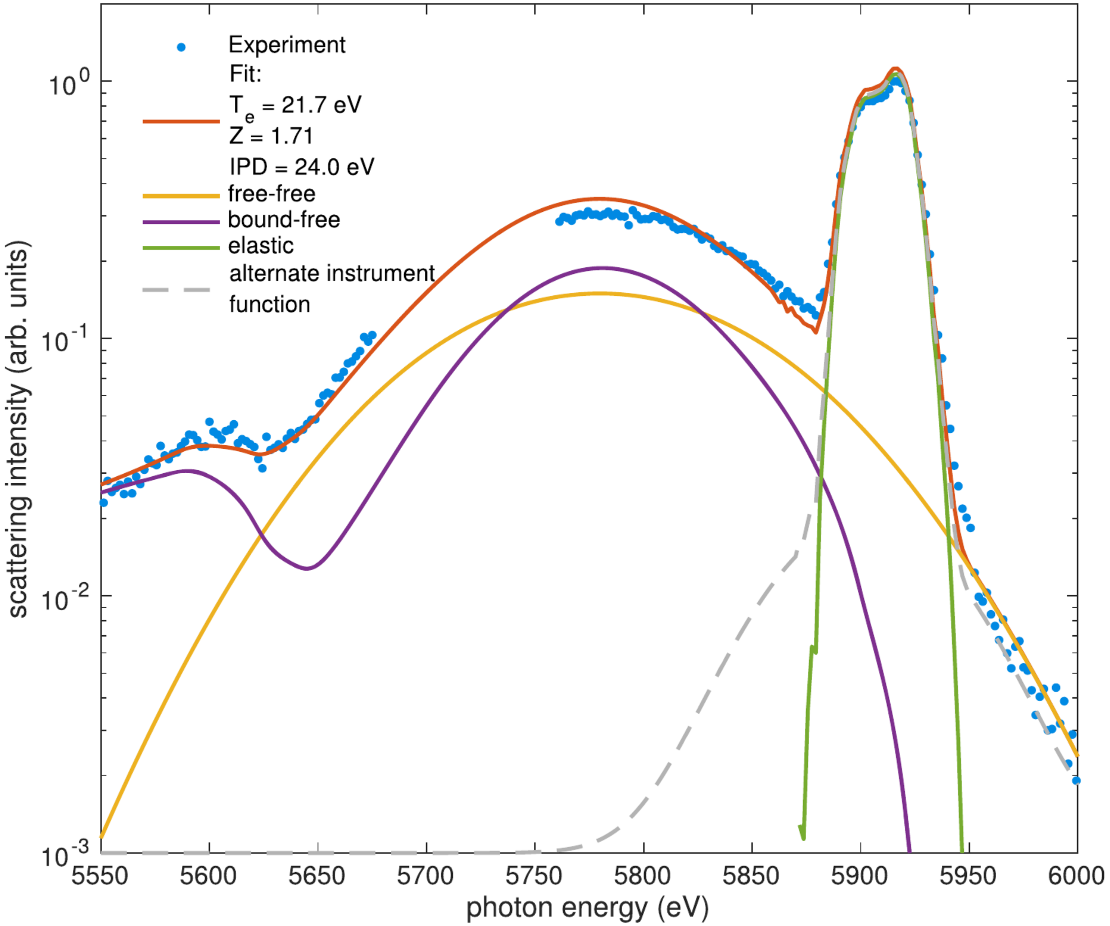

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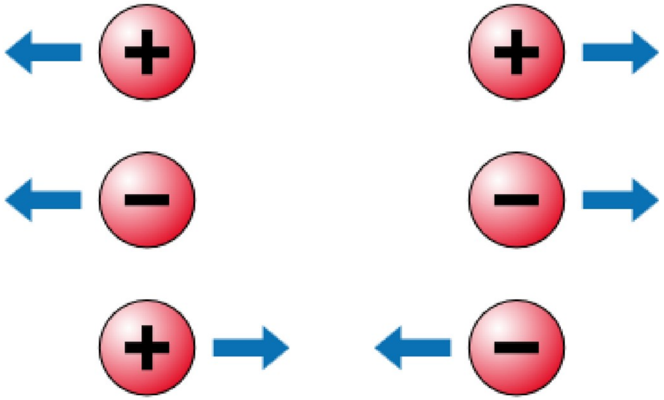

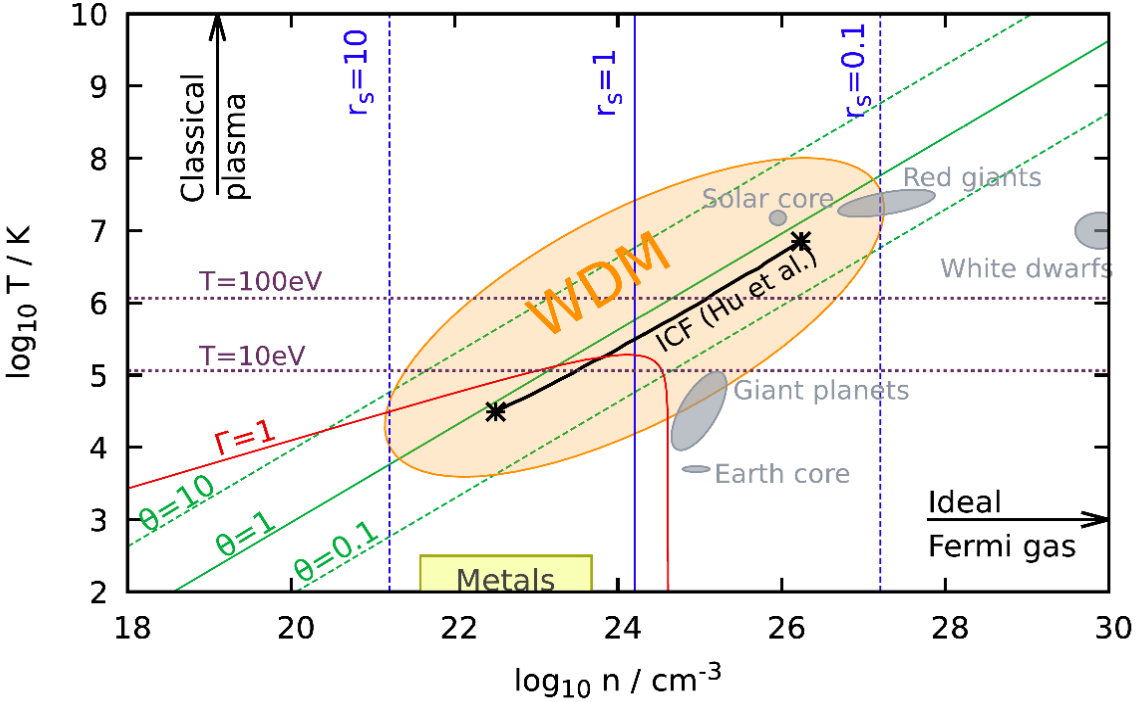

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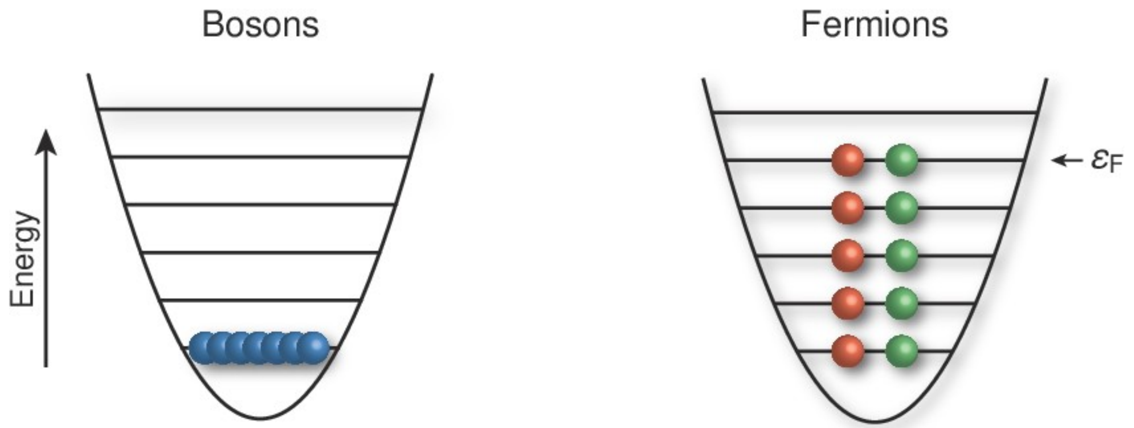

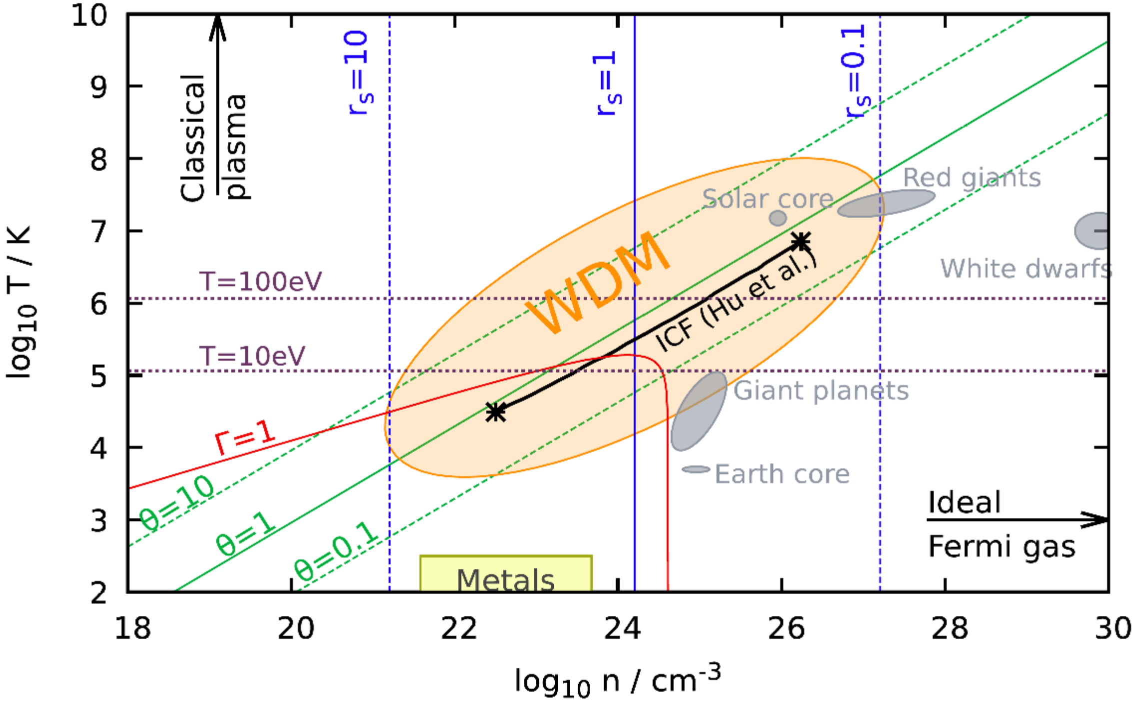

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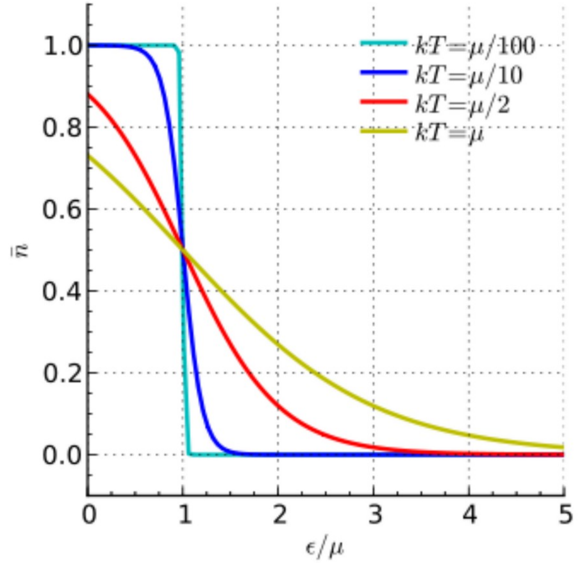

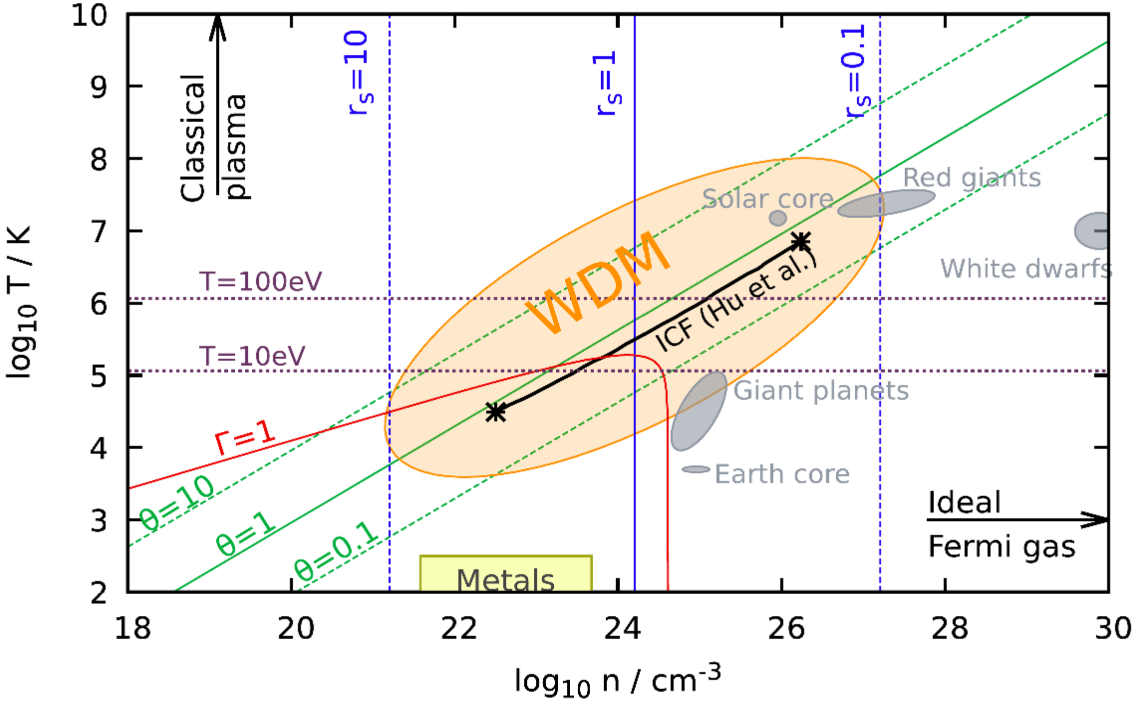

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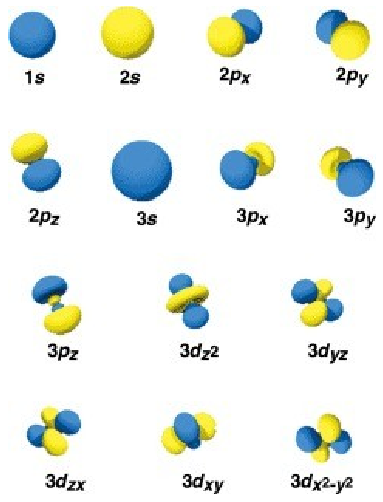

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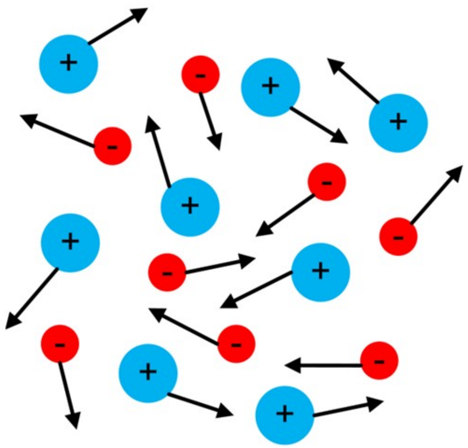

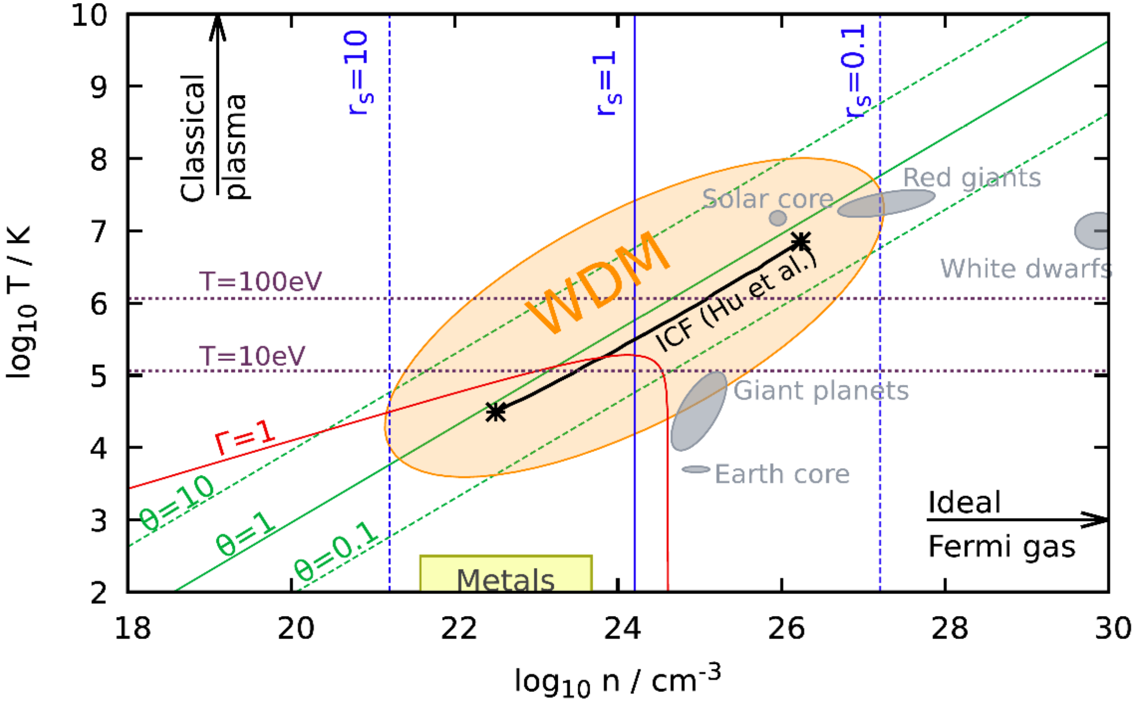

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Outline

Highlight I: **Model-free X-ray scattering diagnostics of warm dense matter**

T. Dornheim, M. Böhme, D. Kraus *et al.*, Nature Commun. 13, 7911 (2022)

T. Döppner, M. Bethkenhagen, D. Kraus *et al.*, Nature 618, 270-275 (2023)

Highlight II: **Exact path integral Monte Carlo simulations of warm dense matter**

T. Dornheim, T. Döppner, P. Tolias *et al.*, Nature Commun. 16, 5103 (2025)

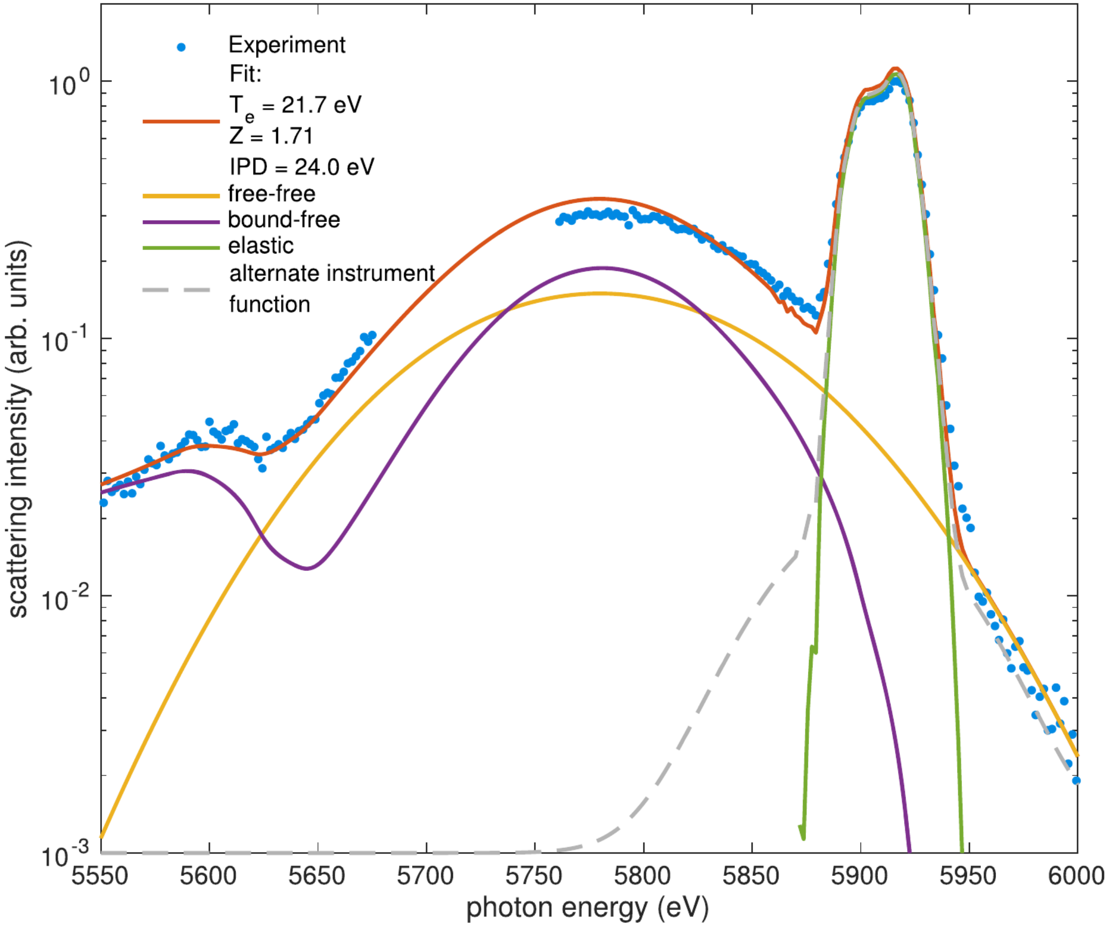
supported by experiments at the National Ignition Facility and European XFEL (HED-HIBEF)

Highlight I: Model-free XRTS diagnostics

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)

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



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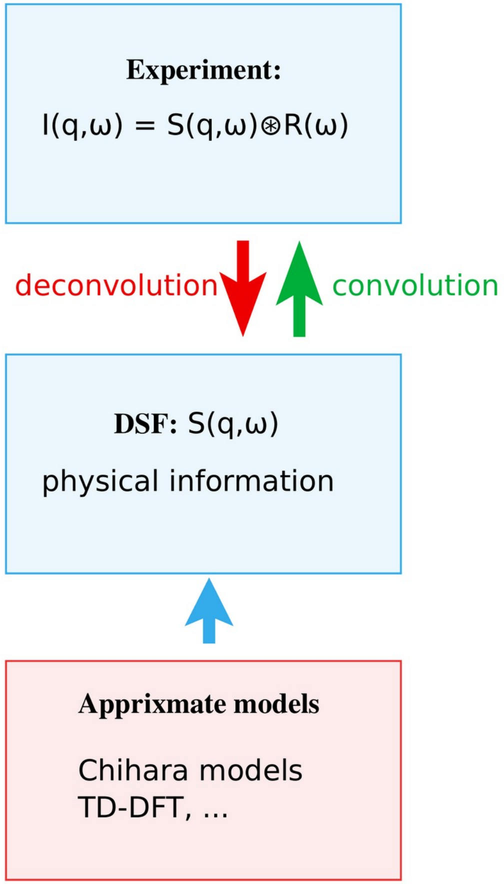
• **<u>Frequency domain:</u>**

→ no direct access to physical information

→ approximate theoretical models



<u>Taken from:</u> **T. Dornheim**, Zh. Moldabekov, P. Tolias, M. Böhme, and J. Vorberger, Matt. Rad. Extremes **8**, 056601 (2023)

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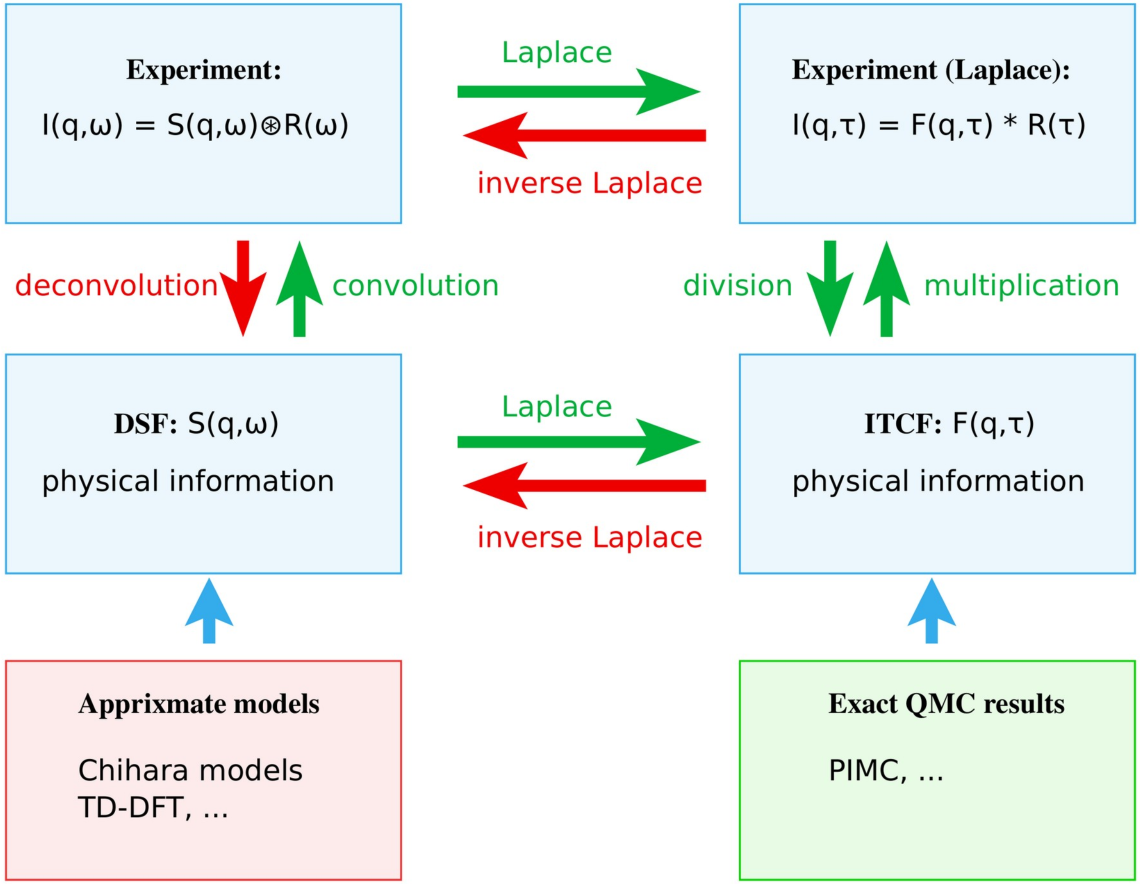
• **Imaginary-time domain:**

→ direct access to physics, e.g. T, ω_p

→ exact PIMC simulations

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



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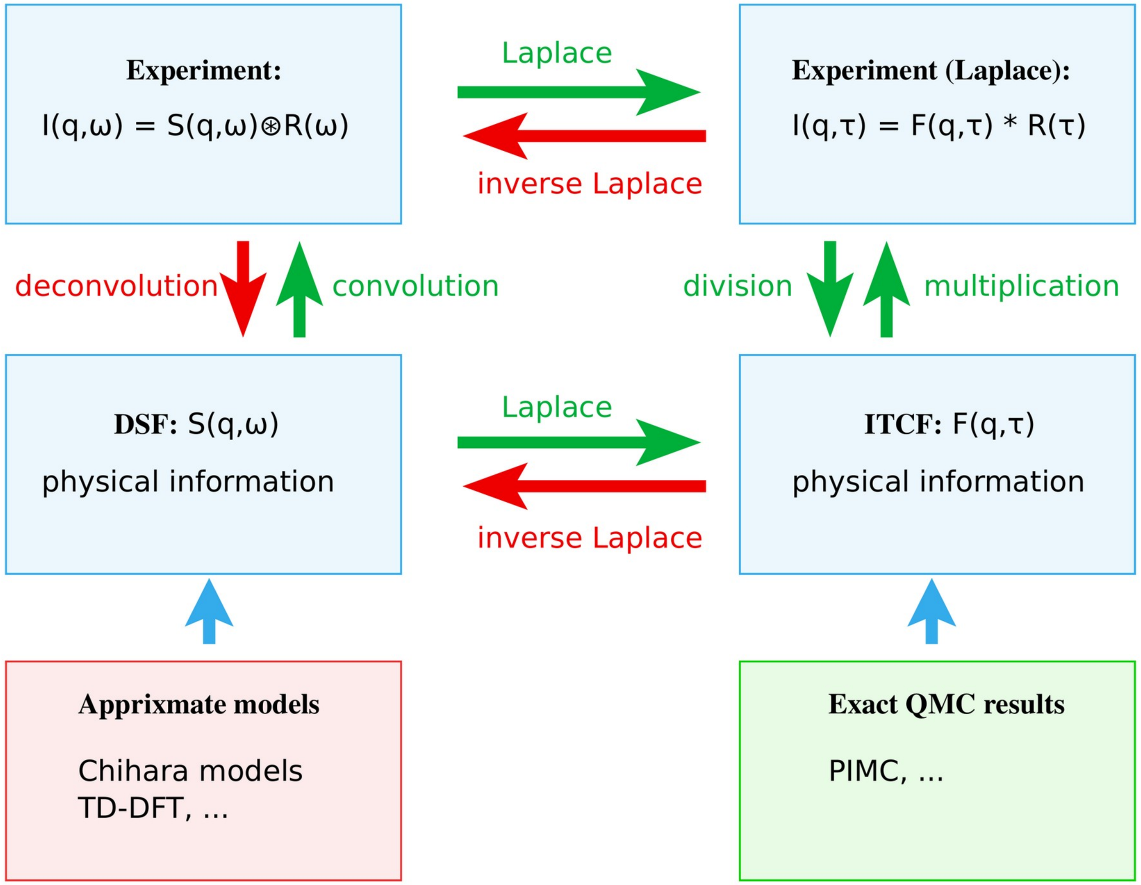

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Highlight I: Model-free XRTS diagnostics

Model-free temperature diagnostics

T. Dornheim et al., *Nature Commun.* 13, 7911 (2022)

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

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

→ works for all wave numbers

→ no explicit resolution of plasmon required

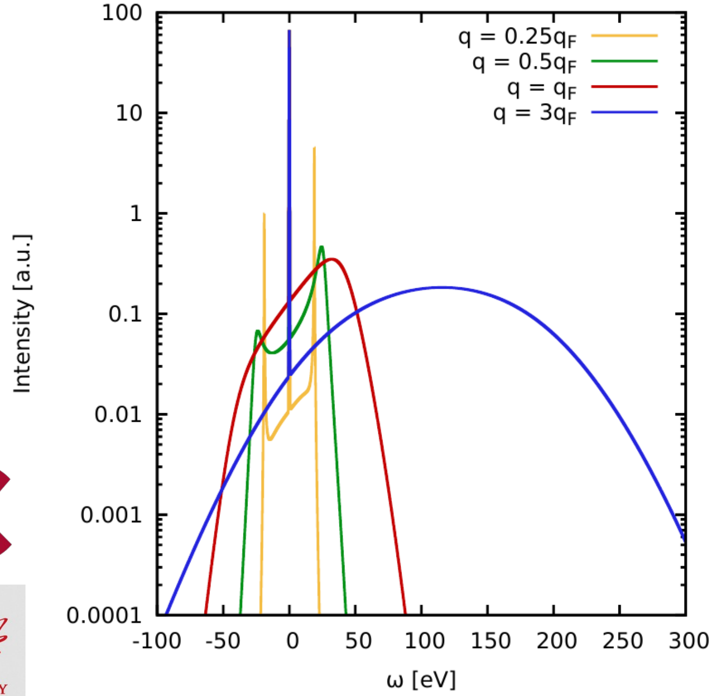
→ other properties possible!

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

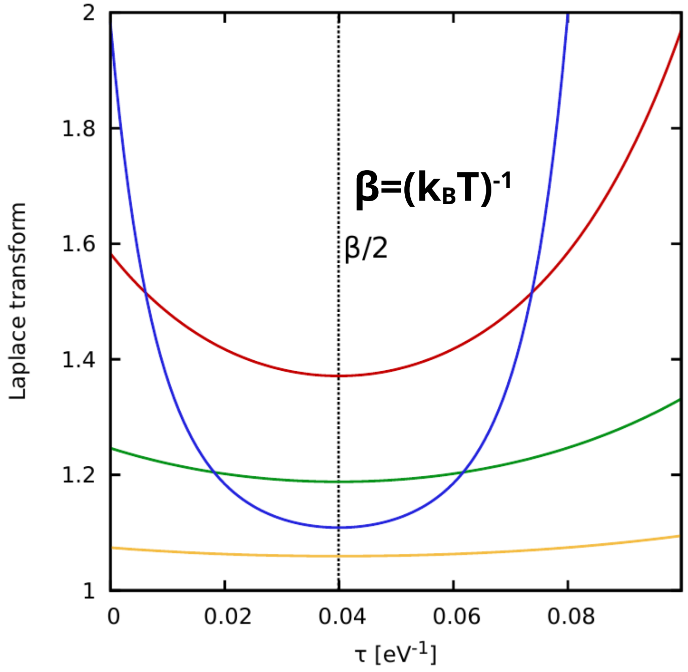
No models and approximations required!

Already implemented at:

SLAC, European XFEL, Lawrence Livermore National Laboratory, 上海交通大學 Shanghai Jiao Tong University



Left: S(q,ω)



Right: Laplace transform

Taken from: **T. Dornheim** et al, Phys. Plasmas **30**, 042707 (2023)

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T. Dornheim et al., *Nature Commun.* 13, 7911 (2022)

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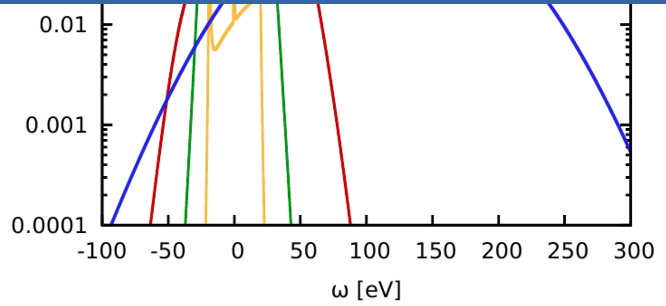
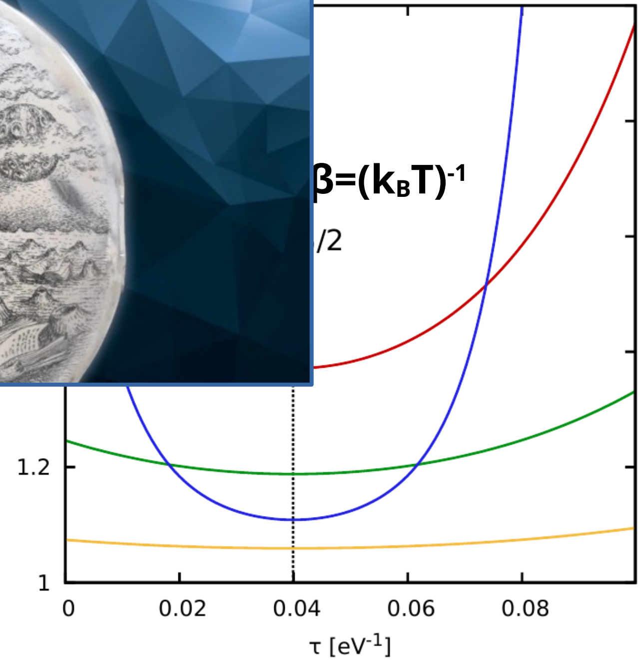




Left: S(q,ω) **Right:** Laplace transform

Already implemented at: European XFEL, Lawrence Livermore National Laboratory, Shanghai Jiao Tong University, SLAC

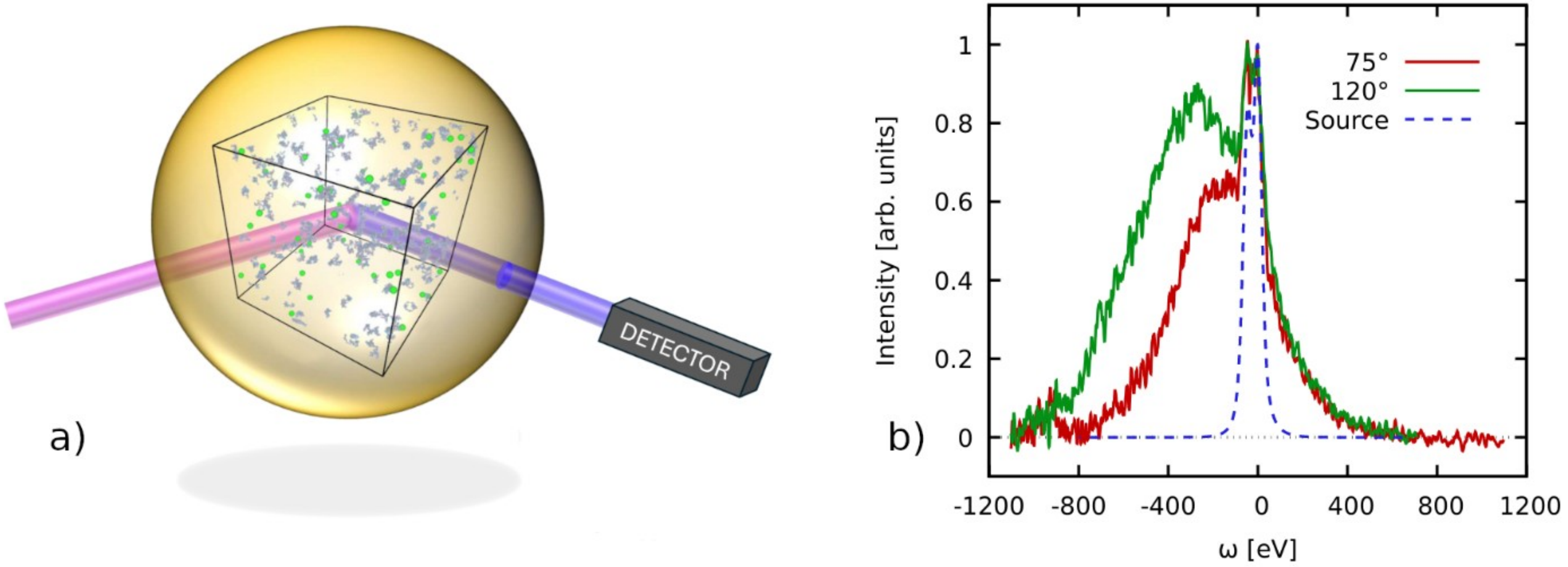
Taken from: **T. Dornheim** et al, Phys. Plasmas **30**, 042707 (2023)

<u>Highlight II:</u> Exact PIMC simulation of WDM

ERC Starting Grant „Predicting the Extreme“ (PREXTREME)

T. Dornheim et al., *Nature Commun.* 16, 5103 (2025)

- <u>New capability:</u> exact PIMC simulation of warm dense beryllium at NIF conditions



NIF Discovery Science Project: Advancing Atomic Physics at Gbar Pressure

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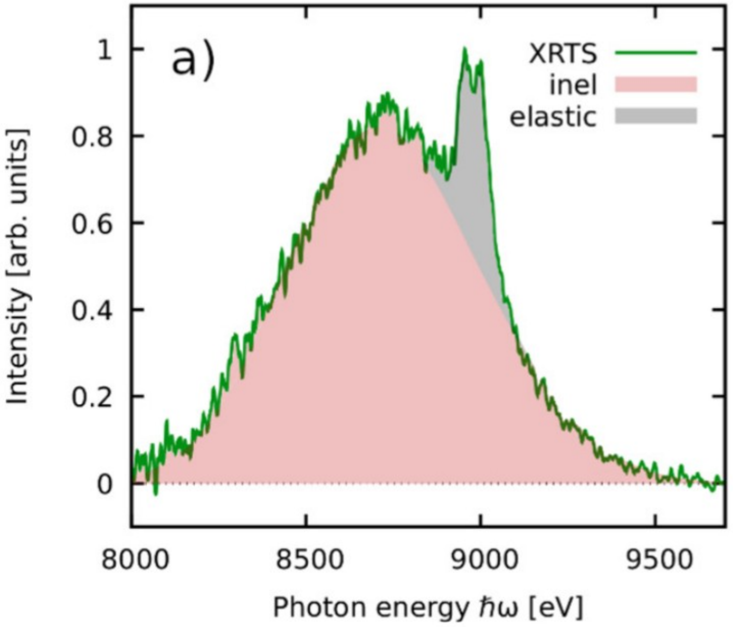
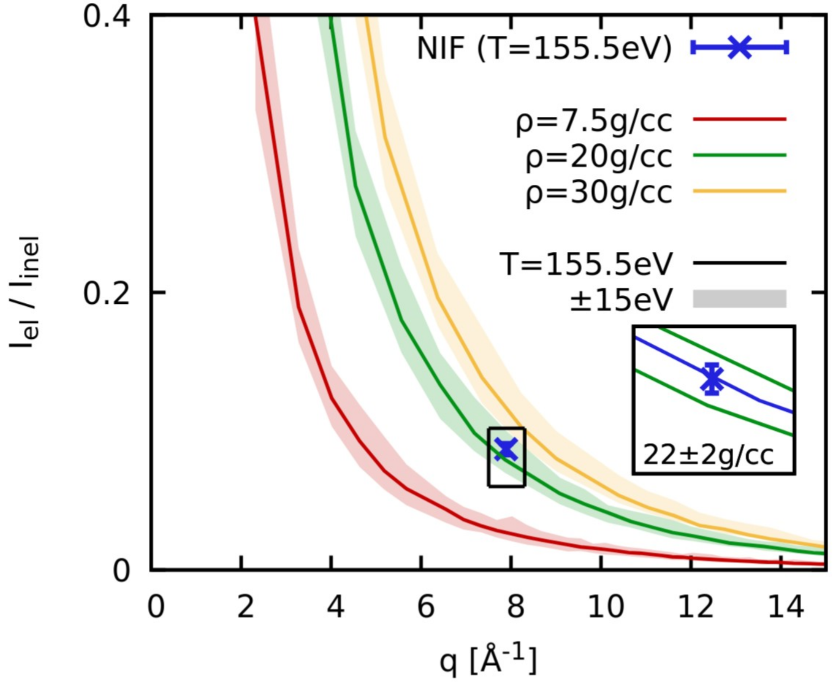
T. Dornheim et al., *Nature Commun.* 16, 5103 (2025)

- New capability: exact PIMC simulation of warm dense beryllium at NIF conditions

→ PIMC consistently gives density ρ~22g/cc, ruling out previously used chemical models (ρ~34g/cc)





NIF Discovery Science Project: Advancing Atomic Physics at Gbar Pressure

New overview article!

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

- **Broad overview of experimental techniques / facilities, numerical methods, and relevant systems**

- **~70 authors from US / Europe / Asia**

- **Context: inertial fusion energy, material science, planetary and astrophysics, …**

- **~1500 relevant citations**

arXiv > physics > arXiv:2505.02494

Physics > Plasma Physics

[Submitted on 5 May 2025]

Roadmap for warm dense matter physics

Jan Vorberger[1], Frank Graziani[2], David Riley[3], Andrew D. Baczewski[4], Isabelle Baraffe[5,6], Mandy Bethkenhagen[7], Simon Blouin[8], Maximilian P. Böhme[2], Michael Bonitz[9,10], Michael Bussmann[1], Alexis Casner[11], Witold Cayzac[11], Peter Celliers[2], Gilles Chabrier[6,5], Nicolas Chamel[12], Dave Chapman[13], Mohan Chen[14], Jean Clérouin[15], Gilbert Collins[16,17,18], Federica Coppari[2], Tilo Döppner[2], Tobias Dornheim[1,19], Luke B. Fletcher[20], Dirk O. Gericke[21], Siegfried Glenzer[20], Alexander F. Goncharov[22], Gianluca Gregori[23], Sebastien Hamel,[2], Stephanie B. Hansen[24], Nicholas J. Hartley[20], Suxing Hu[16,17,18], Omar A. Hurricane[2], Valentin V. Karasiev[16], Joshua J. Kas[25], Brendan Kettle[26], Thomas Kluge[1], Marcus D. Knudson[24], Alina Kononov[4], Zuzana Konôpková[27] Dominik Kraus[28,1], Andrea Kritcher[2], Sophia Malko[29], Gérard Massacrier[30], Burkhard Militzer[31], Zhandos A. Moldabekov[1,19], Michael S. Murillo[32], Bob Nagler[20], Nadine Nettelmann[28], Paul Neumayer[33], Benjamin K. Ofori-Okai[20], Ivan I. Oleynik[34], Martin Preising[28], Aurora Pribram-Jones[35], Tlekkabul Ramazanov[36], Alessandra Ravasio[7], Ronald Redmer[28], Baerbel Rethfeld[37], Alex P. L. Robinson[38], Gerd Röpke[28], François Soubiran[15], Charles E. Starrett[39], Gerd Steinle-Neumann[40], Phillip A. Sterne[2], Shigenori Tanaka[41], Aidan P. Thompson[4], Samuel B. Trickey[42], Tommaso Vinci[7], Sam M. Vinko[43], Lei Wang[44], Alexander J. White[39] Thomas G. White[45], Ulf Zastrau[27], Eva Zurek[46], Panagiotis Tolias[47]

Summary and Outlook

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

• WDM diagnostics challenging; infer parameters like T, n, Z indirectly by modelling XRTS spectra

→ **New:** Model-free ITCF analysis (T, $S_{ee}(q)$, …)

• New, highly accurate PIMC simulations of WDM

→ **New:** XRTS diagnostics of warm dense Be arxiv:2402.19113

→ **New:** Density response + XC-kernel of warm dense hydrogen

T. Dornheim et al., Matter Radiat. Extremes **9**, 057401 (2024) Review article: M. Bonitz, …, and **T. Dornheim**, Phys. Plasmas **30**, 110501 (2024)

European Research Council
Established by the European Commission

→ ERC Starting Grant „Predicting the Extreme“ (PREXTREME)

→ European Union’s Just Transtition Fund Project „X-ray optimization of laserfusion“ (ROLF)

HLRN

KIT NHR
National High-Performance Computing Center

Dr. Tobias Dornheim
Young Investigator Group Leader

Hannah Bellenbaum
PhD Candidate

Thomas M. Chuna
Postdoctoral Researcher

Dr. Thomas Gawne
Postdoctoral Researcher

Dr. Uwe Hernandez Acosta
Postdoctoral Researcher

Dr. Zhandos Moldabekov
Postdoctoral Researcher

Dr. Sebastian Schwalbe
Postdoctoral Researcher

2025 new joiners:

Paul Hamann
Dr. Pontus Svensson

Dornheim Group: Frontiers of Computational Quantum Many-Body Theory

From XRTS to PIMC

X-ray Thomson scattering (XRTS)

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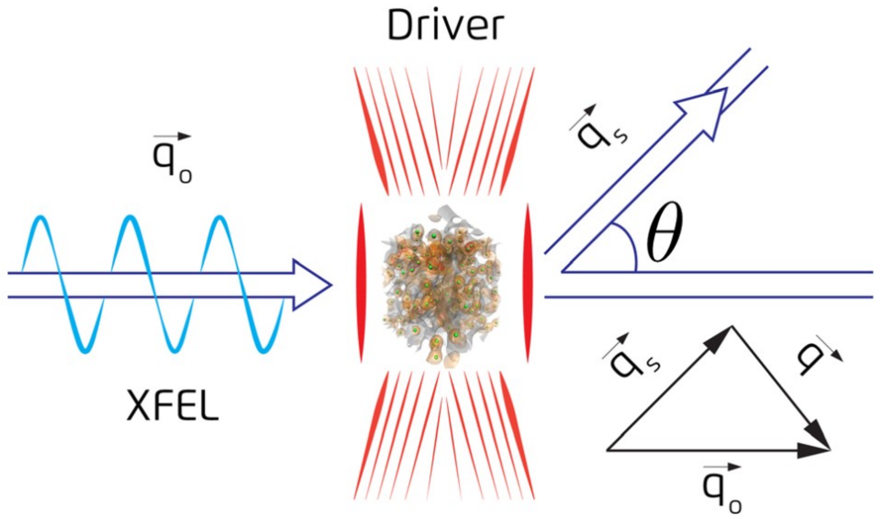
→ X-ray Thomson scattering (XRTS)



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Phys. Plasmas **30**, 042707 (2023)

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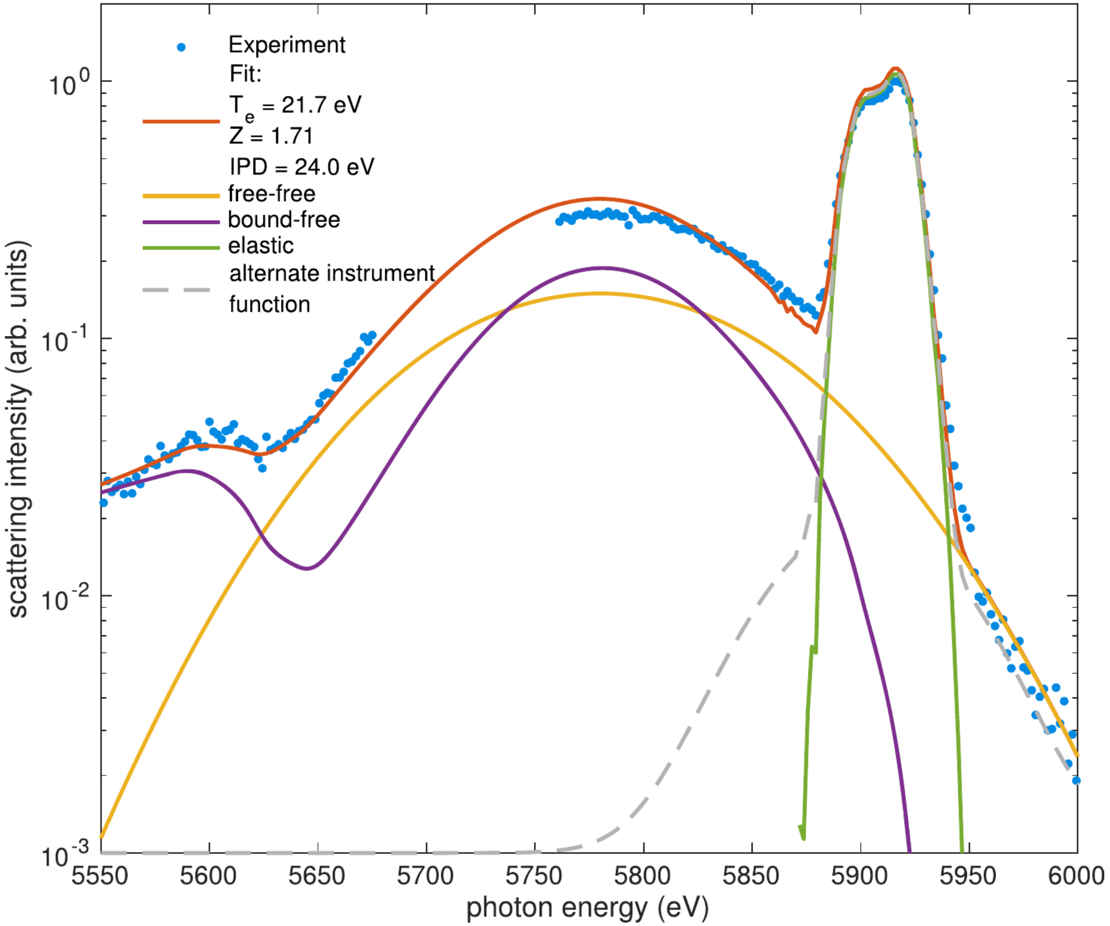

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Plasma Phys. Control. Fusion **61**, 014015 (2019)

Path integral Monte Carlo (PIMC): exact, but difficult!

• Canonical (N,V,T=const) partition function in coordinate representation:

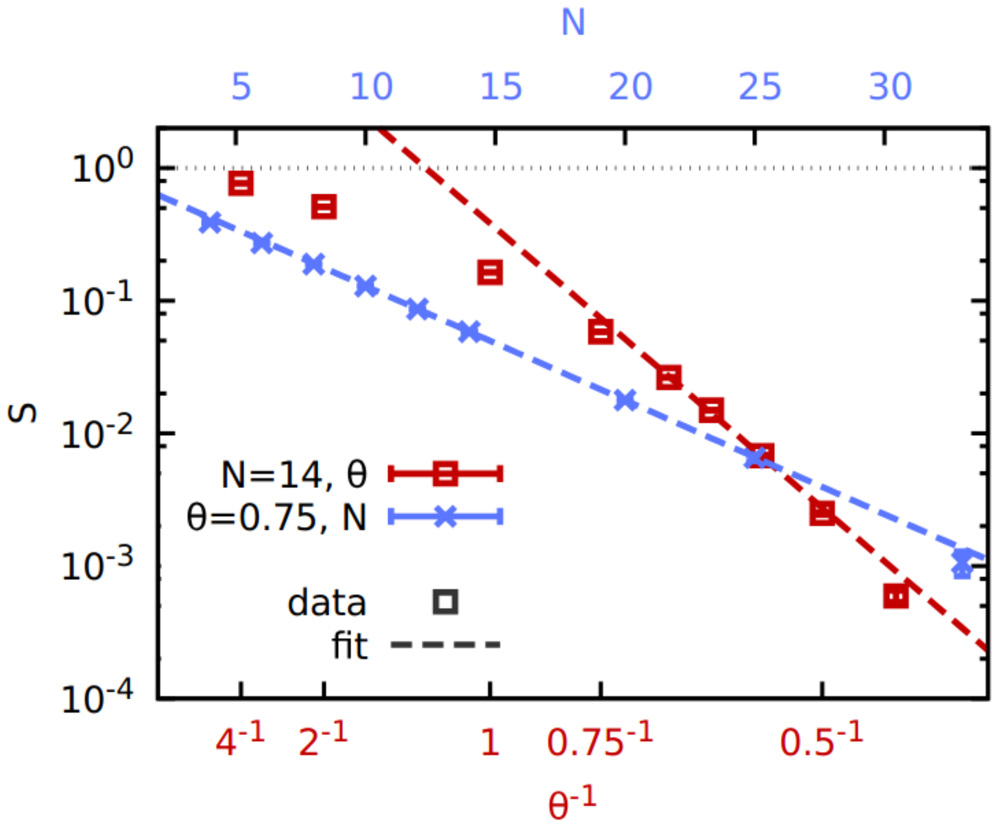
$$Z = \frac{1}{N!} \boxed{\sum_{\sigma \in S_N} \mathrm{sgn}(\sigma)} \int \mathrm{d}\mathbf{R} \; \langle \mathbf{R} | \, e^{-\beta \hat{H}} \, | \hat{\pi}_\sigma \mathbf{R} \rangle$$

→ Trotter-decomposition + group property of ρ lead to imaginary-time path integrals

• **Fermion sign problem:** cancellation of negative terms leading to exponential increase in compute time!

PIMC simulation of WDM possible, but highly challenging!

Average sign of uniform electron gas, rs=2, T-Fermi



Taken from: **T. Dornheim**, Phys. Rev. E **100**, 023307 (2019)