Momentum distribution function and short-range correlations in dense quantum plasmas – ab initio quantum Monte Carlo results

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Plasma Theory and Simulation, PTS–2022

pdf at www.theo-physik.uni-kiel.de/bonitz/research.html

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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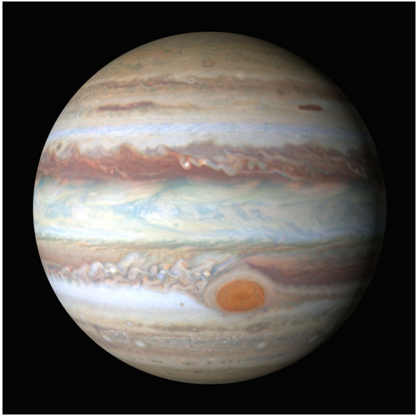
- **What about nonideal Quantum plasmas?**
  - slower non-exponential decay, $\sim p^{-8}$, predicted[1]
  - relevant for threshold processes: dramatic increase of reaction rates, fusion rates could be possible
  - important for electrons under warm dense matter (WDM) conditions or ions in dense stars
  - 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)

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

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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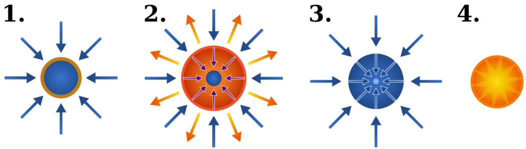
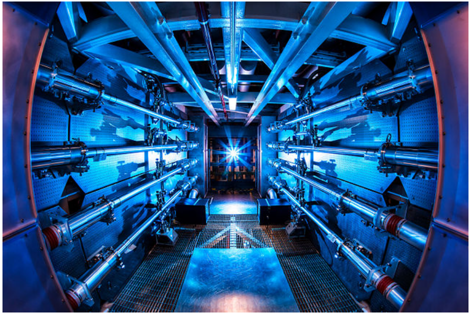
- **Laboratory Experiments, shock compression:**
  - Lasers, FELs, Z-pinch, ion beams
  - Properties of matter under extreme conditions, e.g. Kritcher *et al.*, Nature 2020
  - major driver: Inertial confinement fusion

  Potential abundance of clean energy!





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

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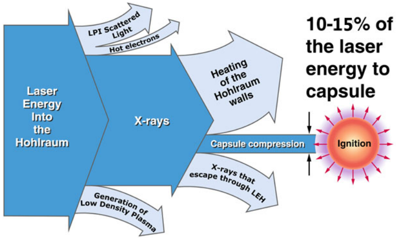
US: NIF, Omega (Rochester), LCLS (Stanford): Fundamental research into WDM properties: $\rightarrow$ Equation of state, $S(\mathbf{q}, \omega)$, conductivity etc.

National Ignition Facility (Livermore, California)

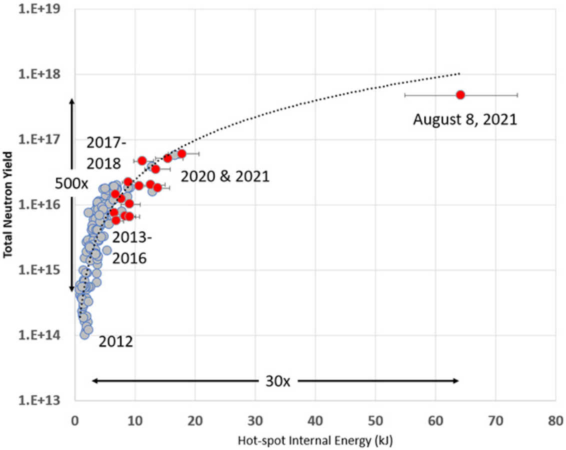
area: $70000 m^2$
cost: $\sim$1 billion Dollar
Source: C. Stolz, *Phil. Trans. R. Soc. A* **370**, 4115 (2012) [Img7]

Progress in Inertial Confinement Fusion



continuous optimization of target design, pulse shape etc.

Record shot on August 8 2021: 1.92 MJ UV laser energy
source: https://lasers.llnl.gov/news/hybrid-experiments-drive-nif-toward-ignition

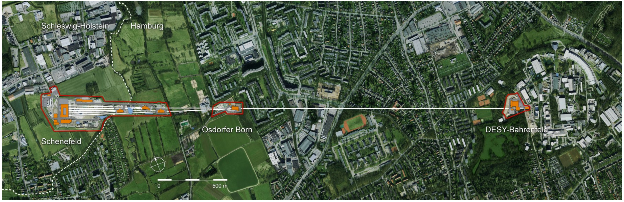


The "Hybrid-E experiment" on Aug. 8 achieved a hot-spot absorbed energy of about 65 kJ—about 20 kJ from the implosion, and the rest from "self-heating" from the fusion reactions (self-sustained burn). 1.35 MJ fusion energy yield, corresponds to 70% of ignition threshold (NAS criterion). Zylstra *et al.*, Nature (2022)

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 first successful experiments
- **Fermi** (Triest, Italy)
- **SACLA** (Riken, Japan)



source: photon-science.desy.de

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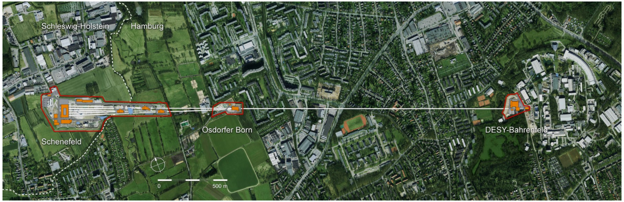

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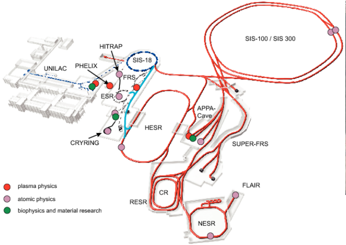
Heavy ion beams:

- **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

source: dw.com

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Warm dense matter: indeed a HOT topic

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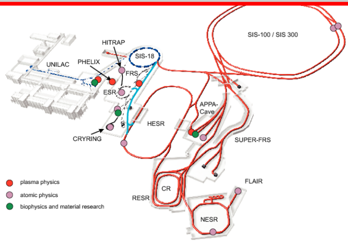

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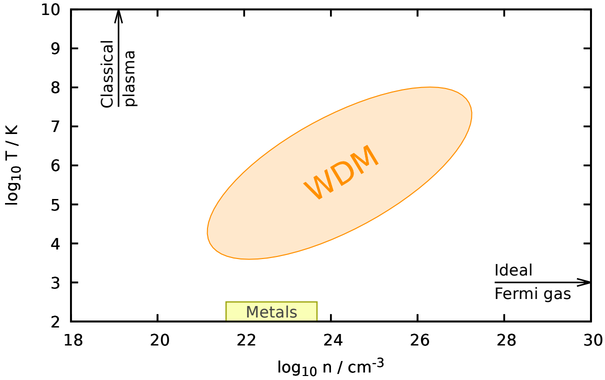
Warm Dense Matter and quantum plasmas: relevant parameters

- **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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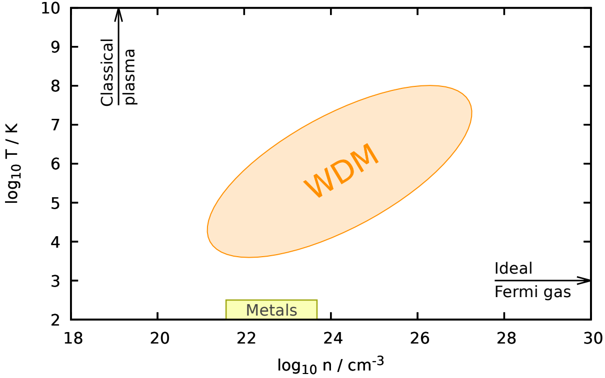

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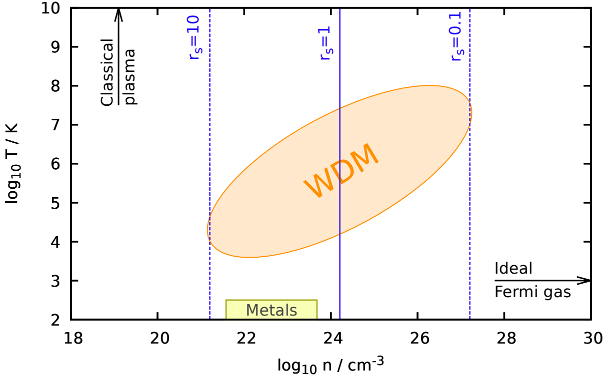

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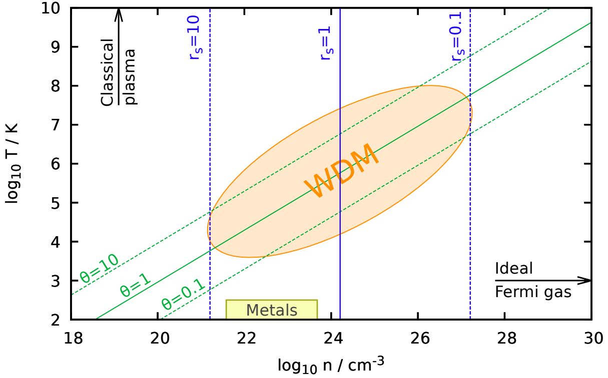

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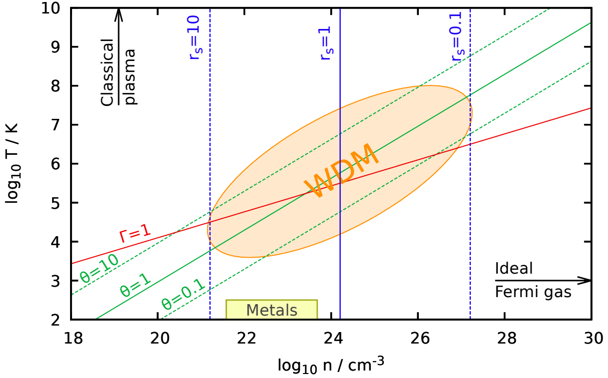

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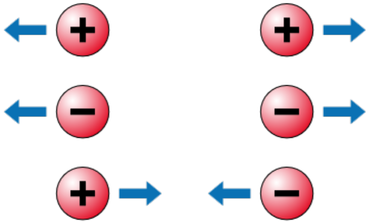
  - Coulomb coupling (non-ideality)



Source: bin-br.at [Img1]

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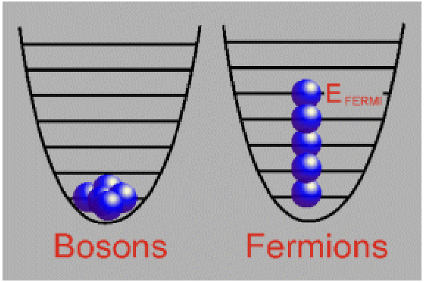

Source: cidehom.com [Img2]

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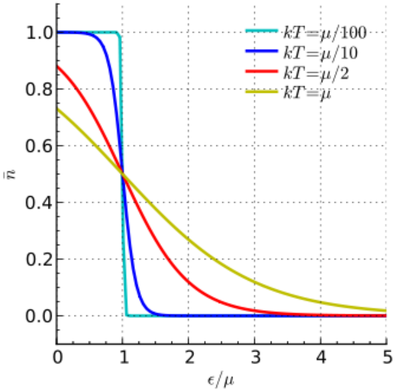
  - Thermal excitations (statistical description)



Source: en.wikipedia.org [Img3]

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**:

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

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

[1] J.P. Perdew and A. Zunger, PRB **23**, 5048 (1981) [2] D.M. Ceperley and B. Alder, PRL **45**, 566 (1980) [3] N.D. Mermin, Phys. Rev **137**, A1441 (1965)
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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:

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

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

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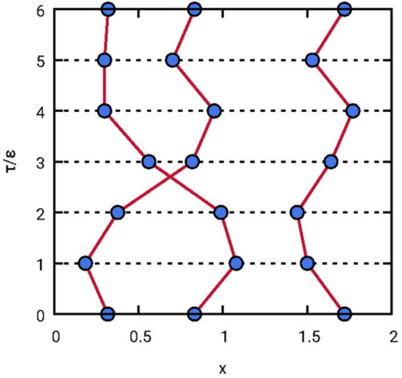
Path Integral Monte Carlo (PIMC): Fermions

- **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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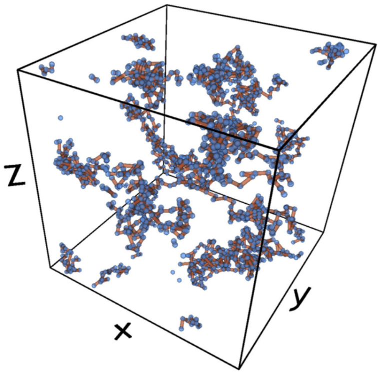

Snapshot of PIMC simulation of UEG with $N = 19$, $r_s = 2$, $\theta = 0.5$ (fluctuating probability density)

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

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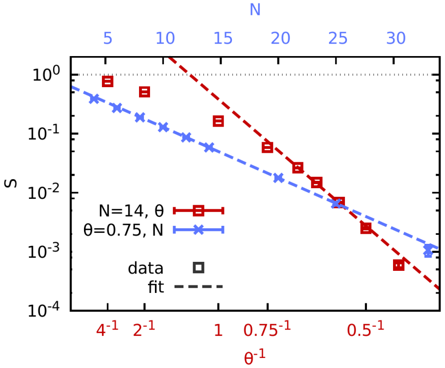
- Sign changes due to particle exchange lead to vanishing signal-to-noise ratio

$\Rightarrow$ **Fermion Sign Problem (unsolved!)**

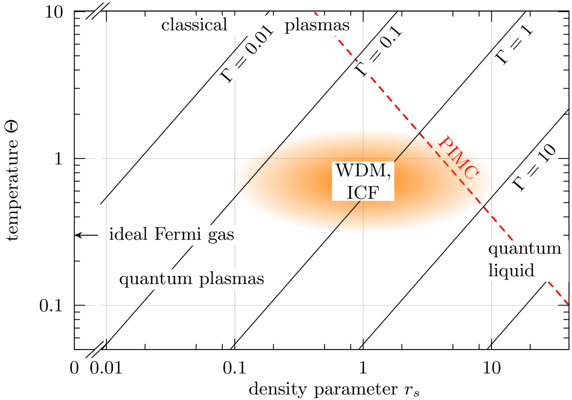


Exponential decrease of the average sign S with system size N and quantum degeneracy θ^{-1}

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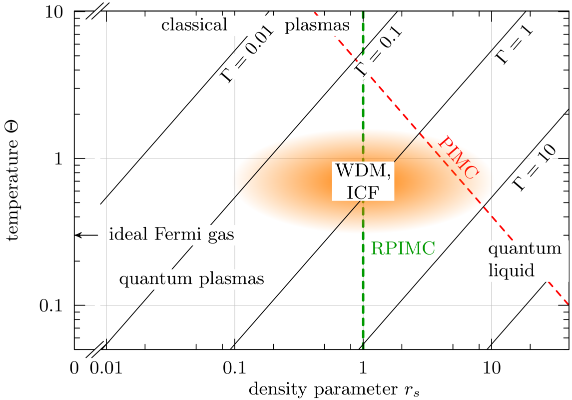
  - First results[1] by E. Brown, D. Ceperley *et al.* (2013) based on ***fixed node approximation*** (**RPIMC**)
  - Induces **systematic errors** of unknown magnitude
  - **RPIMC** limited to $r_s \gtrsim 1$
  - Fermionic **PIMC**: Filinov et al.[2] limited to $r_s \gtrsim 1$



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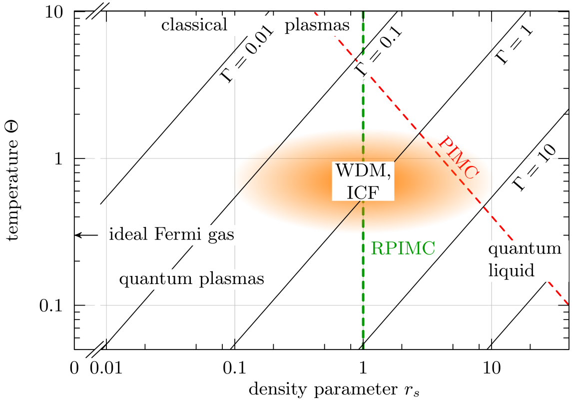
Our approach:

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



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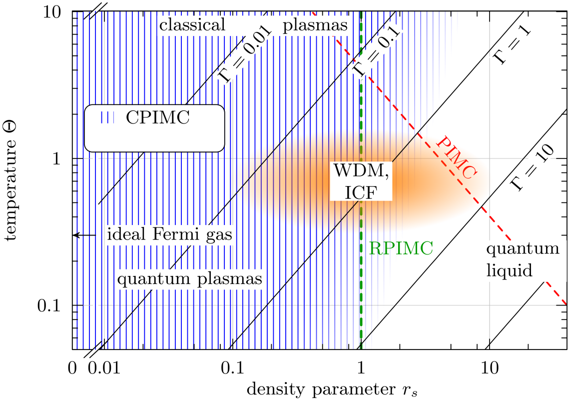
1. **Configuration PIMC (CPIMC)**[3,4]

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



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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 $r_s \gtrsim 1$

Our approach:

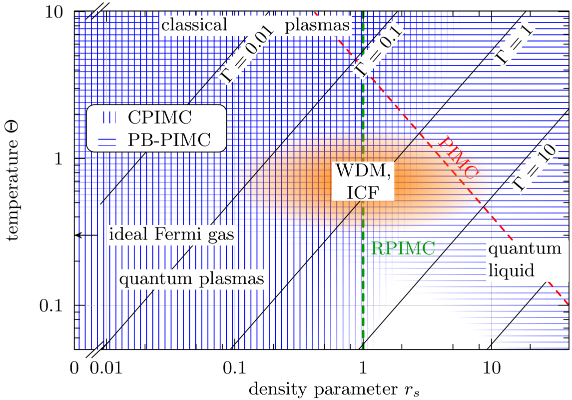
Avoid fermion sign problem by combining two exact and complementary QMC methods:

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

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

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

   $\rightarrow$ Extends standard PIMC towards stronger degeneracy



[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)
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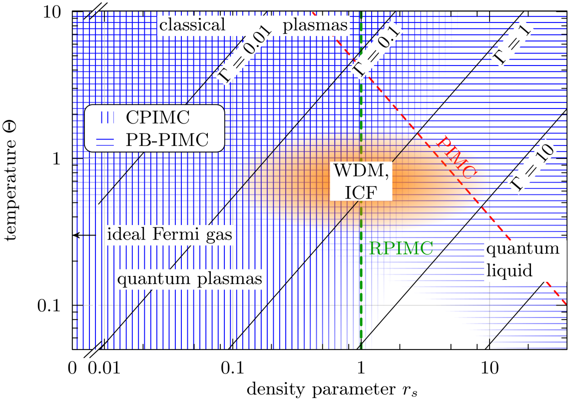

Ab initio simulations over broad range of parameters possible

[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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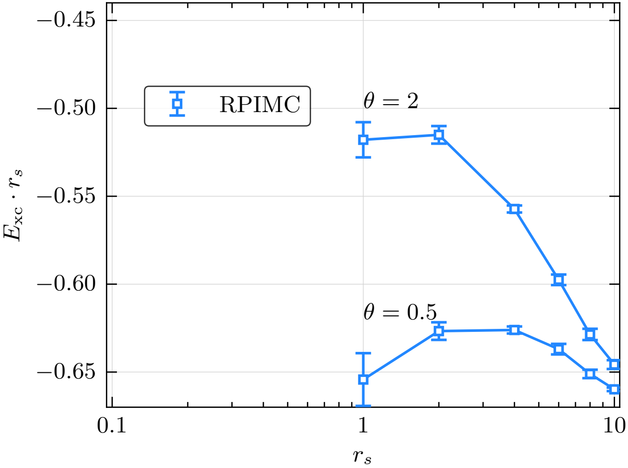
1. Exact exchange-correlation energy $E_{xc} = E - E_0$ (E_0: ideal energy) ($N = 33$ spin-polarized electrons, $\theta \geq 0.5$, $\forall\ r_s$)

- **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) [4] T. Dornheim *et al.*, Phys. Rev. Lett. (2016) [5] S. Groth *et al.*, Phys. Rev. Lett. (2017)

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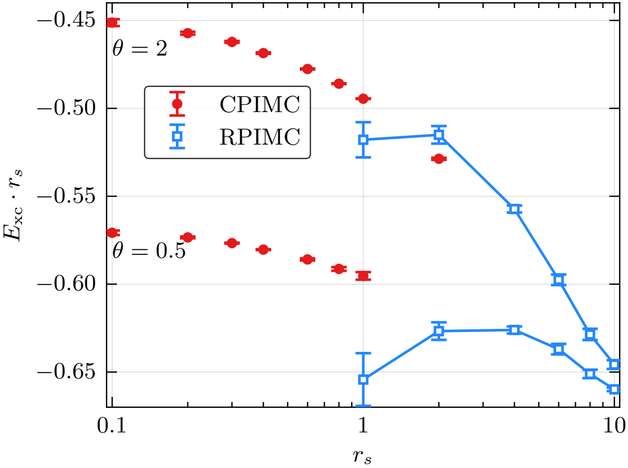

[1] S. Groth *et al.*, Phys. Rev. B **93**, 085102 (2016)
[2] T. Dornheim *et al.*, Phys. Rev. B **93**, 205134 (2016)
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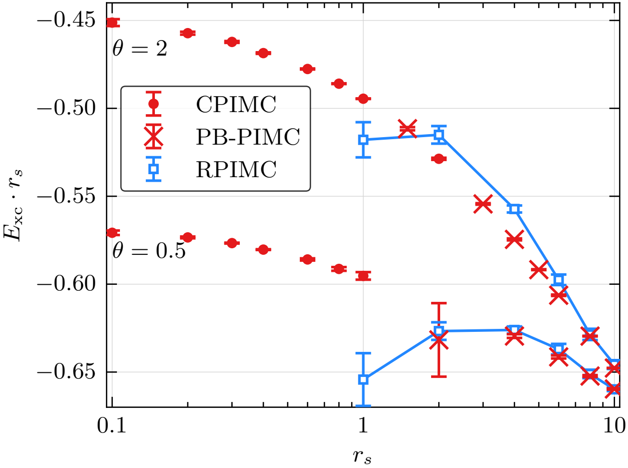

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- **RPIMC** limited to $r_s \geq 1$
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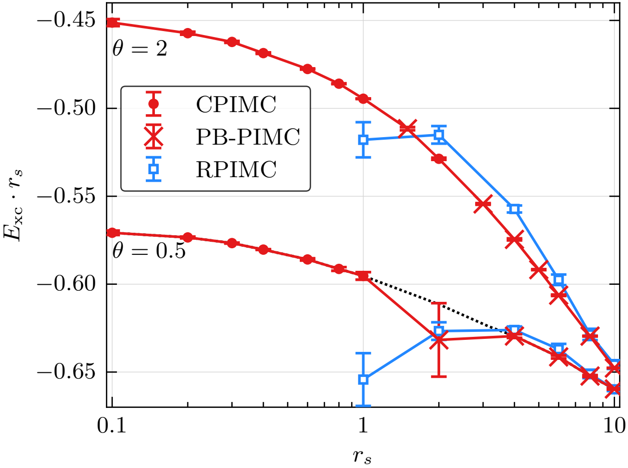
- **PB-PIMC** applicable at $\theta \gtrsim 0.5$

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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Recognition for our work...

APS John Dawson Award 2021

<u>Kiel group</u>:

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.

<u>UK and US collaborators</u>:
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[2], optics etc.: $\chi(\mathbf{q}, \omega)$, $S(\mathbf{q}, \omega)$[3], $\epsilon(\mathbf{q}, \omega)$, $\sigma(\mathbf{q}, \omega)$, plasmon dispersion[4]

PIMC: susceptibilities beyond validity limits of LRT[5]

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

---

[2] Hamann et al., Phys. Rev. B (2020)
[3] Dornheim et al., Phys. Rev. Lett. (2018)
[4] Hamann et al., Contrib. Plasma Phys. (2020)
[5] Dornheim et al., Phys. Rev. Lett. (2020)

Momentum distribution of correlated electrons in WDM[6]

- **Key questions**
  1. Is the large momentum asymptotic of $n(p)$ indeed of order p^{-8}?
  2. How does the asymptotic depend on density and momentum?
  3. How do correlations and quantum effects influence the low-momentum states?

- **Earlier works**
  - non-exponential decay, $\sim p^{-8}$, predicted by Daniel, Vosko (1960); Galitskii, Migdal (1967) and others
  - Many ground state results: analytical and QMC: Gori-Giorgi *et al.*, Calmels, Overhauser, Spink *et al.*
  - Observed also in cold atoms, but there asymptotic $\sim p^{-4}$, e.g. Doggen, Kinnunen, (2015)
  - importance for dense plasmas discussed e.g. by Starostin, Fisch and others
  - recent QMC simulations: Militzer, V. Filinov *et al.*

[6] K. Hunger *et al.*, Phys. Rev. E **103**, 053204 (2021)

Momentum distribution of correlated electrons in WDM[7]

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  - importance for dense plasmas discussed e.g. by Starostin, Fisch and others
  - recent QMC simulations: Militzer, V. Filinov *et al.*
  - Asymptotic given by on-top pair distribution, for all temperatures, via

$$\lim_{p\to\infty} n(p) = \frac{4}{9}\left(\frac{4}{9\pi}\right)^{2/3}\left(\frac{r_s}{\pi}\right)^2 \frac{p_F^8}{p^8} g^{\uparrow\downarrow}(0)\,,$$

  Kimball (1975); Yasuhara, Kawazoe (1976)

- **Tasks**
  - Develop CPIMC and fermionic PIMC simulations for $n(p)$ and $g^{\uparrow\downarrow}(0)$
  - Compute $n(p)$ and $g^{\uparrow\downarrow}(0)$ for WDM parameters, explore density and temperature dependence
  - Generate accurate benchmark data for $n(p)$ for all momenta. Input for models, reaction rates etc.

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[7] K. Hunger *et al.*, Phys. Rev. E **103**, 053204 (2021)

CPIMC approach to the momentum distribution and the on-top PDF[9]

CPIMC is QMC in Fock space (second quantization)[8]
Exact description of quantum electrons at $r_s \lesssim 1$

$$\hat{H} = \sum_{ij} h_{ij} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{ijkl} w_{ijkl}\, \hat{a}_i^\dagger a_j^\dagger \hat{a}_l \hat{a}_k \,, \qquad \hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}} \,,$$

Uniform electron gas: Use plane wave basis.
Generate paths C in Fock space with weight $W(C)$

Estimators for single-particle and two-particle density matrix:

$$n_i = \langle a_i^\dagger a_i \rangle = -\frac{1}{\beta} \frac{\partial}{\partial h_{ii}} \ln Z = \frac{1}{Z} \sum_C \left(\sum_{\nu=0}^{K} n_i^{(\nu)} \frac{\tau_{i+1} - \tau_i}{\beta} \right) W(C)$$

$$d_{ijkl} = \langle a_i^\dagger a_j^\dagger a_k a_l \rangle = -\frac{1}{\beta} \frac{\partial}{\partial w_{ijkl}} \ln Z,$$

$$g^{\uparrow\downarrow}(0, C) = \frac{1}{2N_{\sigma_1}(C) N_{\sigma_2}(C)} \sum_{ijkl} \delta_{s_i, s_l} \delta_{s_j, s_k} (1 - \delta_{s_i, s_j}) d_{ijkl}(C)$$

Illustration for 3 particles

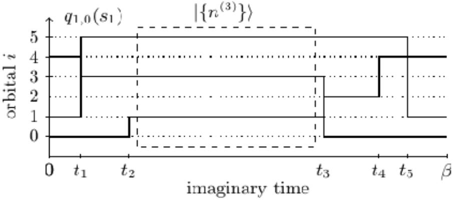


Figure: Continuous time representation of the path integral, for $N = 3$. Paths C are classified by the number K of kinks, their times and involved orbitals.
Ideal Fermi gas: one Slater determinant, corresponds to straight lines (no kinks).
Correlations: mix of Slater determinants, leads to increase or K.

[8] Schoof, Bonitz *et al.*, Contrib. Plasma Phys. (2011)
[9] K. Hunger *et al.*, Phys. Rev. E **103**, 053204 (2021)

Results for the momentum distribution – Overview[10]

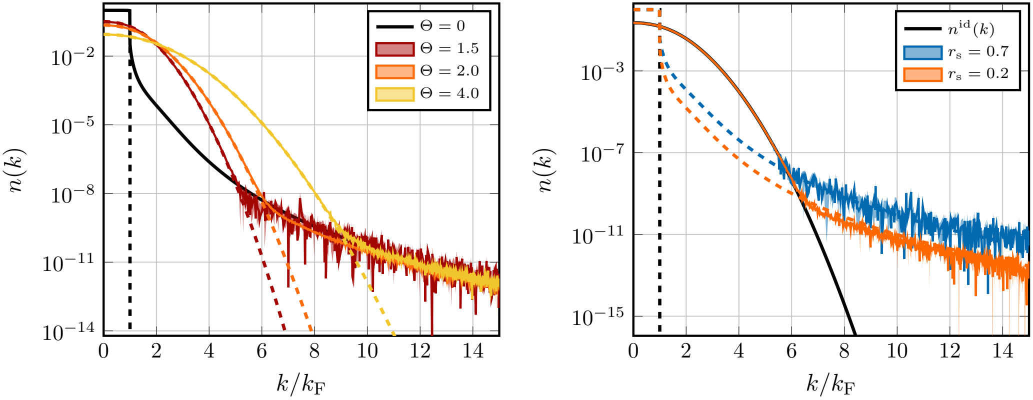
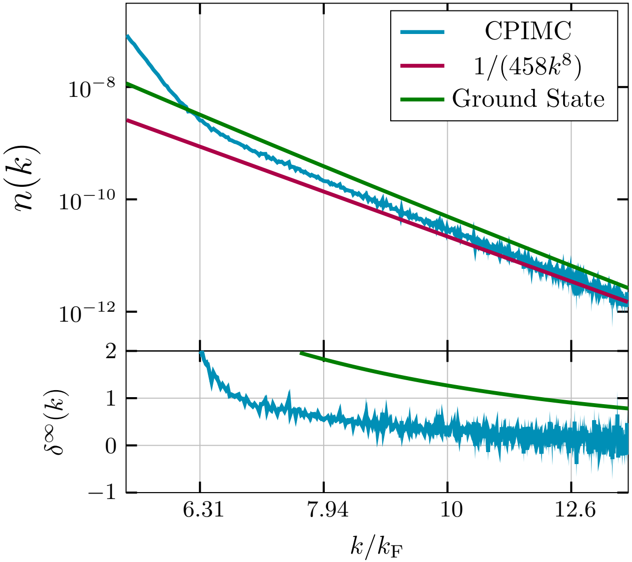


Figure: **Left**: Temperature dependence at $r_s = \bar{r}/a_B = 0.5$. Full lines: CPIMC, dashed: Fermi function n^id.
Right: Density dependence at $\Theta = k_B T/E_F = 2.0$ Full lines: CPIMC, dashed: ground state, black: n^id.

[10] K. Hunger *et al.*, Phys. Rev. E **103**, 053204 (2021)
ground state results: Gori-Giorgi *et al.* (2001)

Results for the momentum distribution – large-k asymptotic[11]



Tail of $n(k)$,

$r_s = 0.5$ and $\Theta = 2$

pink: asymptotic $n^\infty(k)$, using CPIMC result for $g^{\uparrow\downarrow}(0)$

δ^∞ : relative deviation from asymptotic

$$\delta^\infty(k) = \frac{n(k)}{n^\infty(k)} - 1.$$

Ordering of curves determined by $g^{\uparrow\downarrow}(0; \Theta)$

[11] K. Hunger *et al.*, Phys. Rev. E **103**, 053204 (2021), ground state results: Gori-Giorgi *et al.* (2001)

Results for the momentum distribution – low-k states[12]

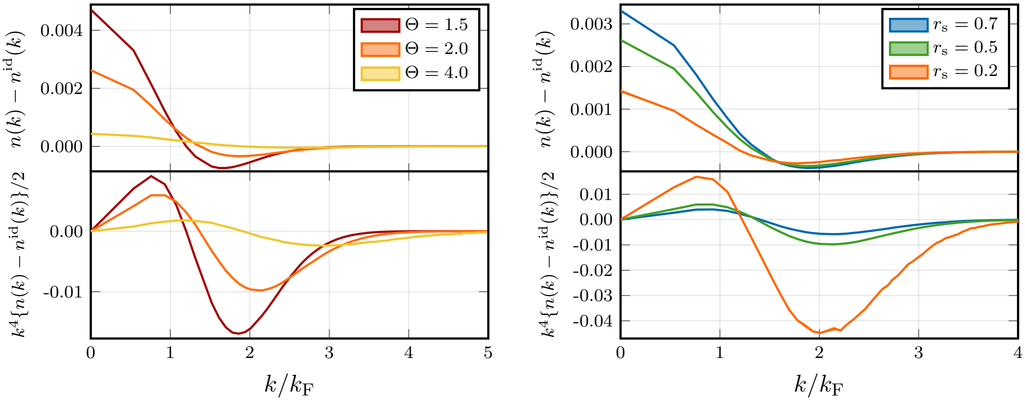
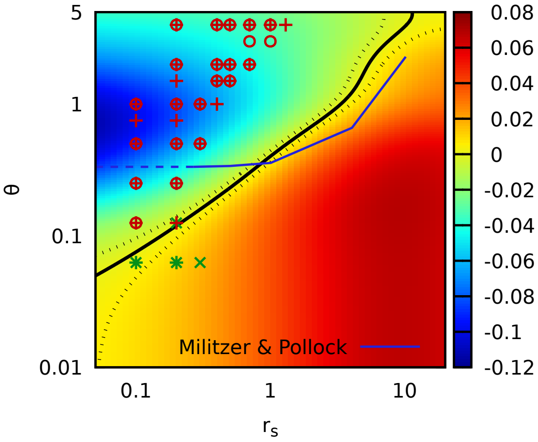


Figure: **Top**: Difference correlated (CPIMC) minus ideal distribution,
Bottom: Difference of kinetic energy densities. Total kinetic energy: area under curve
Left: Temperature dependence at $r_s = 0.5$. **Right**: Density dependence at $\Theta = 2$.

Explanation: negative energy shift of low-momentum states: $E(k) = \frac{k^2}{2m} + \Sigma_F(k) + \ldots$

[12]K. Hunger *et al.*, Phys. Rev. E **103**, 053204 (2021)

Interaction-induced lowering of the kinetic energy[13]



Exchange-correlation contribution to kinetic energy, $K_{\rm xc}$,

Black line: $K_{\rm xc} = 0$,

symbols: CPIMC data points

blue line: Militzer *et al.* (2002)

heat map (and pluses):

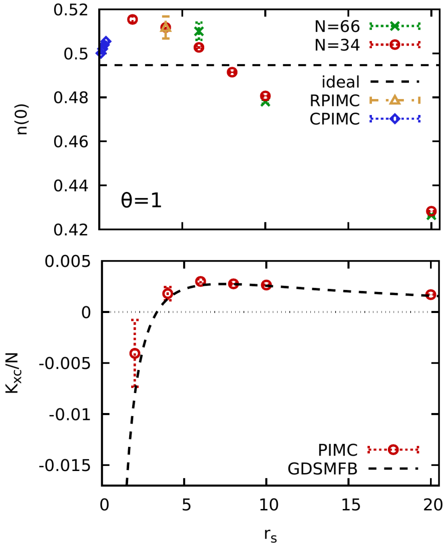
$$K_{xc} = -f_{xc} - \theta \frac{\partial f_{xc}}{\partial \theta}\Big|_{r_s} - r_s \frac{\partial f_{xc}}{\partial r_s}\Big|_{\theta}$$

with f_{xc}: GDSMFB parametrization

red circles: $n(0) > n^{\rm id}(0)$
green crosses: $n(0) < n^{\rm id}(0)$

[13] predicted by Militzer *et al.* (2002), and Kraeft *et al.* (2002),
present results from: K. Hunger *et al.*, Phys. Rev. E **103**, 053204 (2021)

Interaction-induced lowering of the kinetic energy (contd.)[14]



Top: Occupation of lowest momentum orbital

red, green symbols: PIMC data
blue symbols: CPIMC data points

Bottom: Exchange-correlation contribution to kinetic energy, K_{xc},

CPIMC data: minimum at $r_s \approx 0.4$[a]

[a] K. Hunger *et al.*, Phys. Rev. E **103**, 053204 (2021)

[14] predicted by Militzer *et al.* (2002), and Kraeft *et al.* (2002), from: T. Dornheim *et al.*, Phys. Rev. B **103**, 205142 (2021)

On-top pair distribution function $g^{\uparrow\downarrow}(0)$

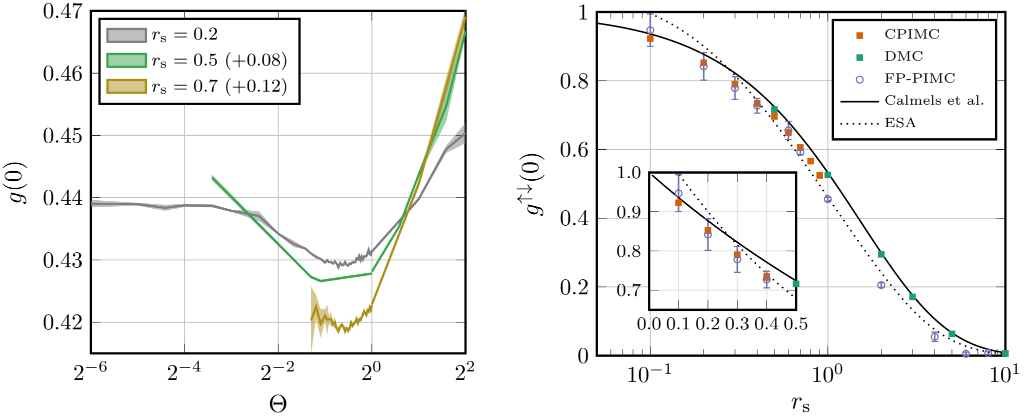
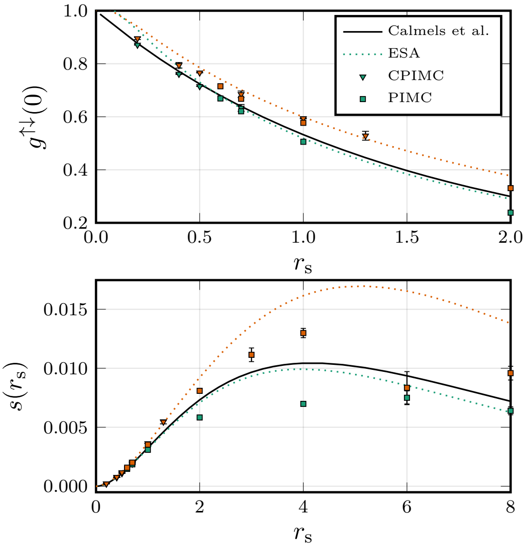


Figure: **Left**: Temperature dependence for three densities (CPIMC data where available, curves shifted vertically).
Right: Density dependence at $\Theta = 1$. Red: CPIMC, blue circles: fermionic propagator PIMC (A. Filinov), green and black line: ground state data of Spink *et al.* (2013) and Calmels *et al.* (1998)
ESA: “effective static approximation” by Dornheim *et al.* (2020)

Minimum due to competition between exchange and Coulomb correlations.

Particle number in the tail: temperature and density dependence



large-momentum asymptotic:

$$n(k) \to s(r_s, \Theta) \cdot \left(\frac{k_F}{k}\right)^{-8}$$

$$\sim r_s^2 \cdot g^{\uparrow\downarrow}(0, r_s, \Theta) \left(\frac{k_F}{k}\right)^{-8},$$

s depends non-monotonically on Θ and r_s

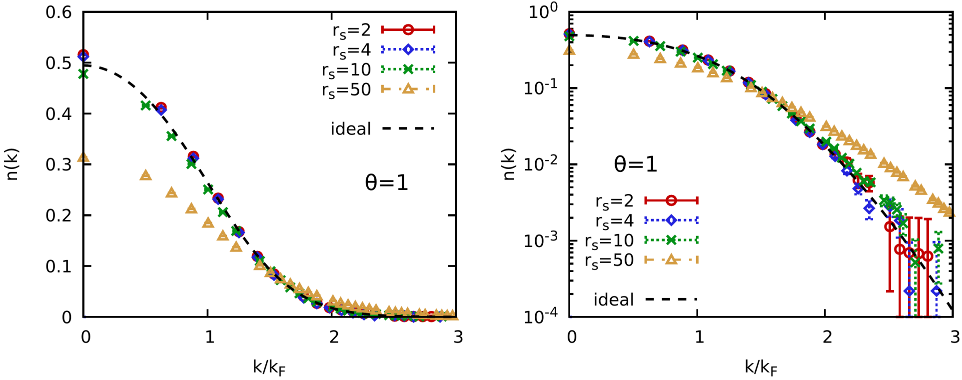
black line: $T = 0$
green symbols: $\Theta = 2$
orange symbols: $\Theta = 4$

minimum around $\Theta \sim 0.65$
maximum around $4 \lesssim r_s \lesssim 5$

Momentum distribution for jellium at strong coupling. . . electron liquid[15]

- Fermionic PIMC simulations in grand canonical ensemble
- Extension of $n(k)$ results to $2 \leq r_s \leq 50$ and $\Theta \geq 0.75$
- Good agreement with RPIMC data of Militzer, Pollock, and Ceperley (HEDP 2019)
- Data limited to moderate k-values

linear vs. log scale



[15] Dornheim *et al.*, Phys. Rev. B **103**, (2021)

Extension to hydrogen plasma

Single-bound electron problem, $T = 0$

ground state wave function: $\psi_{100}(r) = \frac{1}{\sqrt{\pi a_B^3}} e^{-r/a_B}$,   probability density: $g_{100}(r) = r^2 \frac{e^{-2r/a_B}}{\pi a_B^3}$

momentum probability density, p_r: radial momentum:[16]

$$|\langle \mathbf{p}|100\rangle|^2 = \tilde{\rho}_{100}(p_r) = \frac{8}{\pi^2} \frac{p_{\mathrm{Ryd}}^{-3}}{\left(1 + \frac{p_r^2}{p_{\mathrm{Ryd}}^2}\right)^4} , \quad E_{\mathrm{Ryd}} = \frac{m_r}{2} p_{\mathrm{Ryd}}^2 .$$

normalization: $1 = 4\pi \int_0^\infty dp_r p_r^2 \, \tilde{\rho}_{100}(p_r)$,   maximum of $p_r^2 \tilde{\rho}(p_r)$: $p_r^0 = p_{\mathrm{Ryd}}/\sqrt{3}$

asymptotic: $$\lim_{p_r \to \infty} \tilde{\rho}(p_r) \sim \frac{8}{\pi^2 p_{\mathrm{Ryd}}^3} \left(\frac{p_{\mathrm{Ryd}}}{p_r}\right)^8$$

[16] Podolski, Pauling, Phys. Rev. (1929)

Momentum distribution: hydrogen plasma versus jellium, $r_s = 6$

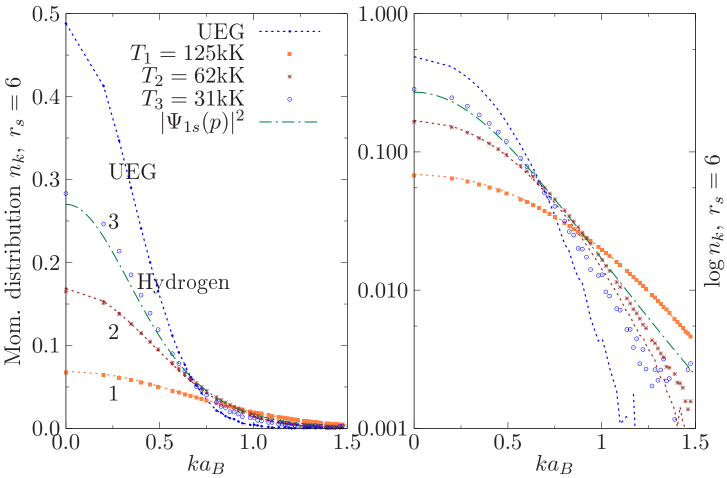


Figure: Grand canonical Fermionic propagator PIMC, A. Filinov

Pair distribution: hydrogen plasma, $r_s = 6$

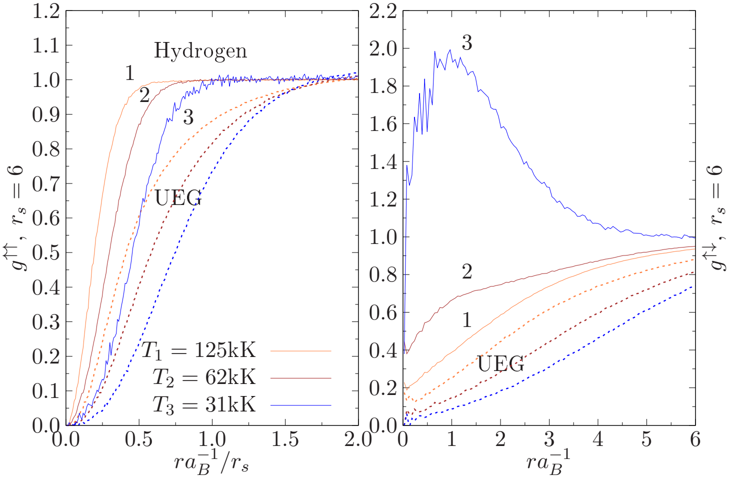


Figure: Grand canonical Fermionic propagator PIMC, A. Filinov

Electron-ion pair distribution: hydrogen plasma, $r_s = 6$

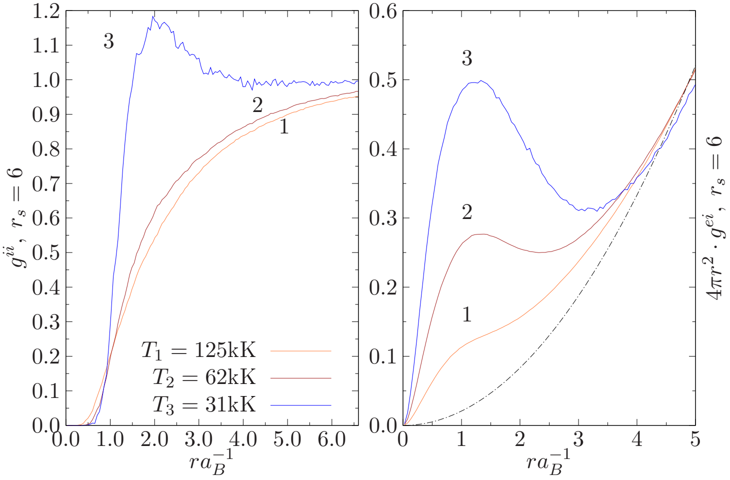
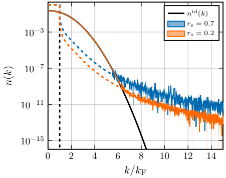
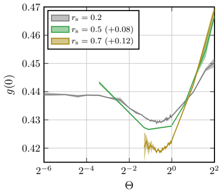


Figure: Grand canonical Fermionic propagator PIMC, A. Filinov

Summary and outlook

- **momentum distribution of quantum electrons in WDM**:
  - tail crucial for rates of threshold processes (e.g. fusion)
  - CPIMC: unprecedented accuracy. Benchmarks, input in analytical models
- **First *ab initio* results**[a] for $n(k)$ and $g^{\uparrow\downarrow}$:
  - based on combination of CPIMC and direct fermionic PIMC, thereby avoiding the fermion sign problem, extending previous thermodynamic results[b]
  - p^{-8}-asymptotic quantified via on-top PDF
  - accurate FPIMC results for hydrogen
- **Outlook**:
  - *ab initio* spectral function, energy dispersion $n(k) = \int d\omega\, a(k,\omega)\, f^{\mathrm{EQ}}(\omega)$
  - further improvement of CPIMC, extension to two-component plasmas





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[a] K. Hunger *et al.*, Phys. Rev. E **103**, 053204 (2021)
[b] T. Dornheim *et al.*, Phys. Reports (2018)