Recent Progress in simulations of dense quantum plasmas and warm dense matter

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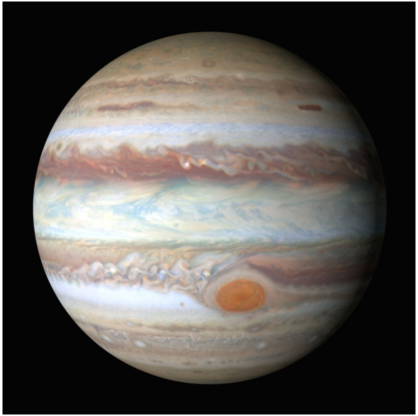
5th AAPS-DPP Meeting, 28 September 2021

DFG DAAD HLRN

Warm Dense Matter: Occurences and Applications [Andrew NG (2000): “missing link between CM, plasmas”]

- **Astrophysics:**
  - Giant planet interiors (e.g. Jupiter)
  - Brown dwarfs
  - Earth interior, Meteor Impacts
  - Recently discovered planets



Source: Sci-News.com [Img4]

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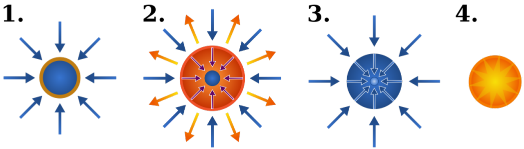
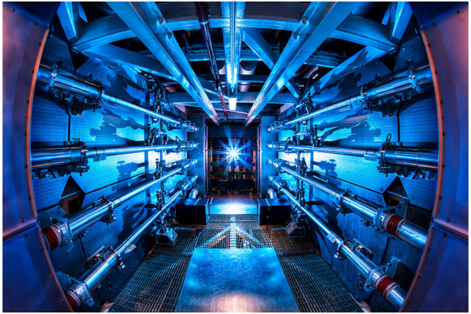
- **Laboratory Experiments, shock compression:**
  - Lasers, FELs, Z-pinch, ion beams
  - Properties of matter under extreme conditions
  - major driver: Inertial confinement fusion

  Potential abundance of clean energy!





Source: en.wikipedia.org [Img5] and arstechnica.com [Img6]

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US: NIF, Omega (Rochester), LCLS (Stanford): Fundamental research into WDM properties: $\rightarrow$ Equation of state, $S(\mathbf{q}, \omega)$, conductivity etc.

National Ignition Facility (Livermore, California)

area: $70000 m^2$
cost: $\sim$1 billion Dollar
Source: C. Stolz, *Phil. Trans. R. Soc. A* **370**, 4115 (2012) [Img7]

Facilities for WDM experiments in Europe and Asia:

Free electron lasers:

- **FLASH** (DESY, Hamburg)
- **E**uropean **X**-ray **F**ree-**E**lectron **L**aser, Hamburg – Schenefeld
- HIBEF Beamline and consortium (2021)
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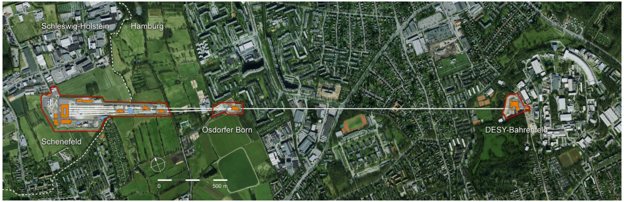

source: photon-science.desy.de

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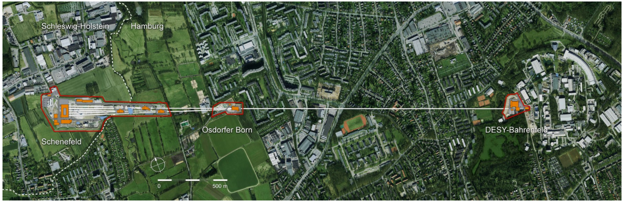

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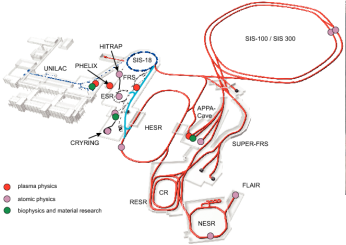
Heavy ion beams:

- **F**acility for **A**ntiproton and **I**on **R**esearch, Darmstadt
- Construction started in 2017
- Heavy ion beams:
  Isochoric heating up to $\sim 10^6 K$



source: inspirehep.net

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Warm dense matter: indeed a HOT topic

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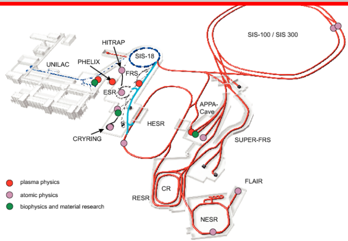

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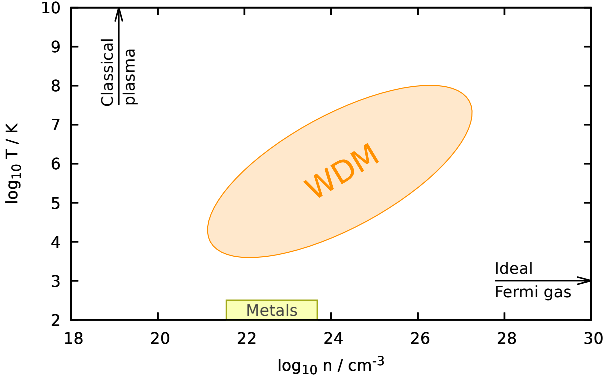
Warm Dense Matter and quantum plasmas: relevant parameters

- **Extreme and exotic state of matter:**
  $\rightarrow$ High temperature: $T \sim 10^3 - 10^8\ K$
  $\rightarrow$ Extreme density: $n \sim 10^{21} - 10^{27}\ cm^{-3}$

Source: T. Dornheim, S. Groth, and M. Bonitz, *Phys. Reports* **744**, 1-86 (2018)



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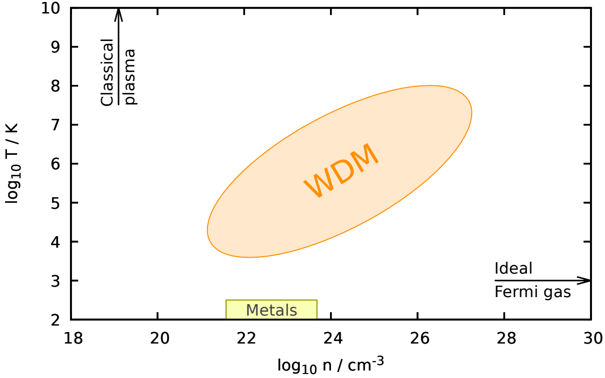

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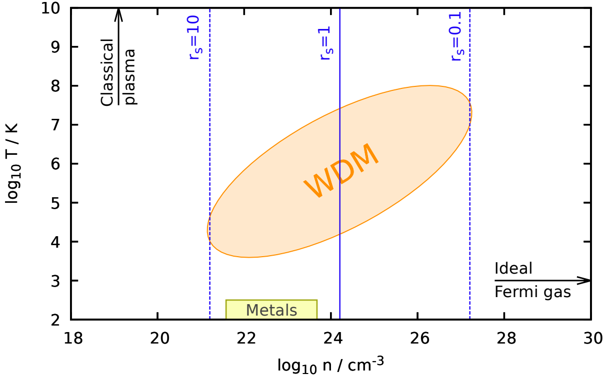

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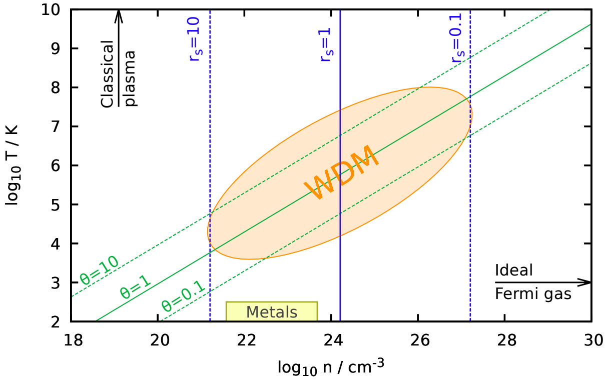

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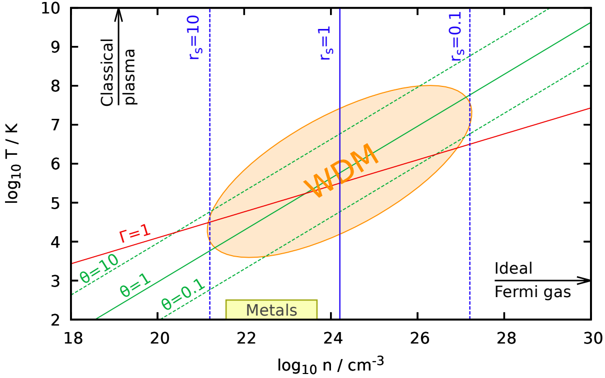

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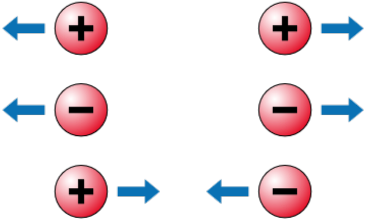
- **Nontrivial interplay of many effects:**
  - Coulomb coupling (non-ideality)



Source: bin-br.at [Img1]

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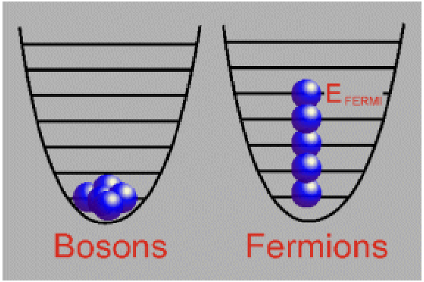

Source: cidehom.com [Img2]

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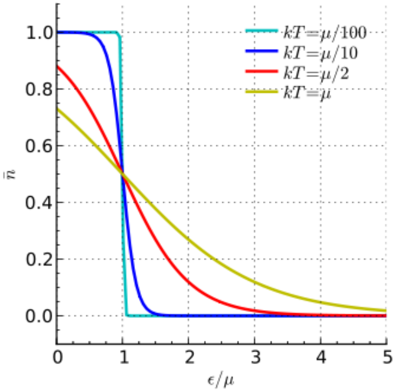
- **Nontrivial interplay of many effects:**
  - Coulomb coupling (non-ideality)
  - Fermionic exchange (anti-symmetry)
  - Thermal excitations (statistical description)



Source: en.wikipedia.org [Img3]

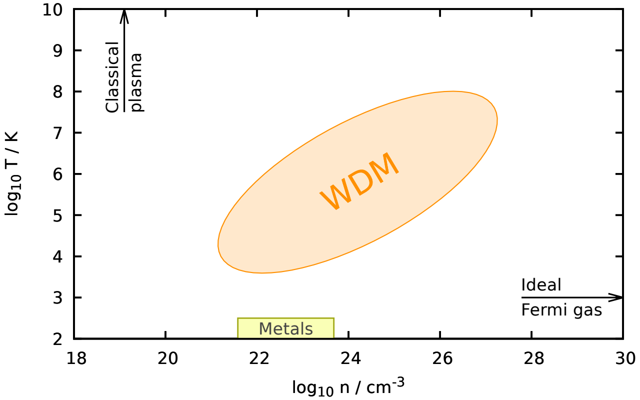
How to experimentally diagnose warm dense matter?

Warm dense matter (WDM) =
highly complex mix of ...

- ... gas phase (atoms, molecules) and plasma: partial ionization, differently charged ions etc.
- ... condensed (crystalline or liquid) phase and gas (plasma) phase

WDM often subject to strong excitation ...

- ... mix of ground state and highly excited phases
- Nonequilibrium: complex time evolution



Experimental strategies: 1. X-ray diffraction: morphology of solid and liquid state,

2. Transport (conductivity) and optics (e.g. X-ray absorption)

3. Recent breakthroughs: light scattering (X-ray Thomson scattering)
temperature, density, charge state, plasmon dispersion/damping...

How to theoretically approach warm dense matter?

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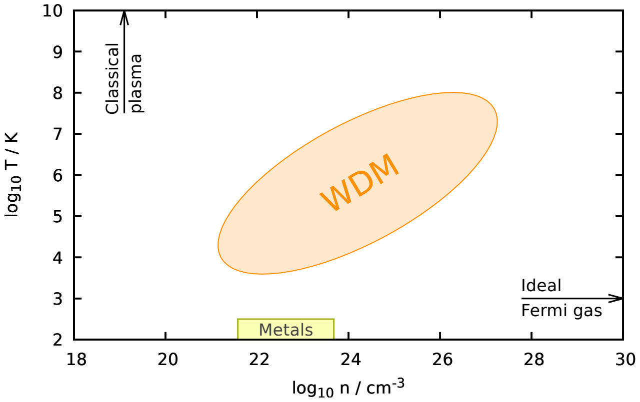

Theoretical strategies: **1. Make a complex (but poor) model of the entire “mess”, e.g. phenomenology, hydrodynamics, DFT, or**

2. Perform an excellent description of one piece of it (our approach)

$\Rightarrow$ **Series of recent breakthroughs: exact quantum Monte Carlo approach: from thermodynamic to dielectric and transport properties**

Importance of the uniform electron gas (UEG)

Model system of Coulomb interacting quantum electrons in a uniform positive background

Ground state ($T = 0$):

- Simple model for conduction electrons in metals
- **Exchange-correlation (XC) energy**:

$$e_{\mathrm{xc}}(r_s) = e_{\mathrm{tot}}(r_s) - e_0(r_s)$$

$\rightarrow$ Input for density functional theory (DFT) simulations (in LDA and GGA)
$\rightarrow$ Parametrization[1] of $e_{\mathrm{xc}}(r_s)$ from ground state quantum Monte Carlo data[2]
$\rightarrow$ this made DFT-MD the basis of modern atomic, molecular physics, chemistry, material science

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Warm dense matter ($T \sim T_{\mathbf{F}}$):

- **Thermal DFT**[3]: minimize free energy $F = E - TS$
  $\rightarrow$ Requires parametrization of XC **free** energy of UEG:

$$\boxed{f_{\mathrm{xc}}(r_s, \theta) = f_{\mathrm{tot}}(r_s, \theta) - f_0(r_s, \theta)}$$

- $f_{\mathrm{xc}}(r_s, \theta)$ direct input for **Equation of state (EOS) models** of astrophysical objects[4]
- $f_{\mathrm{xc}}(r_s, \theta)$ contains **complete thermodynamic information** of UEG

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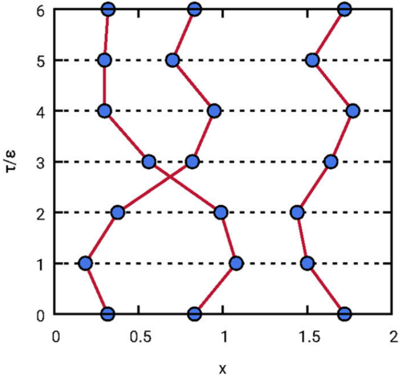
Path Integral Monte Carlo (PIMC): Fermions

- **Fermionic antisymmetry:**

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

$\Rightarrow$ We must include **permutation-cycles**!



PIMC configuration of $N = 3$ particles, $W(\mathbf{X}) < 0$

Taken from: T. Dornheim, S. Groth, A. Filinov, and M. Bonitz, *J. Chem. Phys.* **151**, 014108 (2019)

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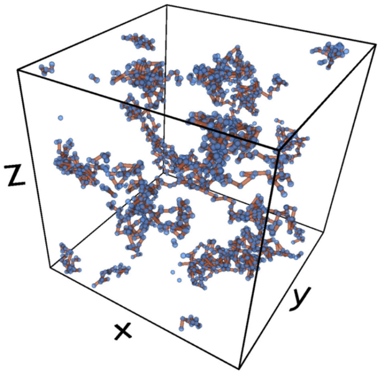

Snapshot of PIMC simulation of UEG with $N = 19$, $r_s = 2$, $\theta = 0.5$ (fluctuating probability density)

Taken from: T. Dornheim, S. Groth, A. Filinov, and M. Bonitz, *J. Chem. Phys.* **151**, 014108 (2019)

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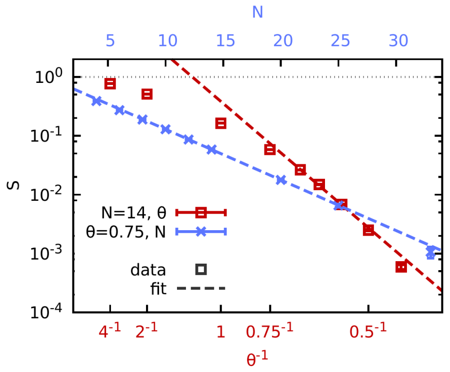
- Sign changes due to particle exchange lead to vanishing signal-to-noise ratio

  ⇒ **Fermion Sign Problem (unsolved!)**

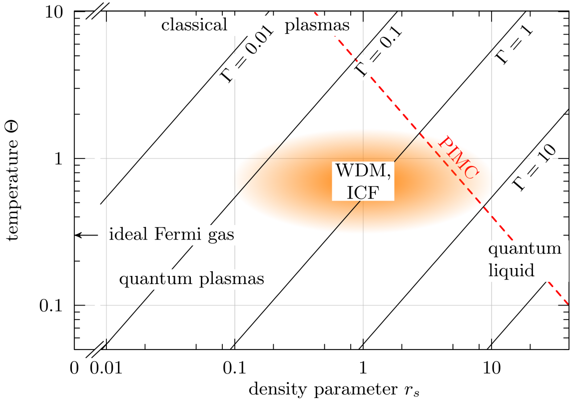


Exponential decrease of the average sign S with system size N and quantum degeneracy θ^{-1}

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

Path integral Monte Carlo (PIMC) simulation of the warm dense UEG

- Standard PIMC in warm dense regime severely hampered by ***fermion sign problem***:



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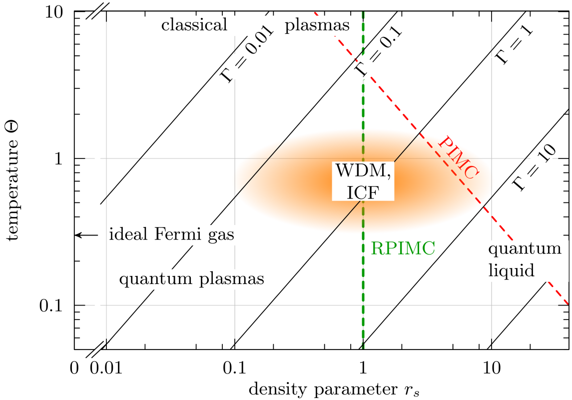
  - Induces **systematic errors** of unknown magnitude
  - **RPIMC** limited to $r_s \gtrsim 1$
  - Fermionic **PIMC**: Filinov et al.[2] limited to $r_s \gtrsim 1$



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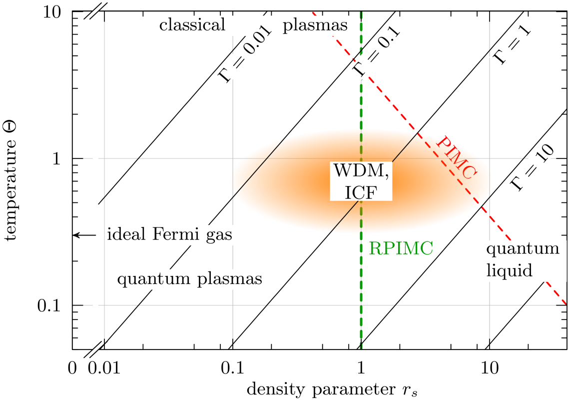
Our approach:

Avoid fermion sign problem by combining two exact and complementary QMC methods:



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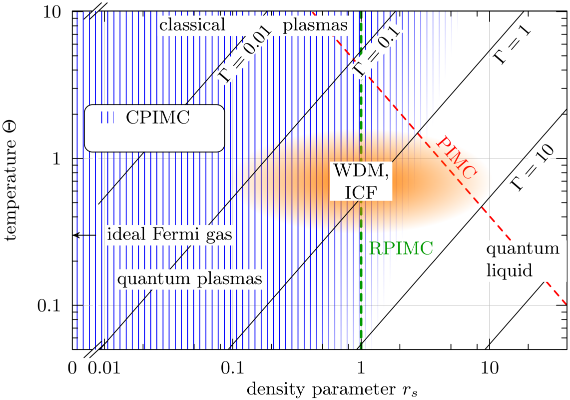
1. **Configuration PIMC (CPIMC)**[3,4]

$\rightarrow$ Excels at high density $r_s \lesssim 1$ and strong degeneracy



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  - Fermionic **PIMC**: Filinov et al.[2] limited to $r_s \gtrsim 1$

Our approach:

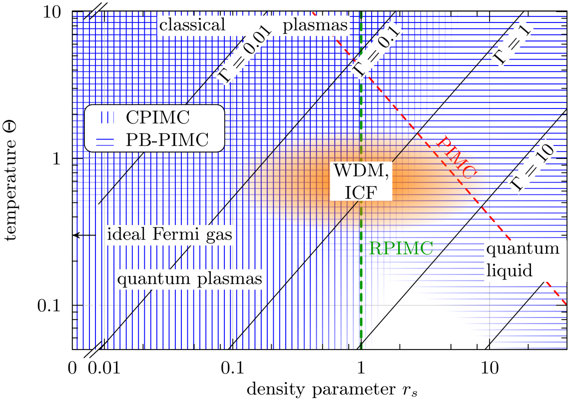
Avoid fermion sign problem by combining two exact and complementary QMC methods:

1. **Configuration PIMC (CPIMC)**[3,4]

   → Excels at high density $r_s \lesssim 1$ and strong degeneracy

2. **Permutation blocking PIMC (PB-PIMC)**[5,6]

   → Extends standard PIMC towards stronger degeneracy



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[1] E.W. Brown *et al.*, PRL **110**, 146405 (2013)
[2] V. Filinov *et al.*, Phys. Rev. E **91**, 033108 (2015)
[3] T. Schoof *et al.*, Phys. Rev. Lett **115**, 130402 (2015)
[4] T. Schoof *et al.*, Contrib. Plasma Phys. **51**, 687 (2011)
[5] T. Dornheim *et al.*, New J. Phys. **17**, 073017 (2015)
[6] T. Dornheim *et al.*, J. Chem. Phys. **143**, 204101 (2015)

Path integral Monte Carlo (PIMC) simulation of the warm dense UEG

- Standard PIMC in warm dense regime severely hampered by ***fermion sign problem***:
  - First results[1] by E. Brown, D. Ceperley *et al.* (2013) based on ***fixed node approximation*** (**RPIMC**)
  - Induces **systematic errors** of unknown magnitude
  - **RPIMC** limited to $r_s \gtrsim 1$
  - Fermionic **PIMC**: Filinov et al.[2] limited to $r_s \gtrsim 1$

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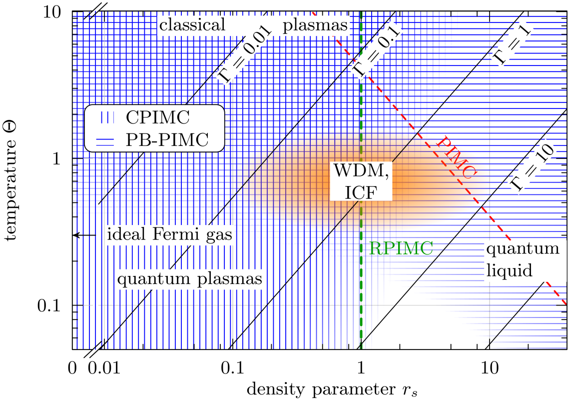

***Ab initio* simulations over broad range of parameters possible**

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[1] E.W. Brown *et al.*, PRL **110**, 146405 (2013)
[2] V. Filinov *et al.*, Phys. Rev. E **91**, 033108 (2015)
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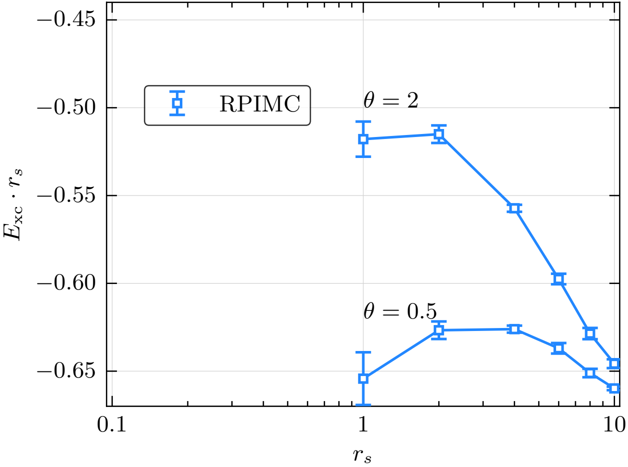
1. Exact exchange-correlation energy $E_{xc} = E - E_0$ (E_0: ideal energy) ($N = 33$ spin-polarized electrons, $\theta \geq 0.5$, $\forall\ r_s$)

- **RPIMC** limited to $r_s \geq 1$



[1] S. Groth *et al.*, Phys. Rev. B **93**, 085102 (2016)
[2] T. Dornheim *et al.*, Phys. Rev. B **93**, 205134 (2016)
[3] F.D. Malone *et al.*, Phys. Rev. Lett. **117**, 115701 (2016)
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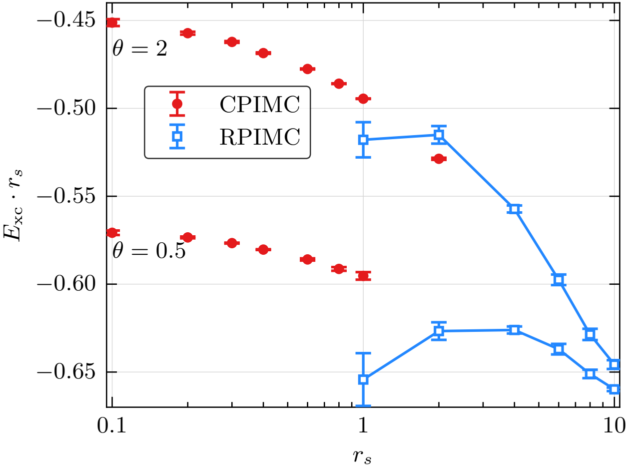
- **CPIMC** excels at high density



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[2] T. Dornheim *et al.*, Phys. Rev. B **93**, 205134 (2016)
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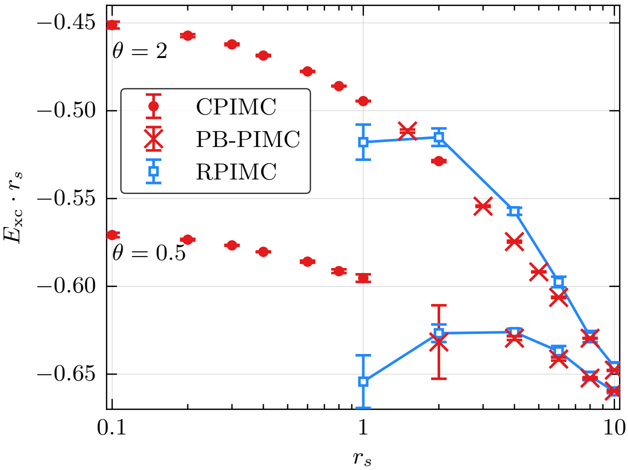

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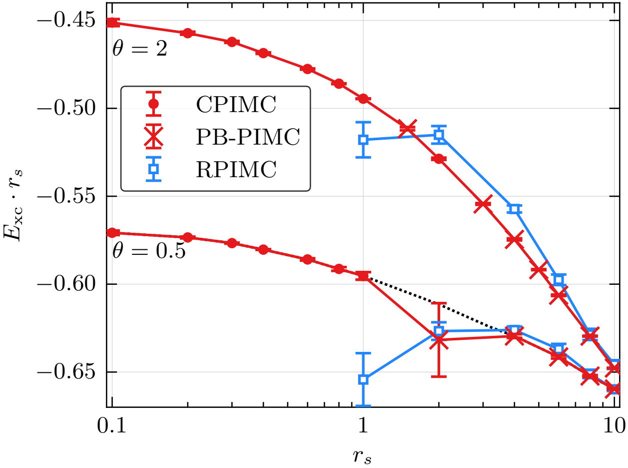
- **CPIMC** excels at high density
- **PB-PIMC** applicable at $\theta \gtrsim 0.5$

Combination[1] yields exact results over entire density range down to $\theta \sim 0.5$

- Also applies to the **unpolarized** UEG[2]
- confirmed by independent **DMQMC** simulations[3]
- Extended to TD Limit[4] and to the ground state[5]
- Analytical parametrization of $f_{xc}(r_s, \theta, \xi)$, "GDSMFB", with error below 0.3%, Integrated in standard DFT libraries[5]



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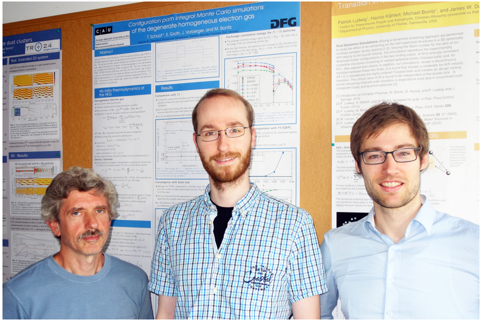
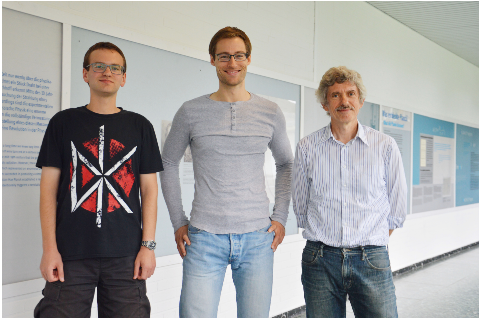
Acknowledgements to those who did most of the work...





Tim Schoof (PhD 2016), **Simon Groth** (PhD 2018):
CPIMC, finite size corrections etc.

Tobias Dornheim (PhD 2018): PB-PIMC
now at CASUS Görlitz, Extension to static and dynamic response, transport, DFT, machine learning, nonlinear density response etc.

Recent review: T. Dornheim, S. Groth, and M. Bonitz, Physics Reports **744**, 1-86 (2018), Photos: J. Siekmann

APS John Dawson Award 2021, together with F. Malone, M. Foulkes and T. Sjostrom

Ab Initio PIMC approach to equilibrium response and transport properties

Quantities accessible in PIMC:

all thermodynamic functions from $F(r_s, \theta)$; structural properties: $g(r)$, $S(q)$

fluctuations in response to excitation: $\delta\hat{H}(\mathbf{q}) \longrightarrow \delta\rho(\mathbf{q})$

correlation functions: e.g. $\langle\delta\rho(\mathbf{q}_1, \tau_1)\rho(\mathbf{q}_2, \tau_2)\rangle$ yield transport properties

Susceptibilites from linear response theory (LRT):

$\delta\rho(\mathbf{q}) = \chi(\mathbf{q})\delta H(\mathbf{q})$, χ: static density response $\longrightarrow$ comparison for PIMC to LRT/experiment

Correlation and exchange effects: encoded in "local field correction" $G(\mathbf{q}, \omega)$

straightforward connection to transport, optics etc.: $\chi(\mathbf{q}, \omega)$, $S(\mathbf{q}, \omega)$, $\epsilon(\mathbf{q}, \omega)$, $\sigma(\mathbf{q}, \omega)$, plasmon dispersion

PIMC: susceptibilities beyond validity limits of LRT

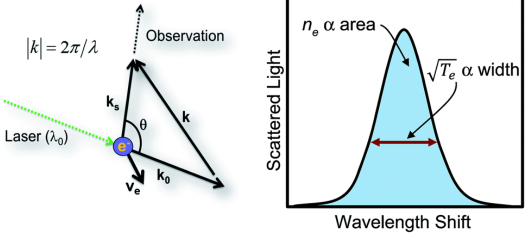
***Ab initio* spectral properties, momentum distribution $n(p)$**

Ab initio dynamic (ω-dependent) results for the warm dense UEG

- **Key quantity:** dynamic structure factor

$$S(\mathbf{q},\omega) := \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t \underbrace{\langle \hat{n}_{\mathbf{q}}(t)\hat{n}_{-\mathbf{q}}(0)\rangle}_{:=F(\mathbf{q},t)} e^{i\omega t}$$

$\rightarrow$ directly measured in **scattering experiments**



X-ray Thomson scattering experiments at free electron laser facilities (e.g. FLASH, X-FEL, LCLS)

yields the most accurate information on plasma density, ionic charge state, and temperature

data analysis requires model input

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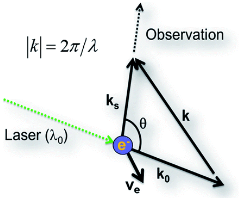
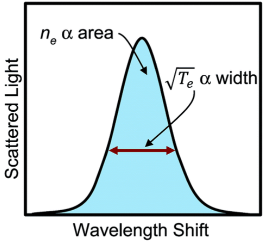
- **Chihara decomposition** applies for non-collective scattering:

$$S(\mathbf{q},\omega) = S_{\text{b-b}}(\mathbf{q},\omega) + S_{\text{b-f}}(\mathbf{q},\omega) + S_{\text{f-f}}(\mathbf{q},\omega)$$

$$\rightarrow S_{\text{f-f}}(\mathbf{q},\omega) \sim S^{\text{UEG}}(\mathbf{q},\omega)$$





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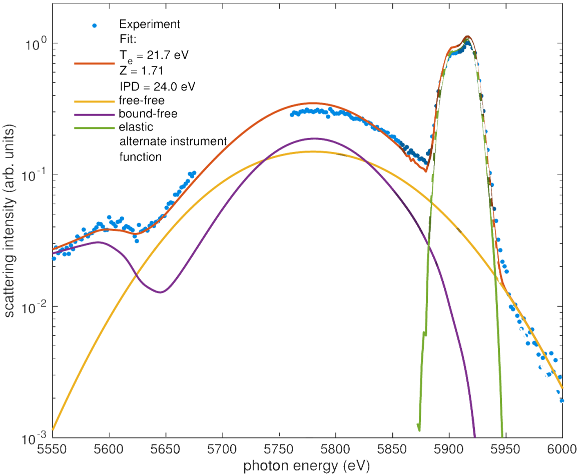
$$\rightarrow S_{\text{f-f}}(\mathbf{q},\omega) \sim S^{\text{UEG}}(\mathbf{q},\omega)$$

- **Practical example:** Fit model for $S(\mathbf{q},\omega;T_\text{e})$ to spectrum to determine electron temperature T_e
- **Problem:**
  $F(\mathbf{q},t)$ requires **real time-dependent simulations**
  $\rightarrow$ with PIMC have to use analytic continuation, reconstruct $F(q,it)$ and 4 frequency moments, but: insufficient information



Scattering spectrum of isochorically heated graphite at LCLS.
From D. Kraus *et al.*, *Plasma Phys. Control. Fusion* (2019)

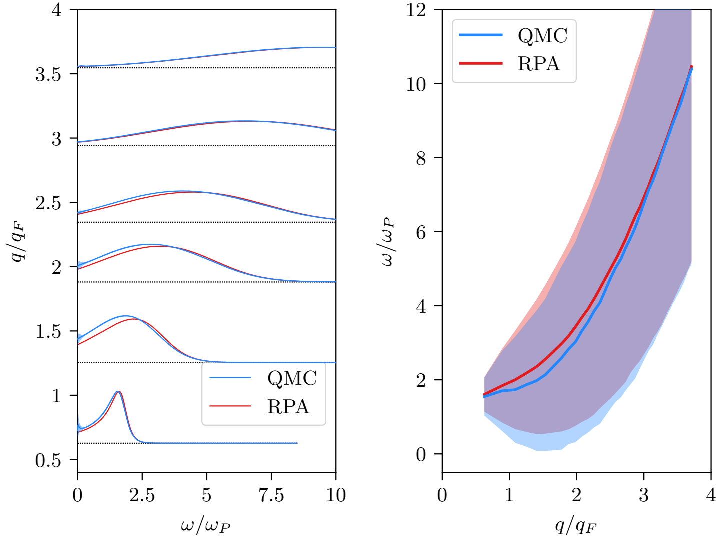
Correlation effects, Landau and collisional damping in $S(q,\omega)$: $\theta = 1$, $r_s = 2$

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

- Slight **correlation induced redshift** of peak for intermediate q (at small r_s)

Dynamic structure factor of the UEG:

Peak position and FWHM:



Correlation effects, Landau and collisional damping in $S(q,\omega)$: $\theta = 1$, $r_s = 10$

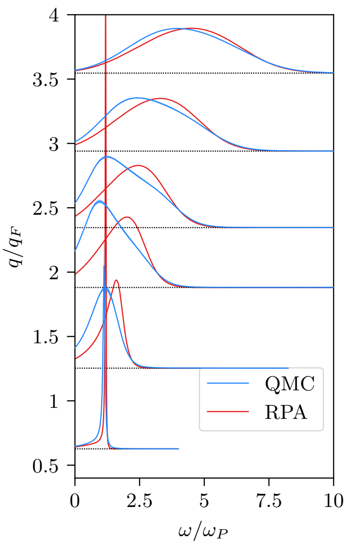
T. Dornheim, S. Groth, J. Vorberger, and M. Bonitz, *Phys. Rev. Lett.* **121**, 255001 (2018)

- Slight **correlation induced redshift** of peak for intermediate q (at small r_s)
- **Pronounced redshift** and **broadening** with increasing r_s
- **Negative dispersion of peak** for large r_s around $q = 2q_F$ **predicted for dense hydrogen**
- **Closely related to plasmons**

Requires dielectric function $\epsilon(q,\omega)$

$$S(\mathbf{q},\omega) = -\frac{\mathrm{Im}\,\epsilon^{-1}(\mathbf{q},\omega)}{\pi n \tilde{v}(q)(1-e^{-\beta\omega})}$$

Dynamic structure factor of the UEG:



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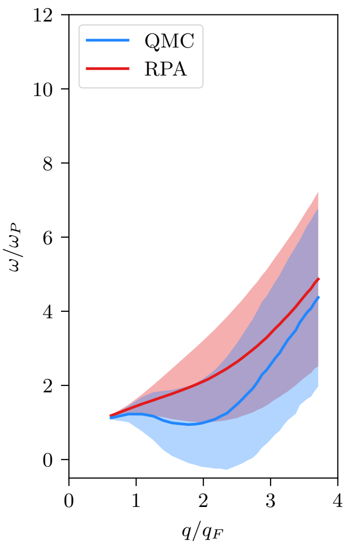


Dielectric function. Plasmons

- Solution of Maxwell's equations: EM field modes, $E(q,t)$, in plasma (isotropic), from

$$\hat{\epsilon}[\vec{q}, \omega(q)] = 0$$

- contains collective excitations (plasmon)
- weak damping approximation (WDA):

$$\mathrm{Re}\,\hat{\epsilon}[\vec{q}, \omega(q)] = 0$$

- roots on real axis vanish for $q \geq q_{\rm cr}$, and damping, $|\mathrm{Im}\,\omega|$, becomes large
- drop WDA and find exact roots

$$\hat{\epsilon}(\vec{q}, z) = 0$$

at complex frequencies $z = \omega - i\gamma$:

$$E(q;t) \sim e^{i\omega(q)t} e^{-\gamma(q)t}, \quad \gamma > 0$$

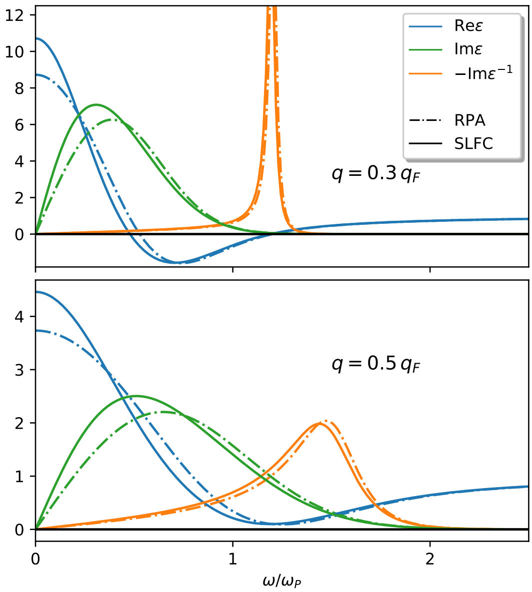
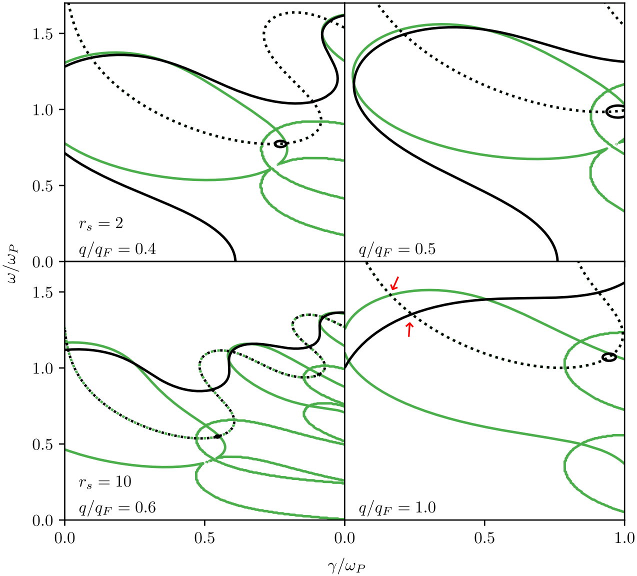


Figure: Moderately correlated electron gas, $\Theta = 1$, $r_s = 2$

Analytic continuation (AC) of the dielectric function[1]

- AC of the retarded DF into the lower frequency half plane, $\gamma > 0$.
- full lines: Re $\epsilon = 0$,
  dotted lines: Im $\epsilon = 0$,
  plasmon = intersection (arrows)
- green: mean field (RPA)
  black: correlated (static LFC)
- complex zeroes may exist, even if Re $\epsilon \neq 0$ on real axis (top right).
- Finite temperature, $\Theta = 1$, $r_s = 2$ (top) and $r_s = 10$ (bottom)



[1] M. Bonitz, Quantum Kinetic Theory, 2nd ed. Springer 2016; P. Hamann *et al.*, Contrib. Plasma Phys. **60**, e202000147 (2020)

Plasmon dispersion (top) and damping (bottom), $\Theta = 1$

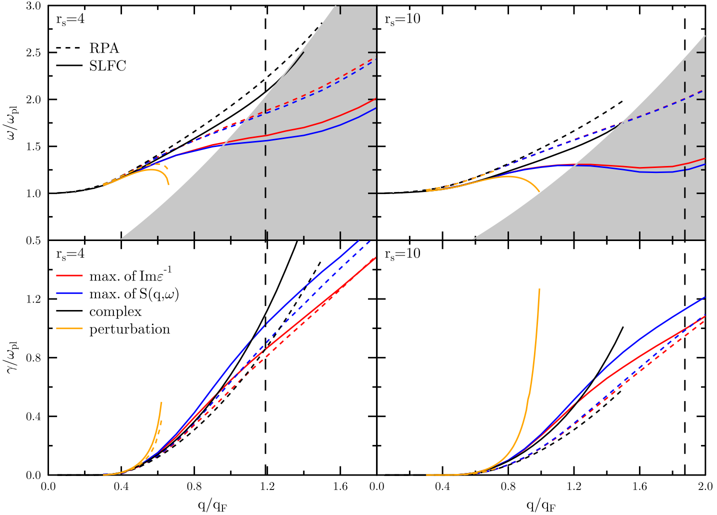


Figure: Black: complex dispersion relation, yellow: weak damping approximation, blue: peak of $S(q, \omega)$, grey area: pair continuum. Work in progress: Plasmon dispersion in two-component plasma (Mermin approach)

The momentum distribution function (thermodynamic equilibrium)

- **Classical plasma**
  - ideal plasma: Maxwell distribution
  - interacting plasma: Maxwell distribution

  $\Rightarrow$ exponential decay for large momenta

- **Quantum plasma**
  - ideal plasma: Fermi/Bose function

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- **What about nonideal Quantum plasmas?**
  - slower non-exponential decay, $\sim p^{-8}$, predicted[2]
  - relevant for threshold processes: dramatic increase of reaction rates, fusion rates could be possible
  - important for electrons under warm dense matter (WDM) conditions or ions in dense stars
  - First *ab initio* Quantum Monte Carlo results for WDM available:
    K. Hunger *et al.*, Phys. Rev. E **103**, 053204 (2021), arXiv:2101.00842
    T. Dornheim *et al.*, Phys. Rev. B **103**, 205142 (2021)

[2] Daniel, Vosko (1960); Galitskii, Migdal (1967)

Ab initio CPIMC-results for the momentum distribution[3]

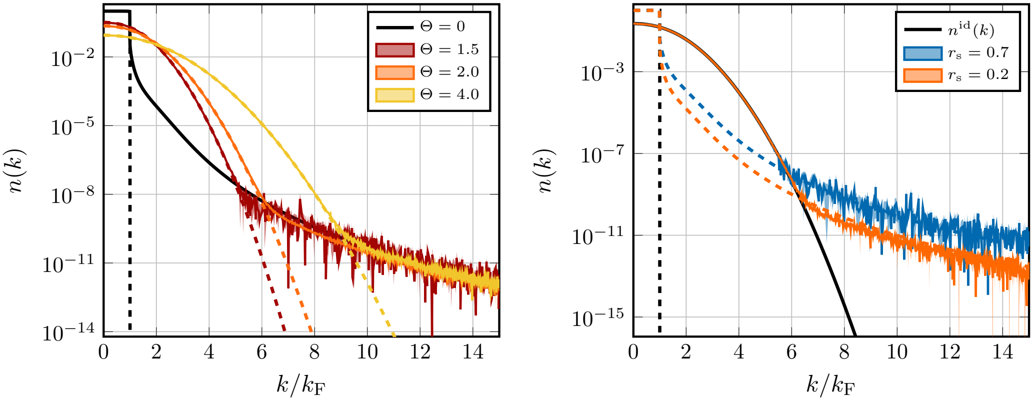

Figure: **Left**: Temperature dependence at $r_s = 0.5$. Full lines: CPIMC, dashed: Fermi function n^{id}.
Right: Density dependence at $\Theta = 2$. Full lines: CPIMC, dashed: ground state, black: n^{id}.

Unprecedented accuracy (11 digits, large k-range), confirm p^{-8} asymptotic, accurate n- and T-dependence
Crucial for reaction rates of threshold processes

[3] K. Hunger *et al.*, Phys. Rev. E **103**, 053204 (2021); T. Dornheim *et al.*, Phys. Rev. B **103**, 205142 (2021)
ground state results: Gori-Giorgi *et al.* (2001)

Summary: *Ab Initio* QMC results for static and dynamic equilibrium properties

Thermodynamic and structural properties of the WD UEG:

- all thermodynamic functions from $f_{xc}(r_s, \theta)$; structural properties: $g(r)$, $S(q)$
- benchmarks and improvements of other models[4]
- Input for two-component approaches including DFT (xc-functionals) or quantum hydrodynamics

Transport, dielectric and optical properties:

- Correlation and exchange effects encoded in "local field correction" $G(\mathbf{q}, \omega)$
- *ab initio* correlated results for: $\chi(\mathbf{q}, \omega)$, $S(\mathbf{q}, \omega)$[5], $\epsilon(\mathbf{q}, \omega)$, $\sigma(\mathbf{q}, \omega)$, plasmon dispersion[6]
- extension to two-component quantum plasma via the Mermin dielectric function[7]
- correlated electron momentum distribution function[8] $n(p)$

Outlook: extension to nonequilibrium electron-ion dynamics

- DFT-MD, time-dependent DFT (TD-DFT)
- Quantum kinetic equations, Nonequilibrium Green functions (NEGF)
- Quantum hydrodynamics (QHD)

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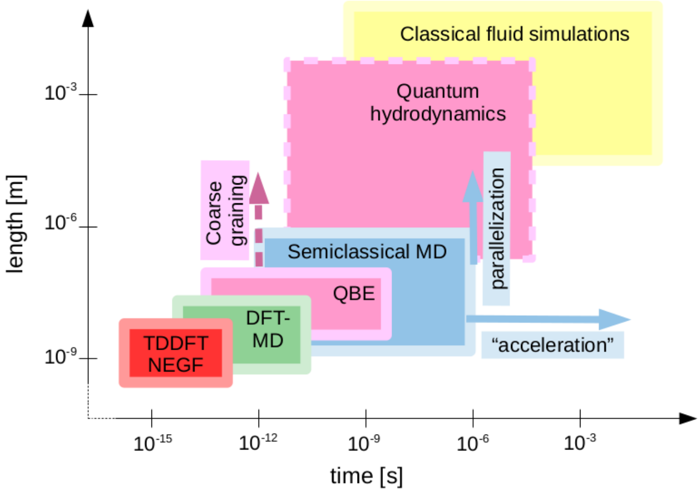
[4] Dornheim *et al.*, Phys. Plasmas (2017); Dornheim *et al.*, Phys. Rep. (2018)
[5] Dornheim *et al.*, PRL 2018
[6] Hamann *et al.*, PRB (2020) and Contrib. Plasma Phys. (2020)
[7] Hamann *et al.*, to be published
[8] Hunger *et al.*, Phys. Rev. E (2021)

Nonequilibrium simulations of warm dense matter



- QBE: Quantum Boltzmann equation
- NEGF: Nonequilibrium Green Functions
- TDDFT: time-dependent DFT

Figure: Approximate range of applicability of different methods; from Bonitz *et al.*, Phys. Plasmas **27** (4), 042710 (2020)

Quantum kinetic theory simulations[9]

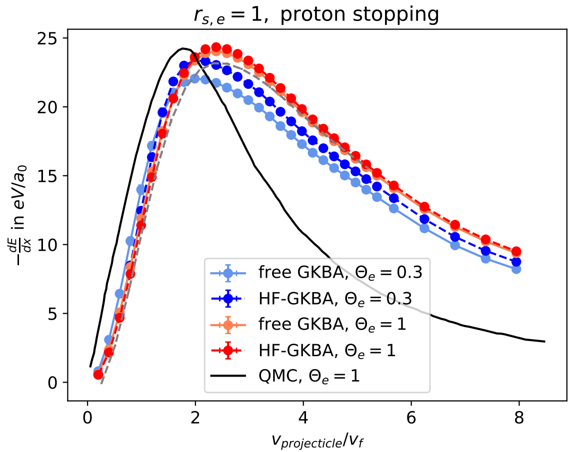


Figure: Stopping power of protons in a dense electron plasma. Time-dependent solution of quantum kinetic equation with the generalized Kadanoff-Baym ansatz, compared to linear response calculations involving *ab initio* QMC-input (C. Makait, Z. Moldabekov, and M. Bonitz, to be published)

- NEGF are the most accurate approach to nonequilibrium quantum plasmas, but very CPU time costly

- recently we achieved a dramatic acceleration [Schlünzen et al., PRL 2020]

⇒ NEGF results will provide benchmarks for real-time TDDFT and deliver improved xc-functionals

⇒ TDDFT results will provide benchmarks for QHD and improved Bohm potential V_B

⇒ Basis for accurate time-dependent quantum simulations over large time and length scales

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[9] M. Bonitz, *Quantum Kinetic Theory*, 2nd ed., Springer 2016

Quantum hydrodynamics for shock propagation

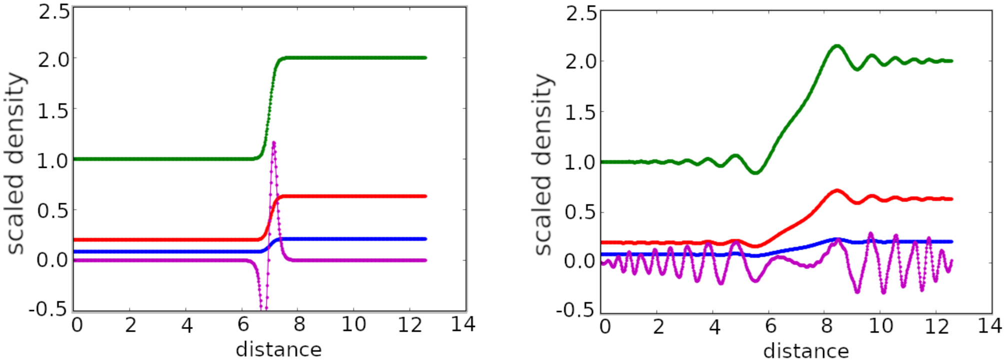


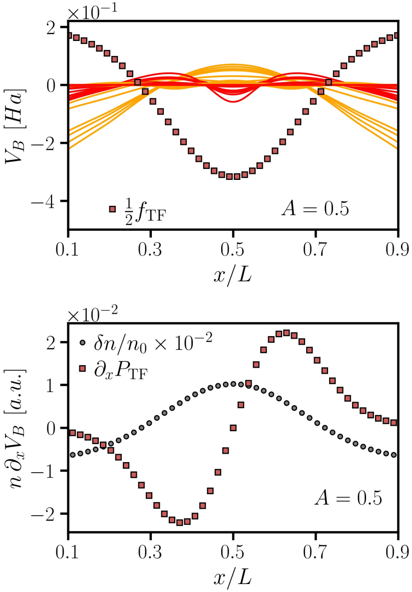
Figure: Influence of th Bohm potential (pink) on the density profile (green) of a running shock. Dense plasma of $r_s = 2$ and $\Theta \approx 0$. Left: initial state, right: $t = 0.62 a_B / c_s$. Red: Thomas-Fermi pressure, blue: exchange pressure.
From: Graziani *et al.*, Contrib. Plasma Phys. (2021), arXiv:2109.09081

The Bohm potential V_B causes a shear force (stretching) of the shock front. Accurate form of V_B is crucial.[10]

[10] Moldabekov *et al.*, Phys. Plasmas **25**, 031903 (2018); Bonitz *et al.*, Phys. Plasmas **26**, 090601 (2019)

Rigorous test of QHD equations using DFT[11]

- Critically assess the validity of the QHD equations for plasmas [Manfredi and Haas, PRB (2001)], $V_B[\bar{n}]$
- $V_B \equiv 0$ in homogeneous system.
  $\Rightarrow$ consider non-uniform electron gas, $r_s = 2$, $\theta = 1$; 1D test case: static perturbation $v(r) = 2A\cos qr$
- Solve finite-temperature Kohn-Sham equations,
  $\Rightarrow$ obtain individual orbitals ϕ_i and densities n_i
  $\Rightarrow$ obtain Bohm potential for each orbital (red and yellow curves in top figure)
- grey circles: mean density, red squares: ideal free energy density (top) and force due to ideal pressure p_{TF} (bottom)

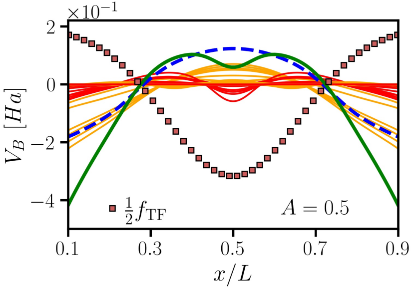


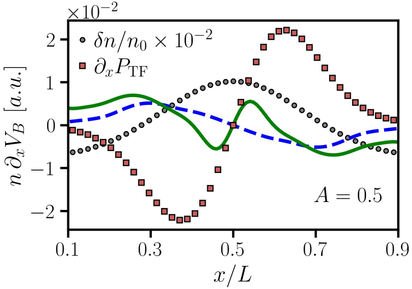
[11] Moldabekov *et al.*, submitted to scipost, arXiv:2103.08523

Rigorous test of QHD equations using DFT[12]

- Bohm potential for each orbital (red and yellow curves)
- blue: Bohm potential with mean density, $V_B(\bar{n})$ (Manfredi, Haas)

  green: many-fermion (microscopic) Bohm potential (average over orbital Bohm potentials)
  [Bonitz *et al.*, Phys. Plasmas **26**, 090601 (2019)]
- $\Rightarrow$ force exhibits more than 100% deviations almost everywhere, despite very weak density modulation
  $\Rightarrow$ previous nonlinear QHD results questionable

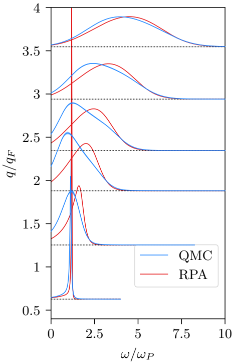


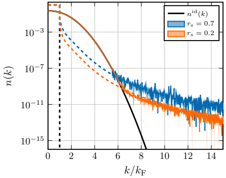


[12] Moldabekov *et al.*, submitted to scipost, arXiv:2103.08523

Warm dense matter and quantum plasmas – Summary and outlook[13]

- **Crucial for astrophysics and laboratory experiments**:
  - complex state of matter, between condensed matter and plasmas
  - New facilities: accurate experimental results (e.g. X-ray Thomson scattering)
- **Accurate simulation results now available**:
  - *Ab initio* QMC results for the electron component, avoid sign problem[a].
  - Benchmarks, input for analytical models and for DFT and QHD
  - *Ab initio* results for transport and dielectric properties, momentum distrib.[b]
- **Outlook: accurate multiscale nonequilibrium simulations**[c]:
  - combination of Green functions, TDDFT, and QHD[d]
  - further improvement of CPIMC, extension to two-component plasmas





[a] Dornheim *et al.*, Phys. Reports (2018)
[b] Dornheim *et al.*, PRL (2018); Hamann *et al.*, PRB (2020); Hunger *et al.*, PRE (2021)
[c] Bonitz *et al.*, Phys. Plasmas (2020)
[d] Bonitz *et al.*, Phys. Plasmas (2019); Moldabekov *et al.*, arXiv:2103.08523

[13] references and talk at http://www.theo-physik.uni-kiel.de/bonitz/research.html