Momentum distribution function and short-range correlations of the warm dense electron gas – ab initio quantum Monte Carlo results

Michael Bonitz, Kai Hunger, Tim Schoof[1], Tobias Dornheim[†], Alexey Filinov

in collaboration with Paul Hamann, Zhandos Moldabekov[**†], Jan Vorberger[*], Pavel Levashov[4]

Institute of Theoretical Physics and Astrophysics, Kiel University
[1] DESY Hamburg
[†] Center for Advanced Systems Understanding, [*] Helmholtz-Zentrum Dresden
[**] Al Farabi University, Almaty, Kazakhstan
[4] IVTAN, Moscow

Hirschegg 2021

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

  $\Rightarrow$ exponential decay for large momenta

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

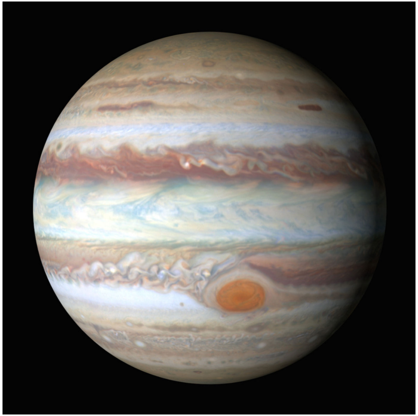
  $\Rightarrow$ exponential decay for large momenta

- **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 (submitted), arXiv:2101.00842

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

Warm Dense Matter: Occurences and Applications

- **Astrophysics:**
  - Giant planet interiors (e.g. Jupiter)
  - Brown dwarfs
  - Meteor Impacts

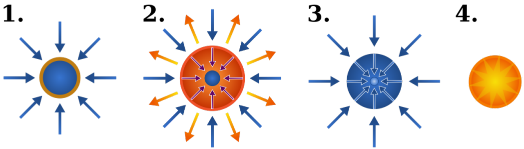


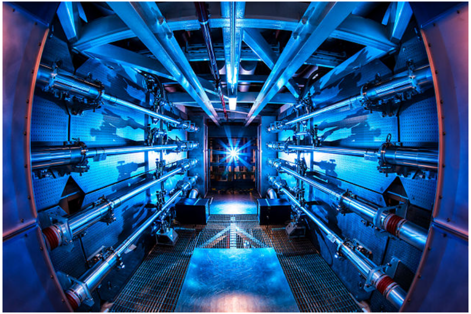
Source: Sci-News.com [Img4]

Warm Dense Matter: Occurences and Applications

- **Astrophysics:**
  - Giant planet interiors (e.g. Jupiter)
  - Brown dwarfs
  - Meteor Impacts
- **Experiments:**
  - Inertial confinement fusion

    Potential abundance of clean energy!





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

Warm Dense Matter: Occurences and Applications

- **Astrophysics:**
  - Giant planet interiors (e.g. Jupiter)
  - Brown dwarfs
  - Meteor Impacts
- **Experiments:**
  - Inertial confinement fusion

    Potential abundance of clean energy!

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

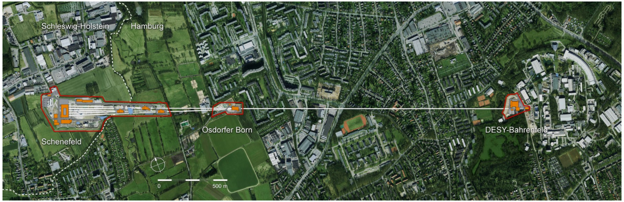
National Ignition Facility (Livermore, California)

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:

European XFEL:

- **E**uropean **X**-ray **F**ree-**E**lectron **L**aser, Hamburg – Schenefeld
- HIBEF Beamline and consortium

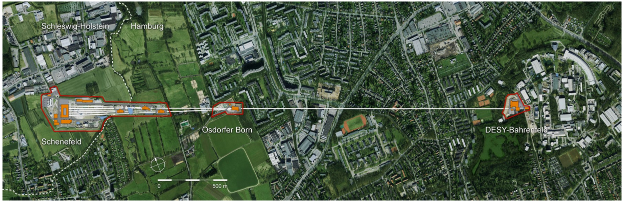


source: photon-science.desy.de

Facilities for WDM experiments in Europe:

European XFEL:

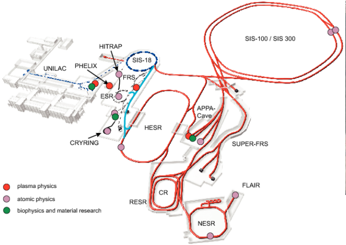
- **E**uropean **X**-ray **F**ree-**E**lectron **L**aser, Hamburg – Schenefeld
- HIBEF Beamline and consortium



source: photon-science.desy.de

FAIR:

- **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

Facilities for WDM experiments in Europe:

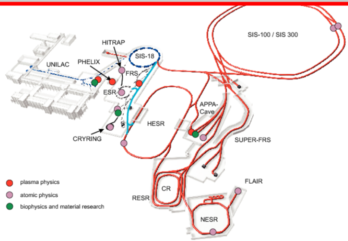
European XFEL:

- **E**uropean **X**-ray **F**ree-**E**lectron **L**aser, Hamburg – Schenefeld
- HIBEF Beamline and consortium

Warm dense matter: indeed a HOT topic

FAIR

- **F**acility
  Research, Darmstadt
- Construction started in 2017
- Heavy ion beams:
  Isochoric heating up to $\sim 10^6 K$



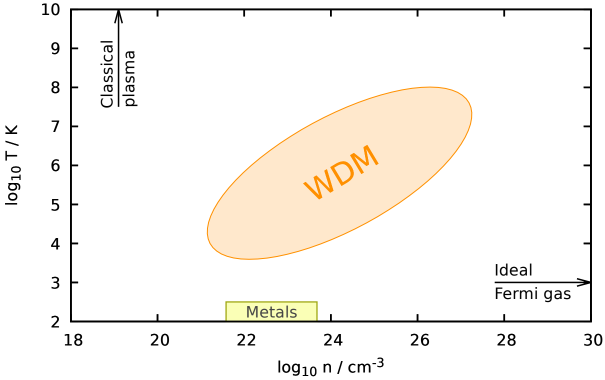
source: inspirehep.net

source: dw.com

Warm Dense Matter and quantum plasmas: relevant parameters

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

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

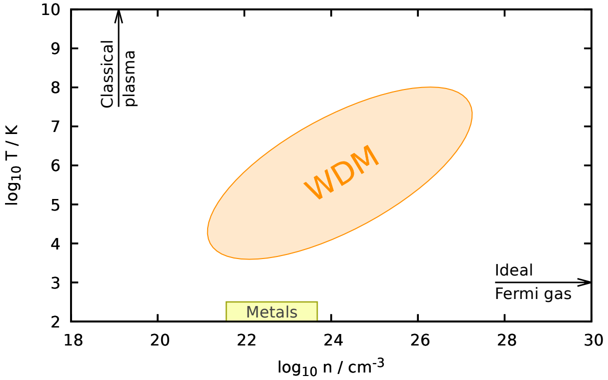


Warm Dense Matter and quantum plasmas: relevant parameters

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

- **Characteristic parameters:**

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

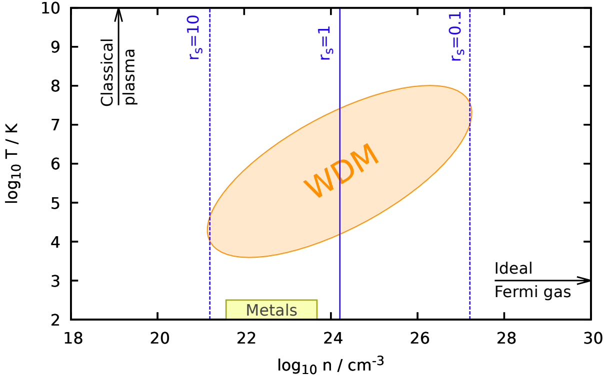


Warm Dense Matter and quantum plasmas: relevant parameters

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

- **Characteristic parameters:**
  - Density (coupling) parameter $r_s = \bar{r}/a_{\mathrm{B}} \sim 1$

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

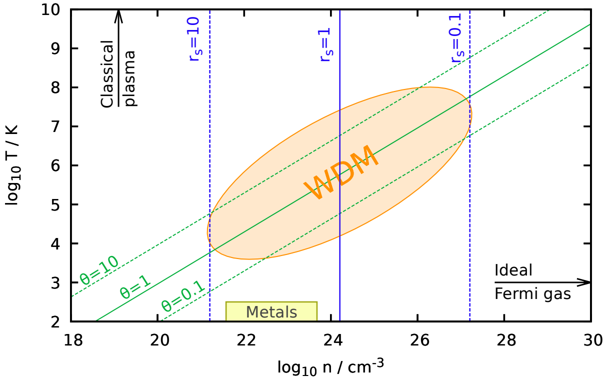


Warm Dense Matter and quantum plasmas: relevant parameters

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

- **Characteristic parameters:**
  - Density (coupling) parameter $r_s = \bar{r}/a_B \sim 1$
  - Degeneracy temperature $\theta = k_B T/E_F \sim 1$

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

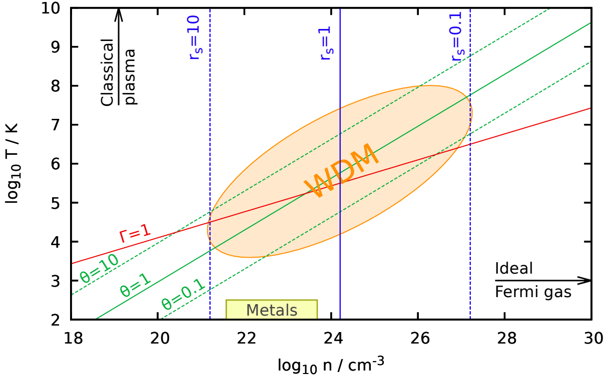


Warm Dense Matter and quantum plasmas: relevant parameters

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

- **Characteristic parameters:**
  - Density (coupling) parameter $r_s = \bar{r}/a_\mathrm{B} \sim 1$
  - Degeneracy temperature $\theta = k_\mathrm{B}T/E_\mathrm{F} \sim 1$
  - $\Theta > 1$: quantum plasma,
    $\Theta < 1$: classical plasma
    Classical coupling parameter $\Gamma = e^2/r_s k_\mathrm{B} T \sim 1$

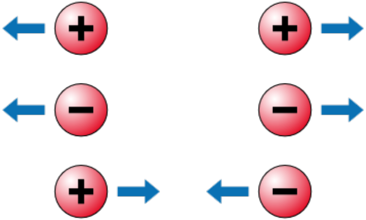
Source: T. Dornheim, S. Groth, and M. Bonitz, *Phys. Reports* **744**, 1-86 (2018)



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: $n \sim 10^{21} - 10^{27}\ cm^{-3}$

- **Characteristic parameters:**
  - Density (coupling) parameter $r_s = \bar{r}/a_\text{B} \sim 1$
  - Degeneracy temperature $\theta = k_\text{B}T/E_\text{F} \sim 1$
  - $\Theta > 1$: quantum plasma,
    $\Theta < 1$: classical plasma
    Classical coupling parameter $\Gamma = e^2/r_s k_\text{B} T \sim 1$



Source: bin-br.at [Img1]

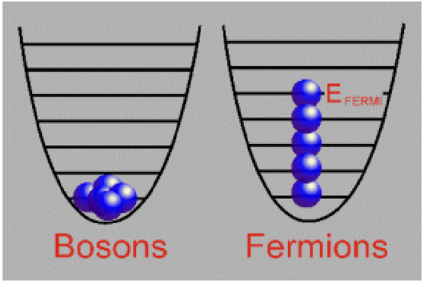
- **Nontrivial interplay of many effects:**
  - Coulomb coupling (non-ideality)

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: $n \sim 10^{21} - 10^{27}\ cm^{-3}$

- **Characteristic parameters:**
  - Density (coupling) parameter $r_s = \bar{r}/a_{\mathrm{B}} \sim 1$
  - Degeneracy temperature $\theta = k_{\mathrm{B}}T/E_{\mathrm{F}} \sim 1$
  - $\Theta > 1$: quantum plasma,
    $\Theta < 1$: classical plasma
    Classical coupling parameter $\Gamma = e^2/r_s k_{\mathrm{B}} T \sim 1$

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



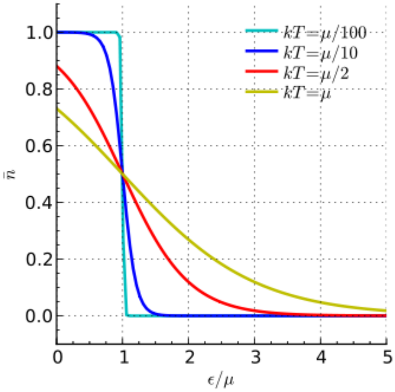
Source: cidehom.com [Img2]

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: $n \sim 10^{21} - 10^{27}\ cm^{-3}$

- **Characteristic parameters:**
  - Density (coupling) parameter $r_s = \bar{r}/a_\mathrm{B} \sim 1$
  - Degeneracy temperature $\theta = k_\mathrm{B}T/E_\mathrm{F} \sim 1$
  - $\Theta > 1$: quantum plasma,
    $\Theta < 1$: classical plasma
    Classical coupling parameter $\Gamma = e^2/r_s k_\mathrm{B} T \sim 1$

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

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

$\rightarrow$ 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

---

[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)
[4] A.Y. Potekhin and G. Chabrier, *A&A **550**, A43* (2013)

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**:

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

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

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

---

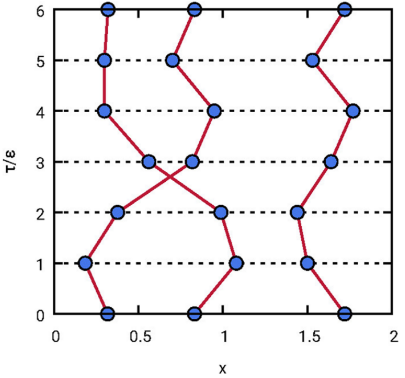
[1] J.P. Perdew and A. Zunger, PRB **23**, 5048 (1981) [2] D.M. Ceperley and B. Alder, PRL **45**, 566 (1980) [3] N.D. Mermin, Phys. Rev **137**, A1441 (1965)
[4] A.Y. Potekhin and G. Chabrier, *A&A* ***550****, A43* (2013)

Path Integral Monte Carlo (PIMC): Fermions

- **Fermionic antisymmetry:**

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

$\Rightarrow$ 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)

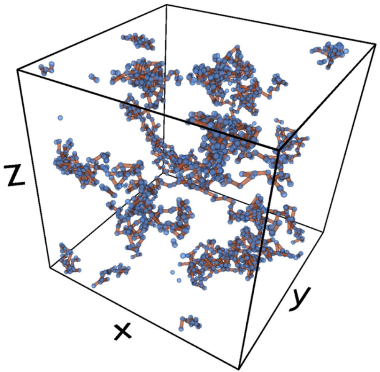
Path Integral Monte Carlo (PIMC): Fermions

- **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**!

- Randomly generate all possible paths **X** using the **Metropolis algorithm**



Snapshot of PIMC simulation of UEG with $N = 19$, $r_s = 2$, $\theta = 0.5$

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

Path Integral Monte Carlo (PIMC): Fermions

- **Fermionic antisymmetry:**

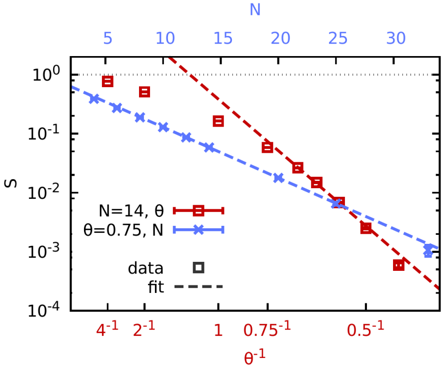
$$Z = \frac{1}{N!} \sum_{\sigma \in S_N} \text{sgn}(\sigma) \int d\mathbf{R} \ \langle \mathbf{R} | \, e^{-\beta \hat{H}} \, | \hat{\pi}_\sigma \mathbf{R} \rangle$$

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

- Randomly generate all possible paths **X** using the **Metropolis algorithm**

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

  $\Rightarrow$ **Fermion Sign Problem**



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): Fermions

- **Fermionic antisymmetry:**

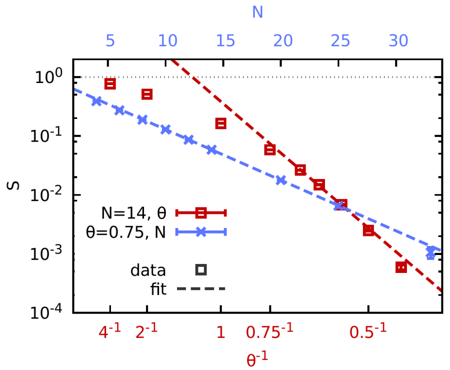
$$Z = \frac{1}{N!} \sum_{\sigma \in S_N} \mathrm{sgn}(\sigma) \int \mathrm{d}\mathbf{R}\ \langle \mathbf{R} | e^{-\beta \hat{H}} | \hat{\pi}_\sigma \mathbf{R} \rangle$$

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

- Randomly generate all possible paths **X** using the **Metropolis algorithm**

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

$\Rightarrow$ **Fermion Sign Problem**



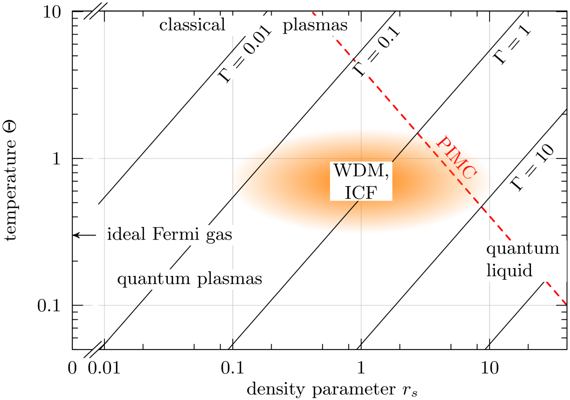
Exponential decrease of the average sign S with system size N and quantum degeneracy θ^{-1}

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

PIMC simulations of WDM very challenging!

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

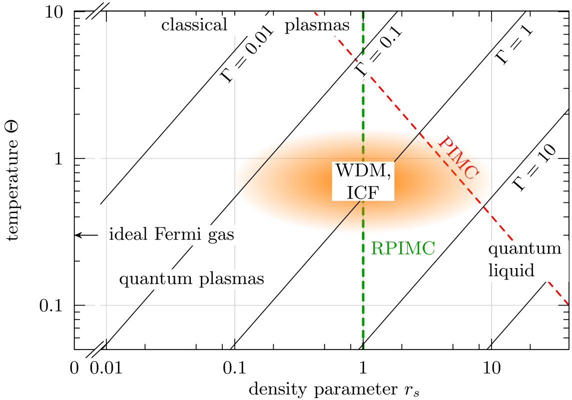
- Standard PIMC in warm dense regime severely hampered by ***fermion sign problem***:



[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 $r_s \gtrsim 1$



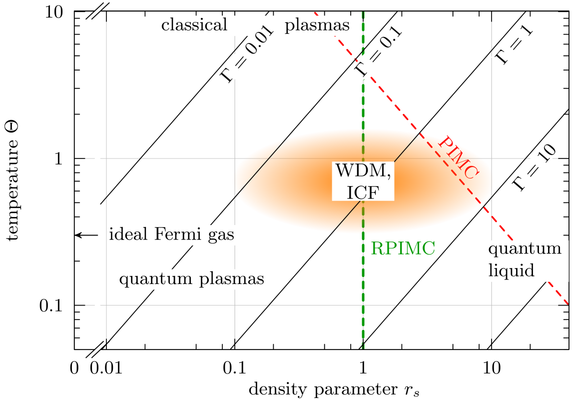
[1] E.W. Brown *et al.*, PRL **110**, 146405 (2013)
[2] V. Filinov *et al.*, Phys. Rev. E **91**, 033108 (2015)
[3] T. Schoof *et al.*, Phys. Rev. Lett **115**, 130402 (2015)
[5] T. Dornheim *et al.*, New J. Phys. **17**, 073017 (2015)
[4] T. Schoof *et al.*, Contrib. Plasma Phys. **51**, 687 (2011)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

Our approach:

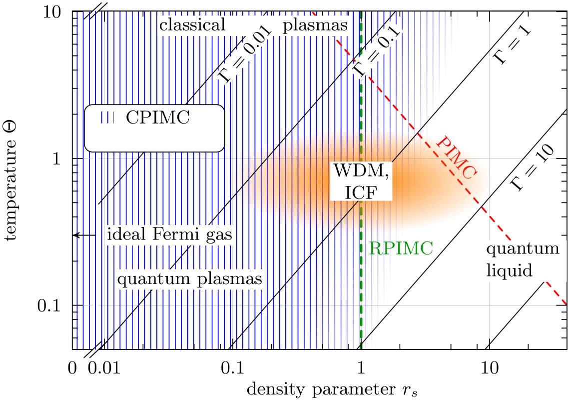
Avoid fermion sign problem by combining two exact and complementary QMC methods:



[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)
[5] T. Dornheim *et al.*, New J. Phys. **17**, 073017 (2015)
[4] T. Schoof *et al.*, Contrib. Plasma Phys. **51**, 687 (2011)
[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 $r_s \gtrsim 1$



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

[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 $r_s \gtrsim 1$

Our approach:

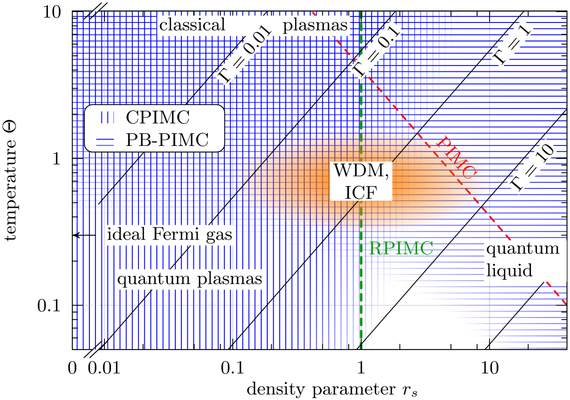
Avoid fermion sign problem by combining two exact and complementary QMC methods:

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



---

[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 $r_s \gtrsim 1$

Our approach:

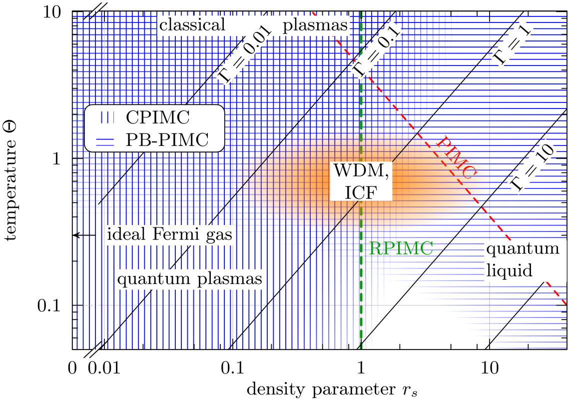
Avoid fermion sign problem by combining two exact and complementary QMC methods:

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

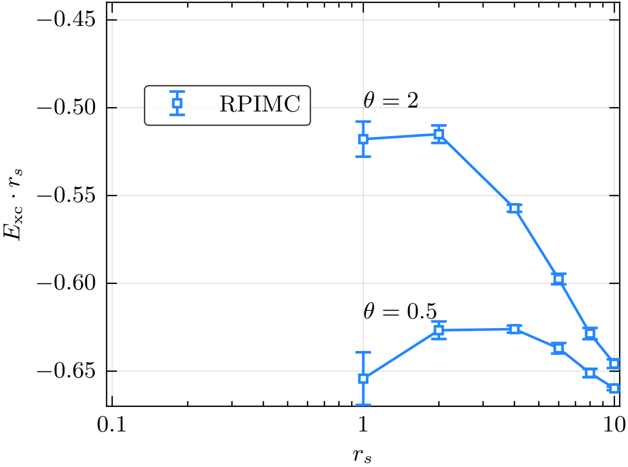


***Ab initio* simulations over broad range of parameters possible**

[1] E.W. Brown *et al.*, PRL **110**, 146405 (2013)
[2] V. Filinov *et al.*, Phys. Rev. E **91**, 033108 (2015)
[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)

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

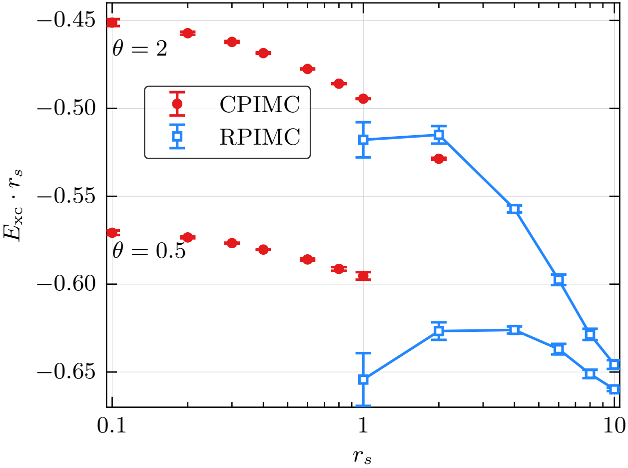
- **RPIMC** limited to $r_s \geq 1$



[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)

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

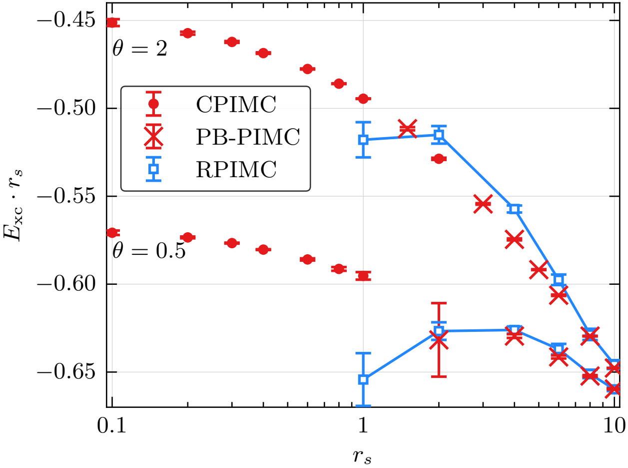
- **RPIMC** limited to $r_s \geq 1$
- **CPIMC** excels at high density



[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)

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 $r_s \geq 1$
- **CPIMC** excels at high density
- **PB-PIMC** applicable at $\theta \gtrsim 0.5$



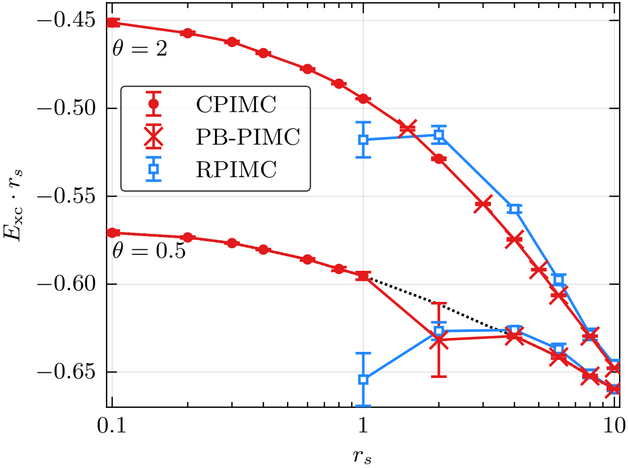
[1] S. Groth *et al.*, Phys. Rev. B **93**, 085102 (2016)
[2] T. Dornheim *et al.*, Phys. Rev. B **93**, 205134 (2016)
[3] F.D. Malone *et al.*, Phys. Rev. Lett. **117**, 115701 (2016)
[4] T. Dornheim *et al.*, Phys. Rev. Lett. (2016)
[5] S. Groth *et al.*, Phys. Rev. Lett. (2017)

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 $r_s \geq 1$
- **CPIMC** excels at high density
- **PB-PIMC** applicable at $\theta \gtrsim 0.5$

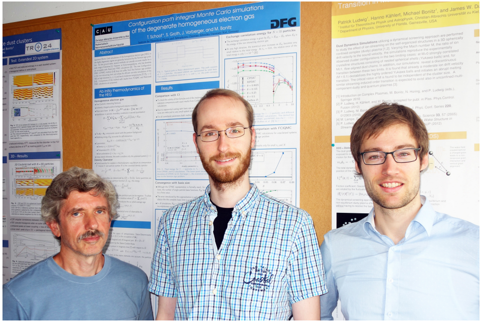
Combination[1] yields exact results over entire density range down to $\theta \sim 0.5$

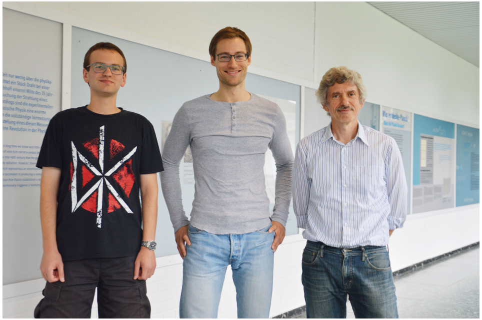
- Also applies to the **unpolarized** UEG[2]
- confirmed by independent **DMQMC** simulations[3]
- Extended to TD Limit[4] and to the ground state[5]
- Analytical parametrization of $f_{xc}(r_s, \theta, \xi)$, with error below 0.3%, Integrated in standard DFT libraries[5]



[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)

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 and Helmholtz-Zentrum Dresden
Extension to static and dynamic response, transport, DFT, machine learning etc.

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

Ab Initio PIMC approach to equilibrium response and transport properties[2]

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**

[2] see talks by Paul Hamann, Tobias Dornheim, Jan Vorberger, Alexey Filinov

Momentum distribution of correlated electrons in WDM[3]

- **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.*

[3] K. Hunger *et al.*, Phys. Rev. E (submitted), arXiv:2101.00842

Momentum distribution of correlated electrons in WDM[4]

- **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.*
  - 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.

---

[4] K. Hunger *et al.*, Phys. Rev. E (submitted), arXiv:2101.00842

CPIMC approach to the momentum distribution and the on-top PDF[6]

CPIMC is QMC in Fock space (second quantization)[5]
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:

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

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

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

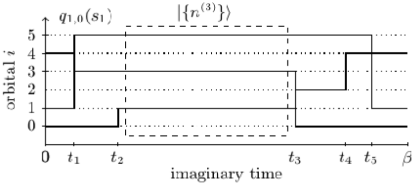


Figure: Continuous time representation of the path integral, for $N = 3$. Paths C are classified by the number K of kinks, their times and involved orbitals. Ideal Fermi gas corresponds to straight lines. Correlations lead to increase or K.

[5] Schoof, Bonitz *et al.*, Contrib. Plasma Phys. (2011)
[6] K. Hunger *et al.*, Phys. Rev. E (submitted), arXiv:2101.00842

Results for the momentum distribution – Overview[7]

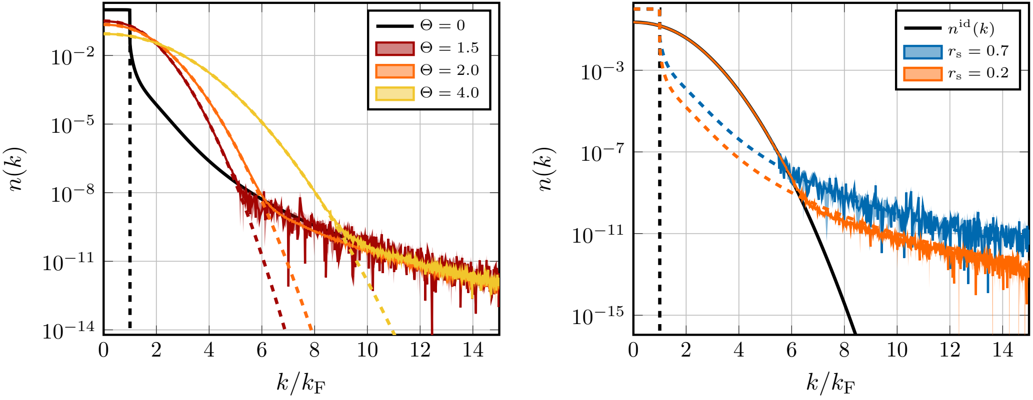
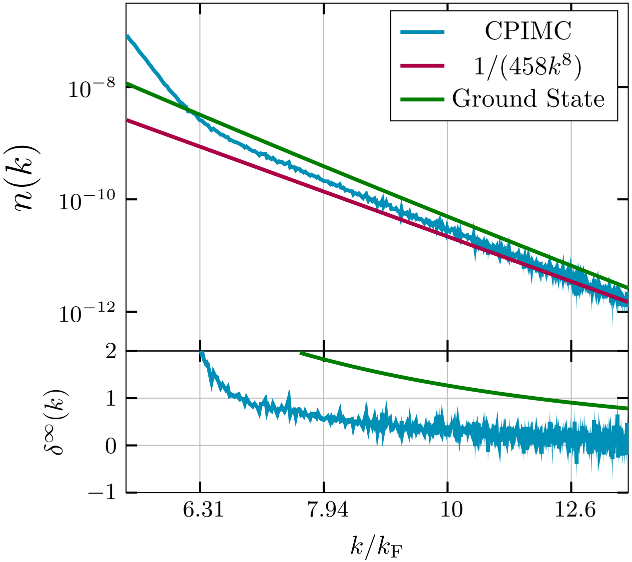


Figure: **Left**: Temperature dependence at $r_s = 0.5$. Full lines: CPIMC, dashed: Fermi function n^{id}.
Right: Density dependence at $\Theta = 2$. Full lines: CPIMC, dashed: ground state, black: n^{id}.

[7] K. Hunger *et al.*, Phys. Rev. E (submitted), arXiv:2101.00842, ground state results: Gori-Giorgi *et al.* (2001)

Results for the momentum distribution – large-k asymptotic[8]



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 $g^{\uparrow\downarrow}(0;\Theta)$

[8] K. Hunger *et al.*, Phys. Rev. E (submitted), arXiv:2101.00842, ground state results: Gori-Giorgi *et al.* (2001)

Results for the momentum distribution – low-k states[9]

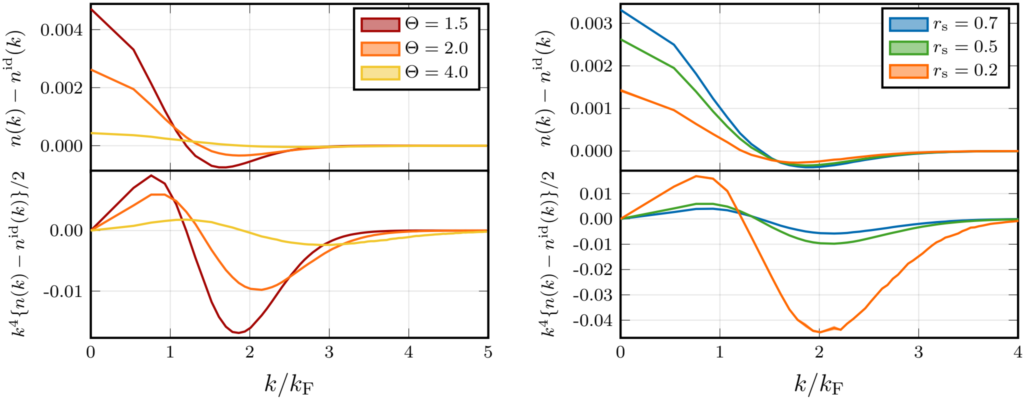
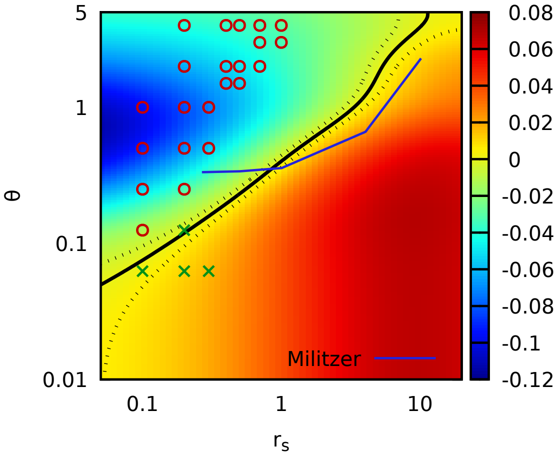


Figure: **Top**: Difference correlated (CPIMC) minus ideal distribution,
Bottom: Difference of kinetic energy densities. Total kinetic energy: area under curve
Left: Temperature dependence at $r_s = 0.5$. **Right**: Density dependence at $\Theta = 2$.

---

[9] K. Hunger *et al.*, Phys. Rev. E (submitted), arXiv:2101.00842

Interaction-induced lowering of the kinetic energy[10]



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

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

symbols: CPIMC data points

blue line: Militzer (2002)

Explanation: negative energy shift of low-momentum states:

$E(k) = \frac{k^2}{2m} + \Sigma_F(k) + \dots$

[10] predicted by Militzer *et al.* (2002), and Kraeft *et al.* (2002), present results from: K. Hunger *et al.*, Phys. Rev. E (submitted), arXiv:2101.00842

On-top pair distribution function[11] $g^{\uparrow\downarrow}(0)$

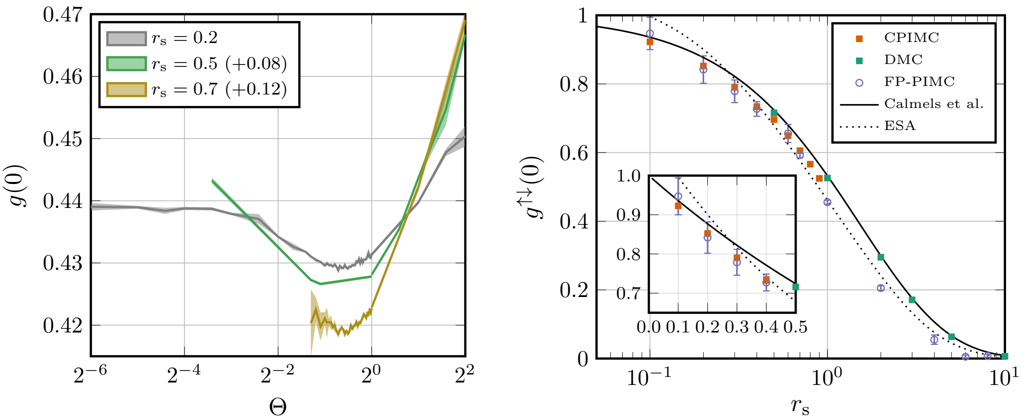
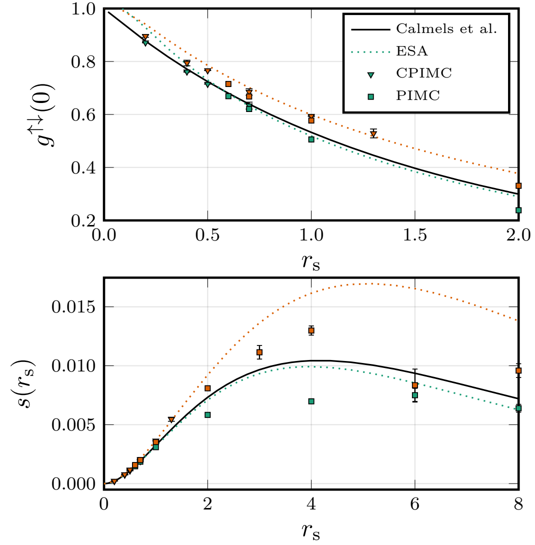


Figure: **Left**: Temperature dependence for three densities (CPIMC data where available, curves shifted vertically).
Right: Density dependence at $\Theta = 1$. Red: CPIMC, blue circles: fermionic propagator PIMC (A. Filinov), green and black line: ground state data of Spink *et al.* (2013) and Calmels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

Minimum due to competition between exchange and Coulomb correlations.

[11] K. Hunger *et al.*, Phys. Rev. E (submitted), arXiv:2101.00842

Particle number in the tail: temperature and density dependence[12]



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 $4 \lesssim r_s \lesssim 5$

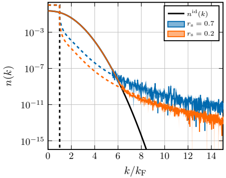
[12] K. Hunger *et al.*, Phys. Rev. E (submitted), arXiv:2101.00842

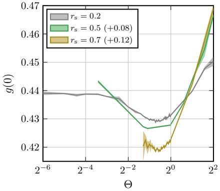
Summary and outlook

- **momentum distribution of quantum electrons in WDM**:
  - crucial for rates of threshold processes (e.g. fusion)
  - 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]
  - non-exponential asymptotic quantified via on-top PDF

- **Outlook**:
  - *ab initio* linear response functions ("exact RPA"),
  - *ab initio* spectral function, energy dispersion
    $n(k) = \int d\omega\, a(k,\omega)\, f^{\mathrm{EQ}}(\omega)$





[a] K. Hunger *et al.*, Phys. Rev. E (submitted), arXiv:2101.00842
[b] T. Dornheim *et al.*, Phys. Reports (2018)