Ab initio thermodynamic results for Warm Dense Matter

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Travis Sjostrom (Los Alamos NL)

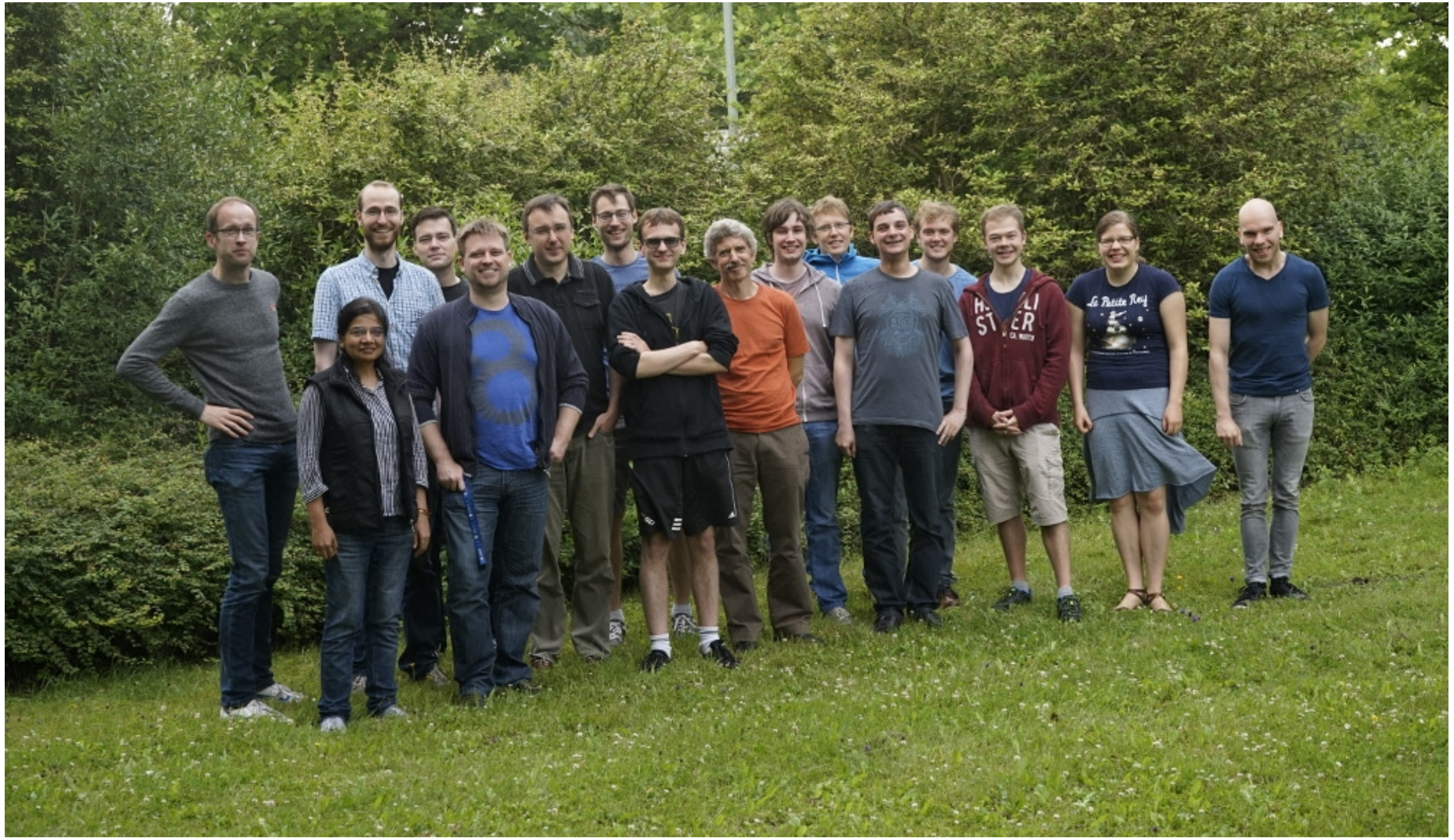
TR 24 complex plasmas

HLRN

DFG

APS-DPP meeting, San Jose, CA, Oct 31 - Nov 4 2016

Acknowledgements



Main contributions:

Tim Schoof,

Tobias Dornheim,

Simon Groth

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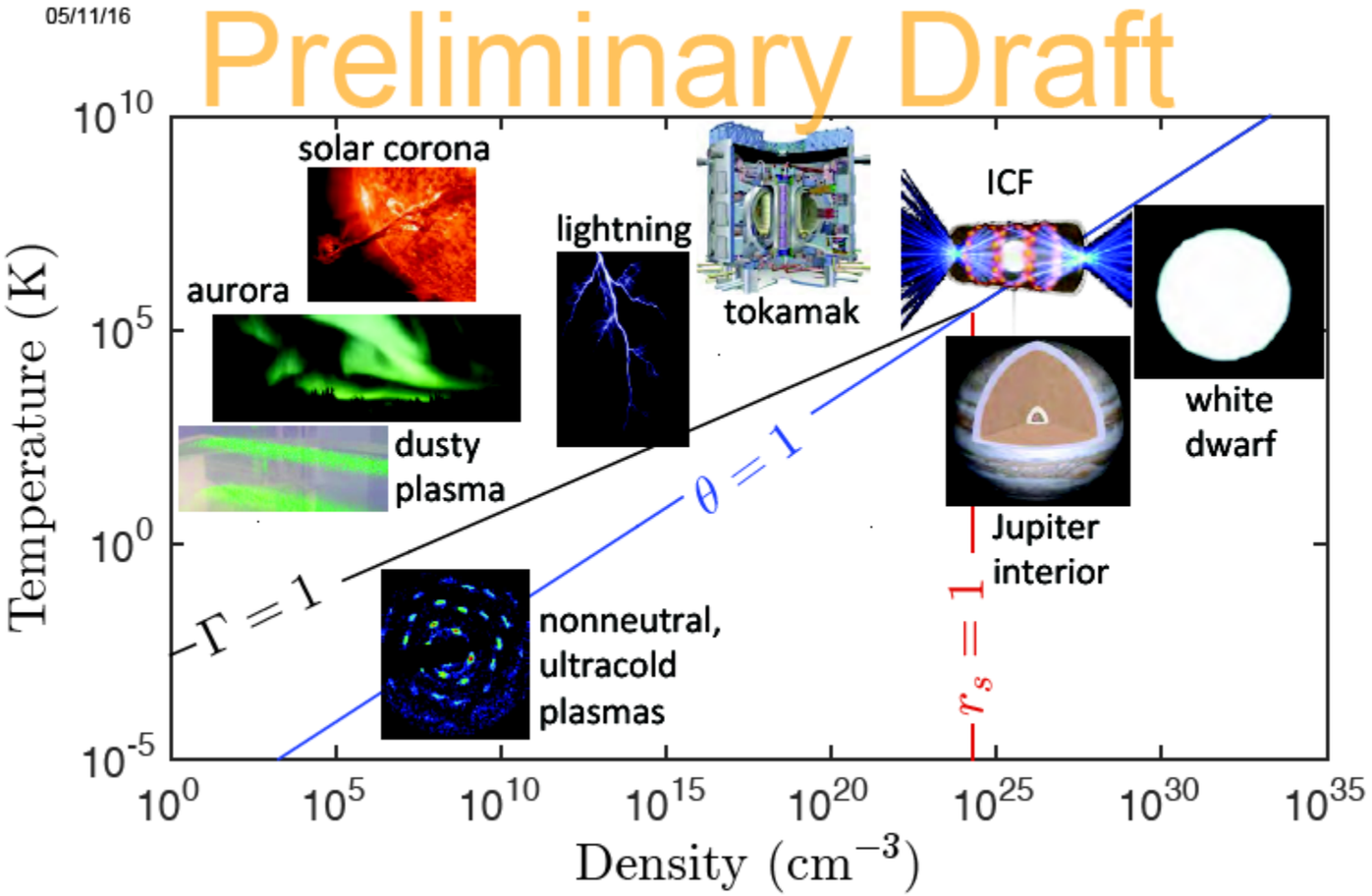
3. Path integral Monte Carlo simulations (PIMC)

4. New developments in PIMC for the electron gas (finite N)

5. Removing finite size errors in PIMC
   Achieving exact thermodynamic results (accuracy of ~ 0.1%)

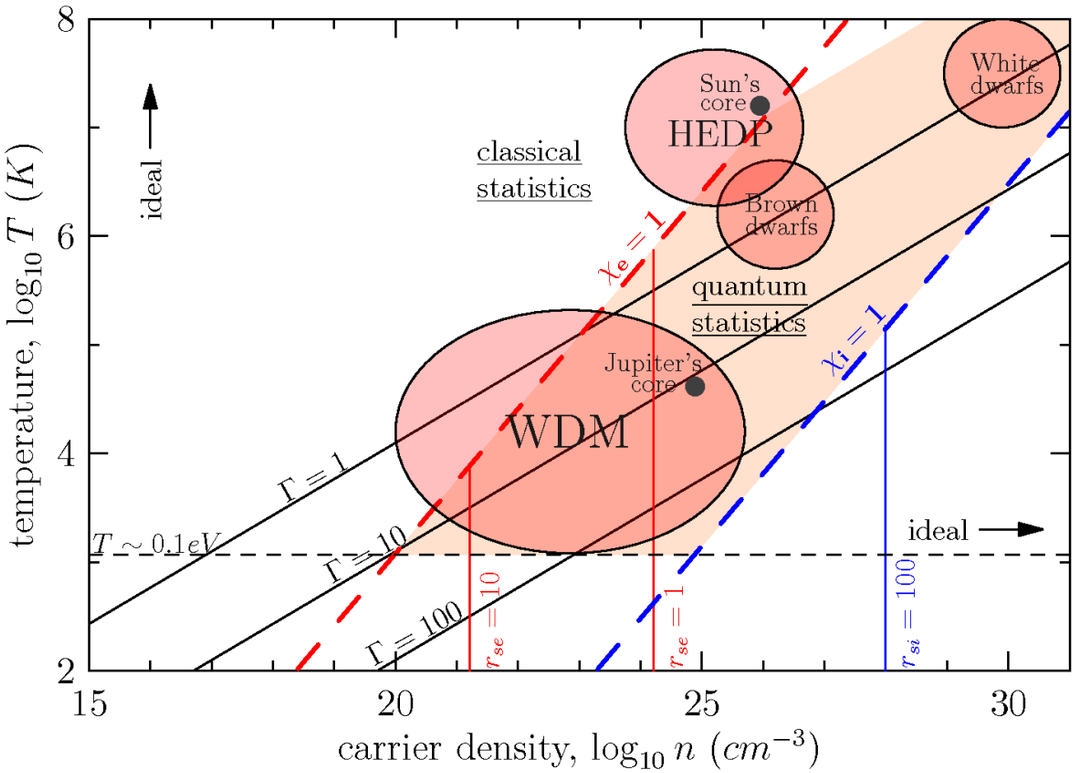
6. Open questions. Outlook

1. Introduction: warm dense matter*



* Term due to A. Ng 1999, figure from *Frontiers of Plasma Science report* (draft) https://www.orau.gov/plasmawkshps2015/report.htm

Warm dense matter: 2 main components

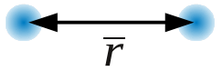


Coulomb coupling parameters:

$$\Gamma \equiv \frac{Q^2}{\bar{r}\, k_B T} > 1 \qquad r_s \equiv \frac{\bar{r}}{a_B} \sim 0.1 \ldots 10$$

Quantum degeneracy parameters:

$$\chi \equiv n \Lambda^{dim} \sim \left(\Lambda / \bar{r}\right)^{dim}$$



$$\Lambda = h / \sqrt{2\pi m k_B T}$$

$$\Theta = k_B T / E_F$$

In quantum system: $\chi \geq 1, \Theta \leq 1$

WDM: $\Theta \sim 0.1 \ldots 10$

Warm dense matter:

- **degenerate nonideal electrons**
- nearly classical ions

- Example: Hydrogen

$$\Lambda_e^3 / \Lambda_p^3 \sim 80{,}000$$

Perturbation theory and ground-state approaches (DFT etc.) fail

Introduction to Complex Plasmas, MB, N. Horing, and P. Ludwg (eds.), Springer 2010
MB, *Quantum Kinetic Theory,* Teubner 1998, 2nd ed. Springer 2016

2. Thermodynamics of warm dense electron gas

- Coulomb interacting electrons in a uniform positive background

I. <u>Ground state:</u> model description of metals and input for density Functional Theory (DFT)
→ correlation expansions (beyond Hartree-Fock)

$$E = \frac{2.21}{r_s^2} - \frac{0.916}{r_s} + 0.0622\ln(r_s) - 0.096 + O(r_s)$$

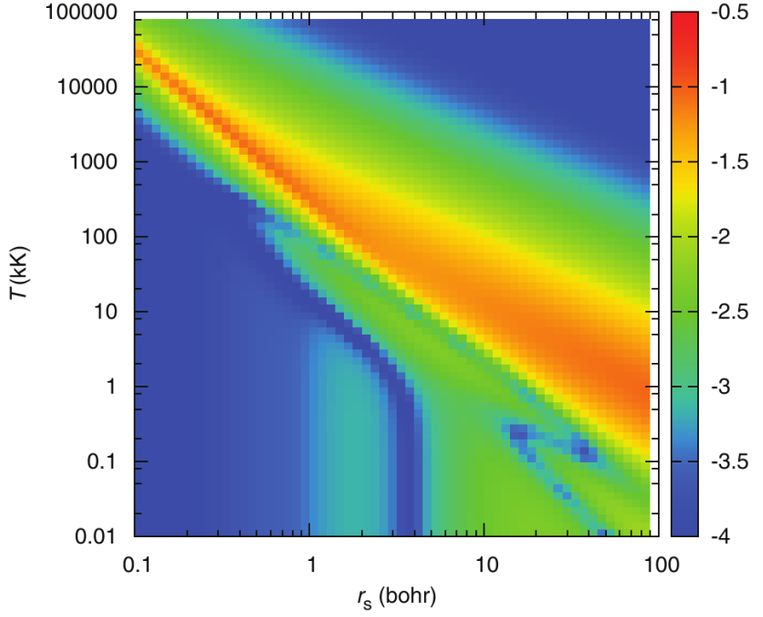
→ Combination with accurate Quantum Monte Carlo data [1] allows for a parametrization of XC-energy [2] for all r_s
→ DFT simulations of real materials

II. <u>Warm dense matter:</u> Thermal DFT [3]

→ ground state XC-energy not sufficient [4]
→ finite-T DFT (KS-DFT, OF-DFT) requires accurate parametrization of the XC-free energy of the UEG in WDM regime

accurate thermodynamic description of the warm dense electron gas required

$\log_{10}\left(|f_{xc}(r_s,T) - e_{xc}(r_s)|/[|f_s(r_s,T)| + |e_{xc}(r_s)|]\right)$



relative importance of finite-T XC-functional [4]

[1] D.M. Ceperley and B. Alder, PRL **45**, 566 (1980)
[2] J.P. Perdew and A. Zunger, PRB **23**, 5048 (1981)
[3] N.D. Mermin, Phys. Rev **137**, A1441 (1965)
[4] V. Karasiev *et al.,* PRE **93**, 063207 (2016)

Standard semi-analytical approaches

Selected parametrizations of f_{xc}

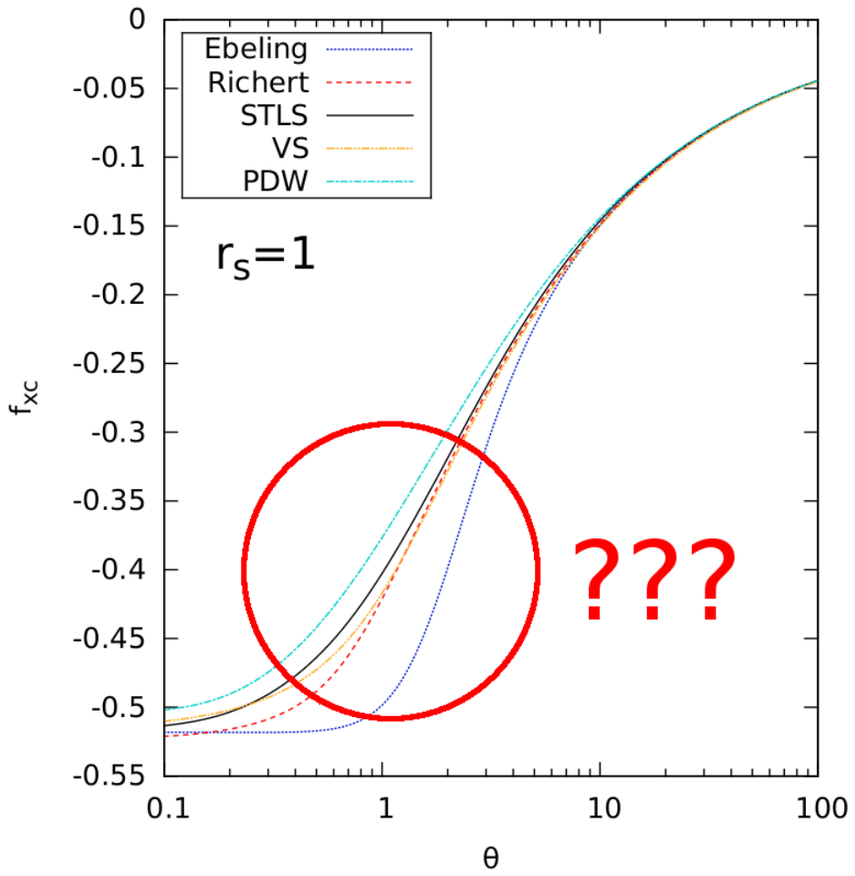
→ Green functions results (De Witt, Montroll/Ward) Kremp, Kraeft, Ebeling
→ Padé approximations by Ebeling [1], Ichimaru
→ Functional fits to dielectric approaches, e.g. Singwi-Tosi-Land-Sjölander (STLS) [2] and Vashista-Singwi (VS) [3,4]
→ Quantum-Classical mappings, e.g. Perrot and Dharma-wardana (PDW) [5]

Known asymptotics:

$$\lim_{T\to 0} f_{xc}(r_s,T) = E_{xc}(r_s)$$

$$\lim_{T\to\infty} f_{xc}(r_s,T) = -\frac{1}{\sqrt{3}} r_s^{-3/2} T^{-1/2}$$

$$\lim_{r_s\to 0} f_{xc}(r_s,T) = \frac{a_{\mathrm{HF}}(T)}{r_s}$$ but...



Exact behavior in the warm dense regime has remained unclear!

→

Quantum Monte Carlo simulations

[1] W. Ebeling and H. Lehmann, Ann. Phys. **45**, 529 (1988)
[2] S. Tanaka, S. Ichimaru, J. Phys. Soc. Jpn. **55**, 2278 (1986)
[3] W. Stolzmann and M. Rösler, Contrib. Plasma Phys. **41**, 203 (2001)
[4] T. Sjostrom and J. Dufty, PRB **88**, 115123 (2013)
[5] F. Perrot and MWC Dharma-wardana, PRB **62**, 16536 (2000)

3. Path integral Monte Carlo (PIMC)

Ab initio simulations of the thermodynamic properties

Feynman's Path integral representation of quantum mechanics

+ Metropolis Monte Carlo

pioneered by Ceperley, Filinov, Imada and others

Equilibrium quantum statistical theory using Feynman's path integrals

- Equilibrium properties described by the density operator:

$$\hat{\rho} = e^{-\beta \hat{H}} \qquad \text{Hamiltonian} \quad \hat{H} = \hat{K} + \hat{V}$$

(kinetic and potential energy)

- The quantum partition functions is defined as the trace over the density matrix:

$$Z = \mathrm{Tr}\left(\hat{\rho}\right) = \int \mathrm{d}\mathbf{R} \ \langle \mathbf{R} | \, \hat{\rho} \, | \mathbf{R} \rangle$$

R: 3N coordinates of all particles, „Micro state“

- Compute expectation values of operators:

$$\langle A \rangle = \frac{1}{Z} \mathrm{Tr}\left(\hat{\rho}\hat{A}\right) = \frac{1}{Z} \int \mathrm{d}\mathbf{R} \ \langle \mathbf{R} | \, \hat{\rho}\hat{A} \, | \mathbf{R} \rangle$$

- Problem: density operator does not factorize, matrix elements are unknown

$$e^{-\beta \hat{H}} \neq e^{-\beta \hat{V}} e^{-\beta \hat{K}} \neq e^{-\beta \hat{K}} e^{-\beta \hat{V}} \rightarrow \langle \mathbf{R} | \, e^{-\beta \hat{H}} \, | \mathbf{R} \rangle = ?$$

- Solution: Exploit group property of the density matrix:

$$e^{-\beta \hat{H}} = \prod_{i=0}^{P-1} e^{-\epsilon \hat{H}} \quad \text{mit} \quad \epsilon = \beta / P \ , \quad \text{z.B. } e^{-\beta \hat{H}} = e^{-\beta \hat{H}/2} e^{-\beta \hat{H}/2}$$

Quantum statistics and Feynman-Path integrals

- Interim result: Partition function = product of *P* density matrices at *P*-times higher temperature (reduced quantum effects):

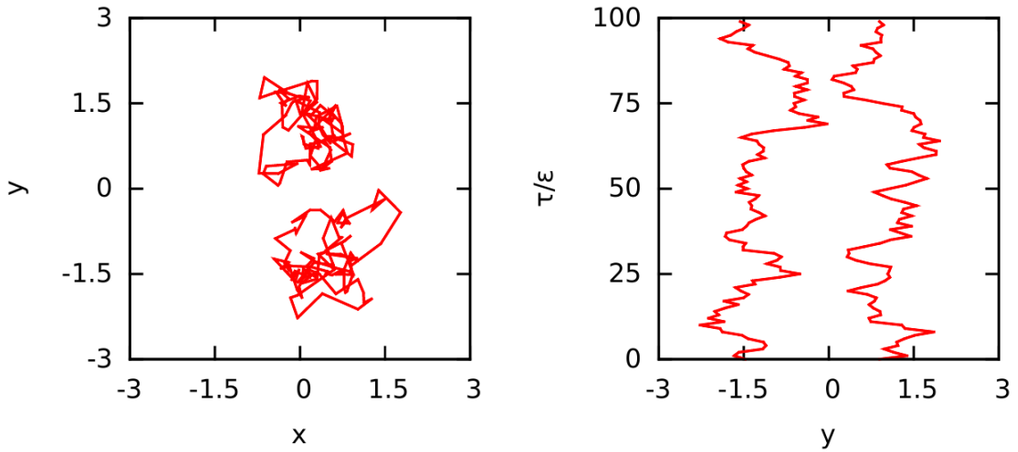
$$Z = \int \mathrm{d}\mathbf{R}_0 \ldots \mathrm{d}\mathbf{R}_{P-1} \left(\langle \mathbf{R_0} | \, e^{-\epsilon \hat{H}} \, | \mathbf{R_1} \rangle \, \langle \mathbf{R_1} | \ldots \langle \mathbf{R_{P-1}} | \, e^{-\epsilon \hat{H}} \, | \mathbf{R_0} \rangle \right)$$

- For a sufficient number of factors *P*, the density operator can be factorized:

Trotter-Formula: $$\lim_{P \to \infty} \left(e^{-\epsilon \hat{K}} e^{-\epsilon \hat{V}} \right)^P = e^{-\beta(\hat{K}+\hat{V})} \, , \quad \epsilon = \beta / P$$

- Final result: Partition function = integral over all closed paths **X** in „imaginary time“, with the appropriate configuration weight *W*(**X**):

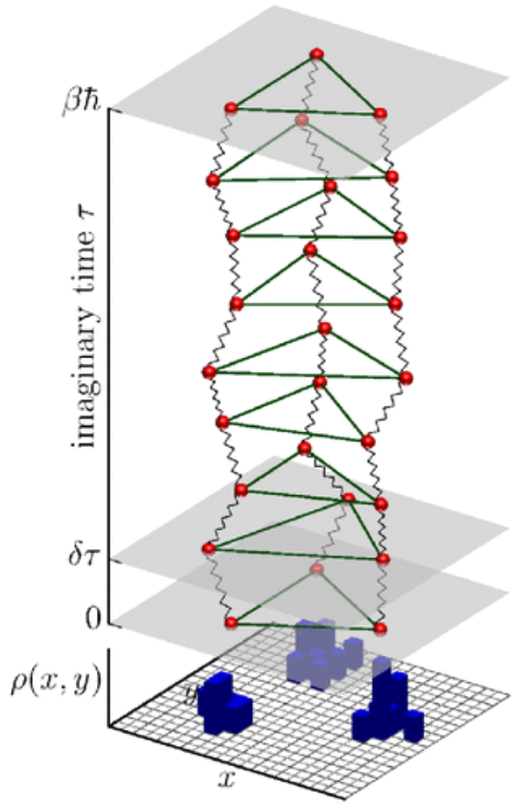
$$Z = \int \mathrm{d}\mathbf{X} \; W(\mathbf{X})$$



Quantum statistics and Feynman-Path integrals

Feynman's quantum mechanics: map delocalized quantum-particles to „classical ring-polymeres“

$$Z = \int \mathrm{d}\mathbf{X}\; W(\mathbf{X})$$



- Path integral-Monte Carlo (PIMC):
use Metropolis-algorithm to randomly generate all closed paths ***X*** from ***W(X)*** (dim=3NP)

Exact simulations of quantum systems of up to *N*=10⁴ distinguishable particles feasible

PIMC for Bosons and Fermions

- Include all *N*-particle permutations into the partition function („exchange“):

$$Z = \frac{1}{N!} \sum_{\sigma \in S_N} \mathrm{sign}(\sigma) \int \mathrm{d}\mathbf{R} \, \langle \mathbf{R} | \, \hat{\rho} \, | \hat{\pi}_\sigma \mathbf{R} \rangle$$

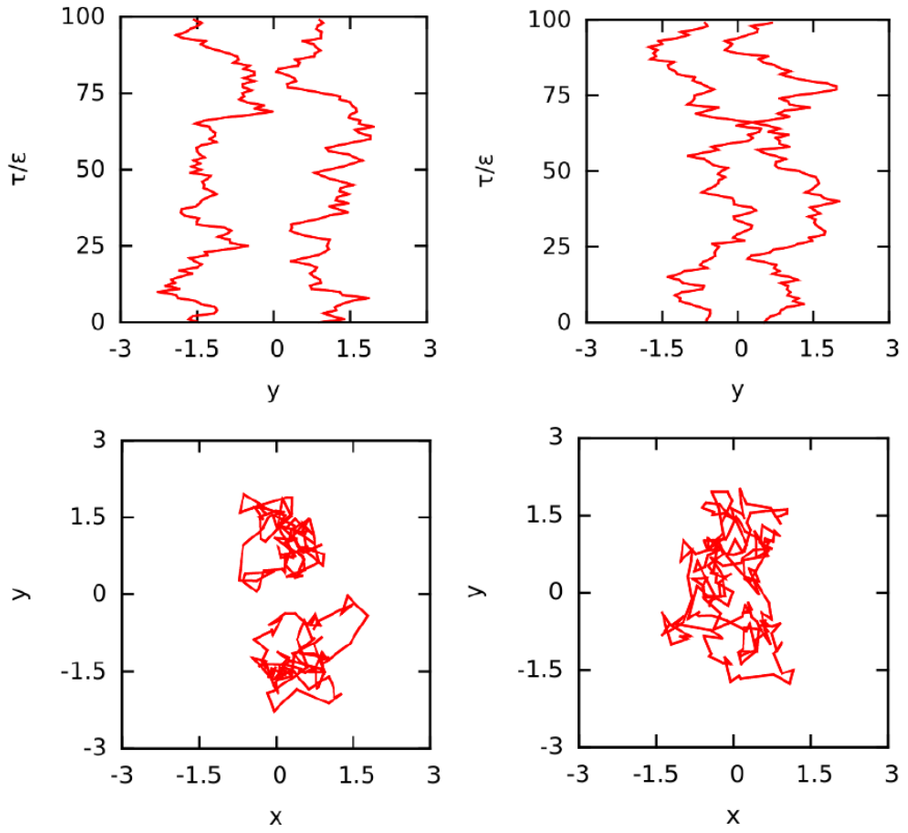
- **PIMC-Simulations** of bosons and fermions require the additional generation of all possible closed many-body paths („exchange cycles“)

$$Z = \sum_{\mathbf{X}} W(\mathbf{X})$$

- **Bosons:** All contributions are positive
→ Exact simulations of up to $N=10^4$ particles are, in principle, feasible (investigation of suprafluidity, etc.)

- **Fermions:** Odd permutations have a negative weight

How to generate configurations with positive and negative weights?



PIMC for fermions: fermion sign problem

- Solution: generate configurations according to their modulus weights

$$Z' = \sum_{\mathbf{X}} |W(\mathbf{X})| \quad \Rightarrow \quad \langle A \rangle = \frac{\langle As \rangle'}{\langle s \rangle'}$$

$$\langle s \rangle' = \frac{1}{Z'} \sum_{\mathbf{X}} |W(\mathbf{X})| \mathrm{sign}(\mathbf{X}) = \frac{Z}{Z'} \propto e^{-\beta N (f - f')}$$

- Average sign, reflecting numerical cancellations

- Monte-Carlo error increases exponentially with particle number and inverse temperature

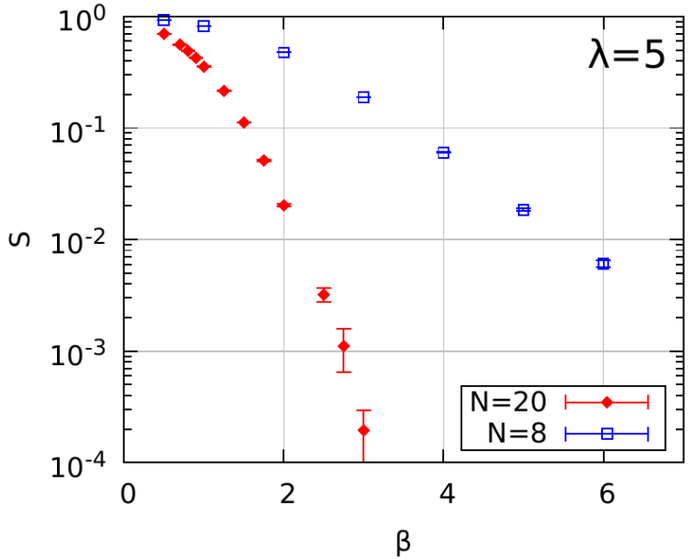
$$\Delta A \propto \frac{e^{\beta N (f - f')}}{\sqrt{N_{\mathrm{MC}}}}$$

- this exponential increase cannot be compensated by more computation time

„Fermion Sign Problem“!

- sign problem ***NP*-hard for a given representation**
(Troyer, Wiese 2005)

Average sign in QMC
Example: Electrons in a quantum dot



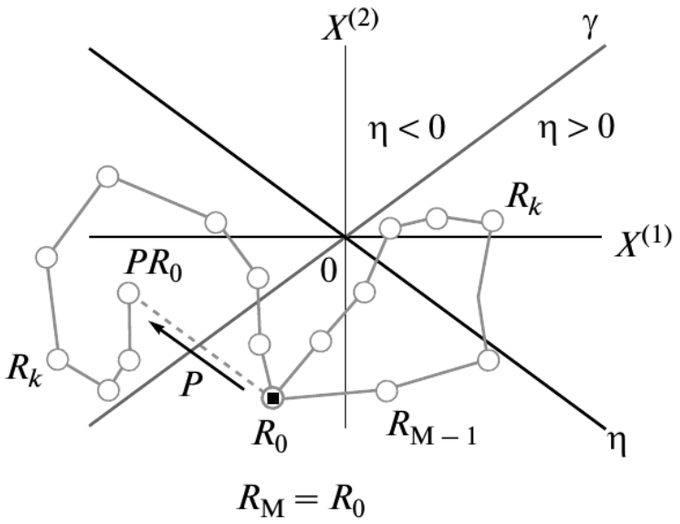
PIMC for Fermions (1): Fixed node approximation

„**Fixed Node Approximation**“, Restricted PIMC (RPIMC [1])

→ Separation of positive and negative contributions

→ exact (?), if using the correct nodes (a-priori unknown)

→ **uncontrolled systematic error** („nodal error“)



[1] D.M. Ceperley J. Stat. Phys. (1991)

RPIMC results for the warm dense UEG

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→ exact (?), if using the correct nodes (a-priori unknown)
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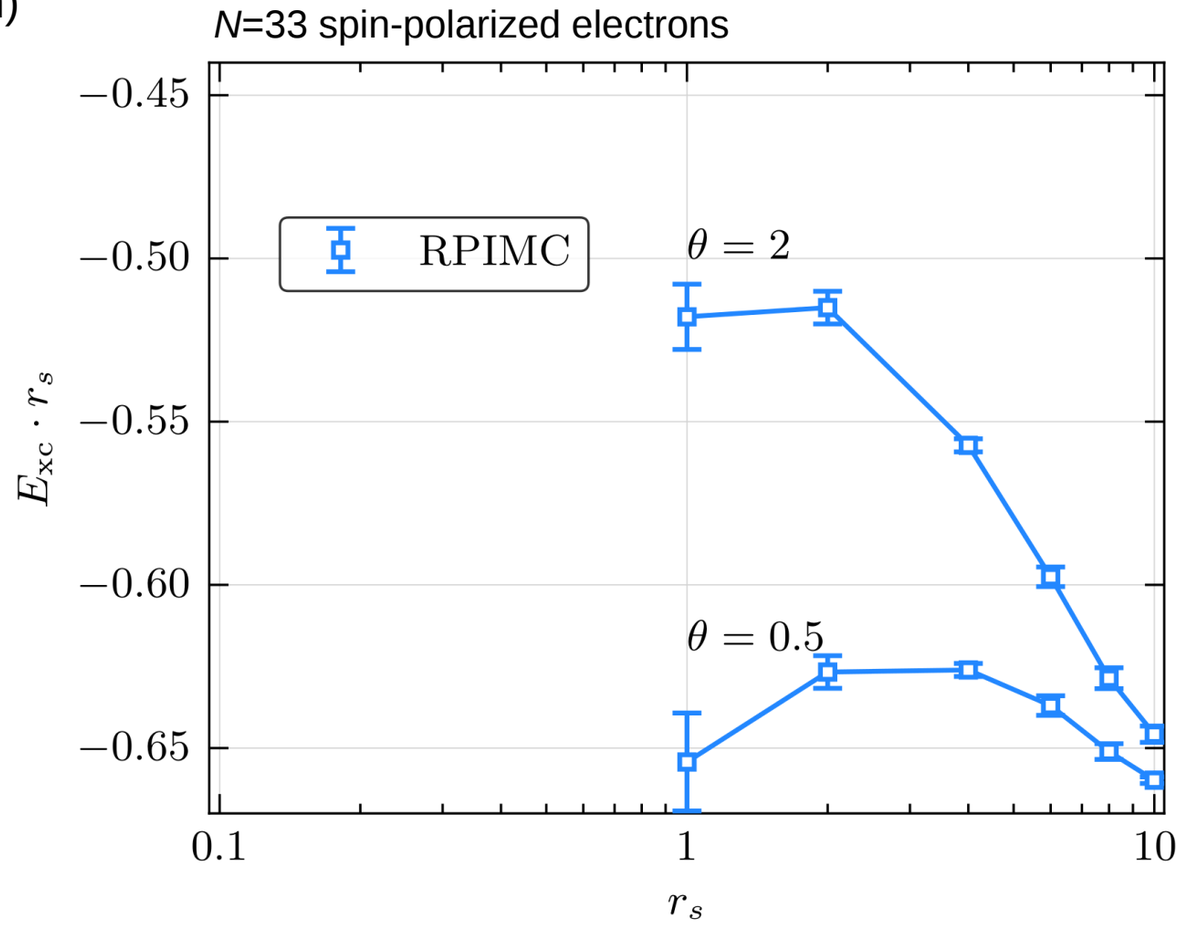
→ **first RPIMC simulations for the UEG**:
Brown, Ceperley and co-workers [2]:
N=33 (66), $T/T_F = 0.0625 \ldots 8$
extrapolation to macroscopic system
→ used as input for new parametrizations [2a,3,4] of $f_{xc}(rs,T)$

→ **Problems of the RPIMC data:**
- limited to rs >= 1
- accuracy unknown
- asymptotics questionable
- finite size correction only partly valid



[1] D.M. Ceperley J. Stat. Phys. (1991)
[2] E.W. Brown *et al.*, PRL **110**, 146405 (2013)
[2a] E.W. Brown *et al.*, PRB **88**, 081102(R) (2013),
[3] T. Sjostrom and J. Dufty, PRB **88**, 115123 (2013)
[4] V.V. Karasiev *et al.*, PRL **112**, 076403 (2014)

4. New developments in QMC simulations of the warm dense electron gas

Goal: QMC simulations without additional approximations

1) Change the QM representation:

„Configuration PIMC“ (CPIMC) [1,2]

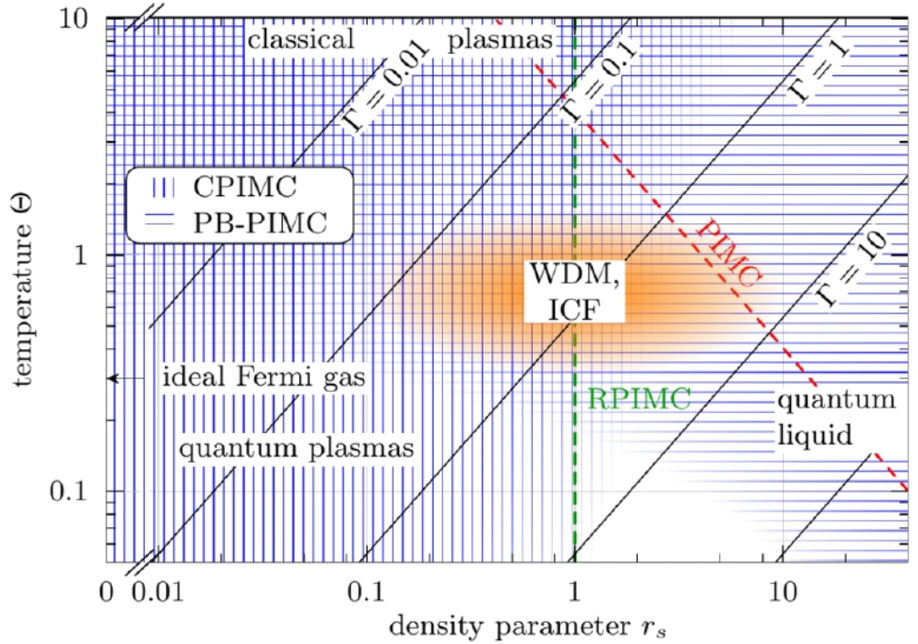
→ evaluation of the trace in antisymmetrized Fock-Space:

$$Z = \mathrm{Tr}\hat{\rho}^{-} = \mathrm{Tr}^{-}\hat{\rho}$$

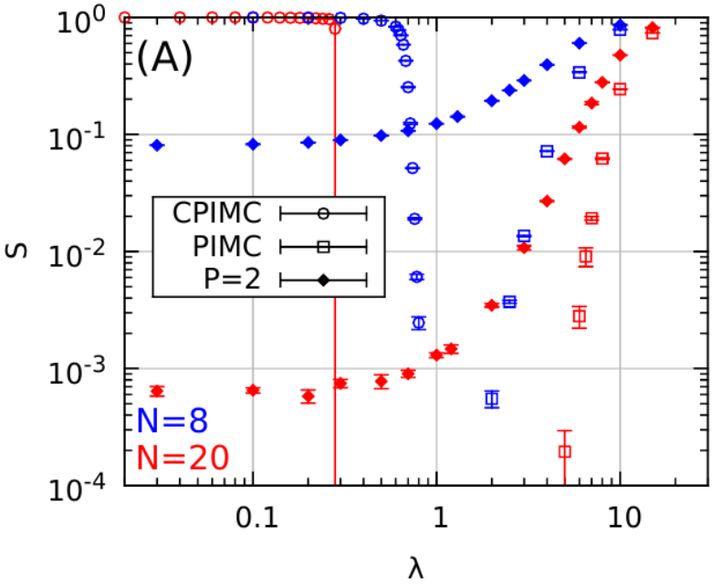
→ Complementary sign problem to standard PIMC

→ Extremely efficient at high degeneracy/ weak coupling [3]

Availability of QMC simulations [5]



Example: Electrons in a quantum dot [4]



[1] T. Schoof *et al.,* Contrib. Plasma Phys. **51**, 687 (2011)
[2] T. Schoof *et al.*, Contrib. Plasma Phys. **55**, 136 (2015)
[3] T. Schoof *et al.*, PRL **115**, 130402 (2015)
[4] T. Dornheim *et al.*, New J. Phys. **17**, 073017 (2015)
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„Permutation blocking PIMC“ (PB-PIMC) [4,5]
→ extends standard PIMC towards lower T and higher density

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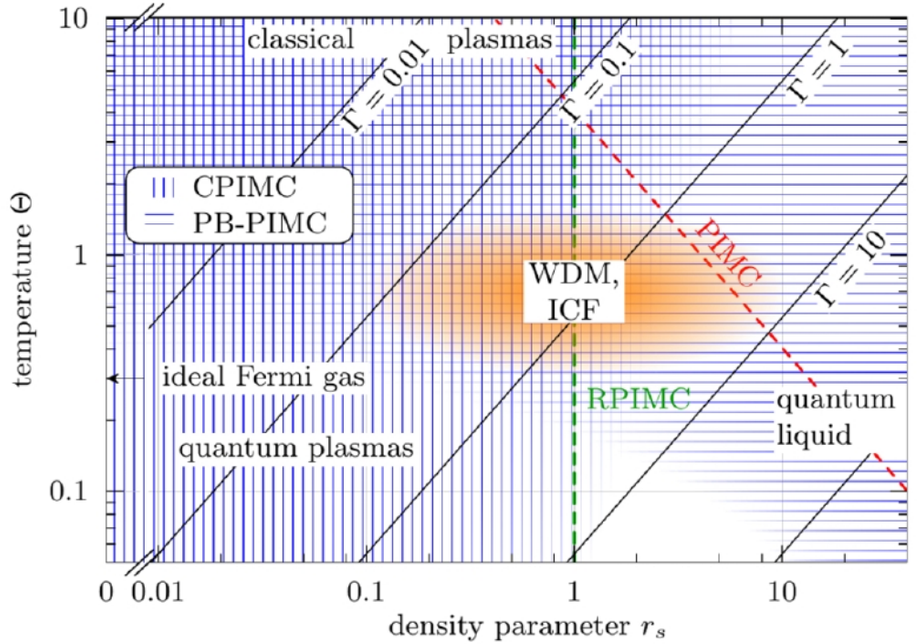

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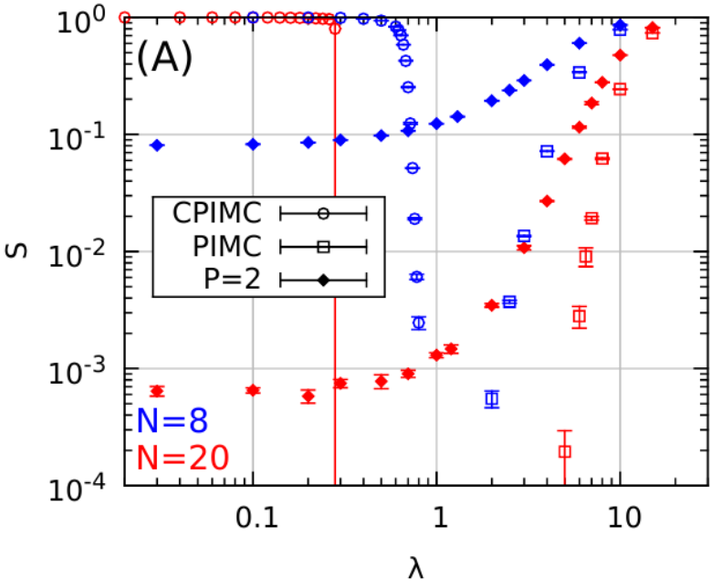

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3) Idea: Circumvent the sign problem by combining two complementary methods!

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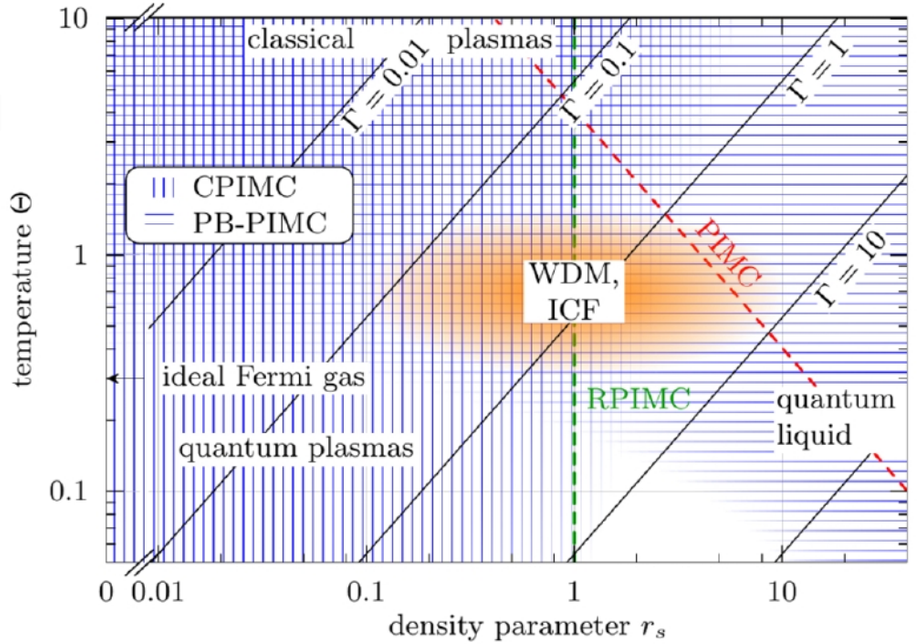

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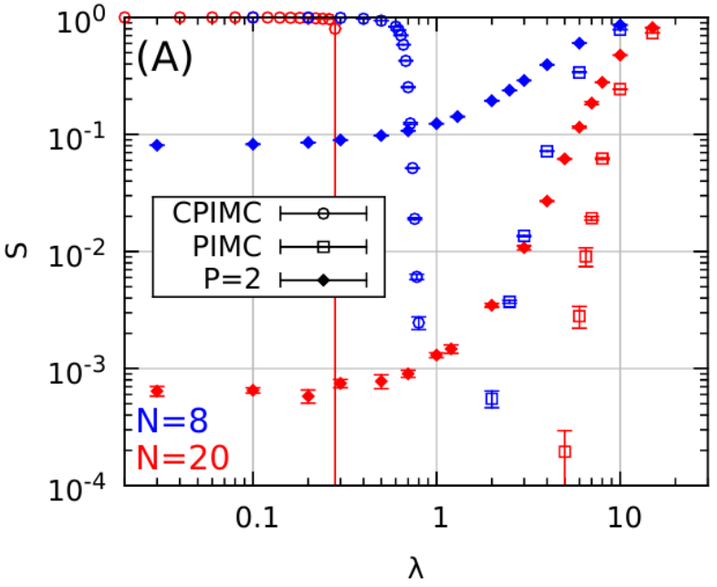

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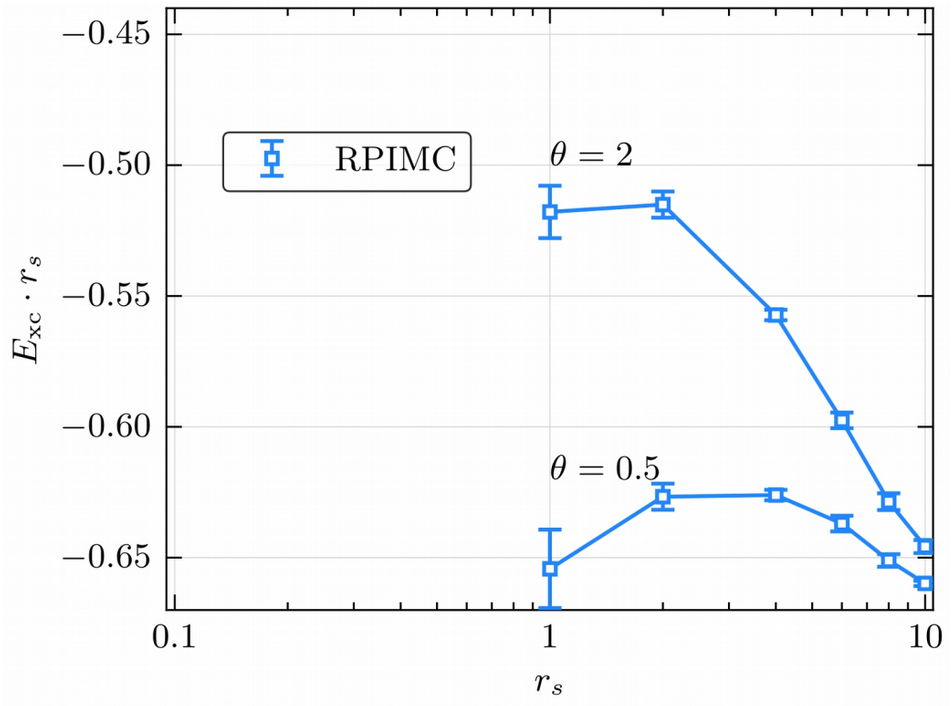
New QMC results for the warm dense electron gas without fixed nodes

QMC simulation of a finite system

→ **RPIMC** simulations by Brown *et al.* [1] are limited to rs >= 1

N=33 spin-polarized electrons



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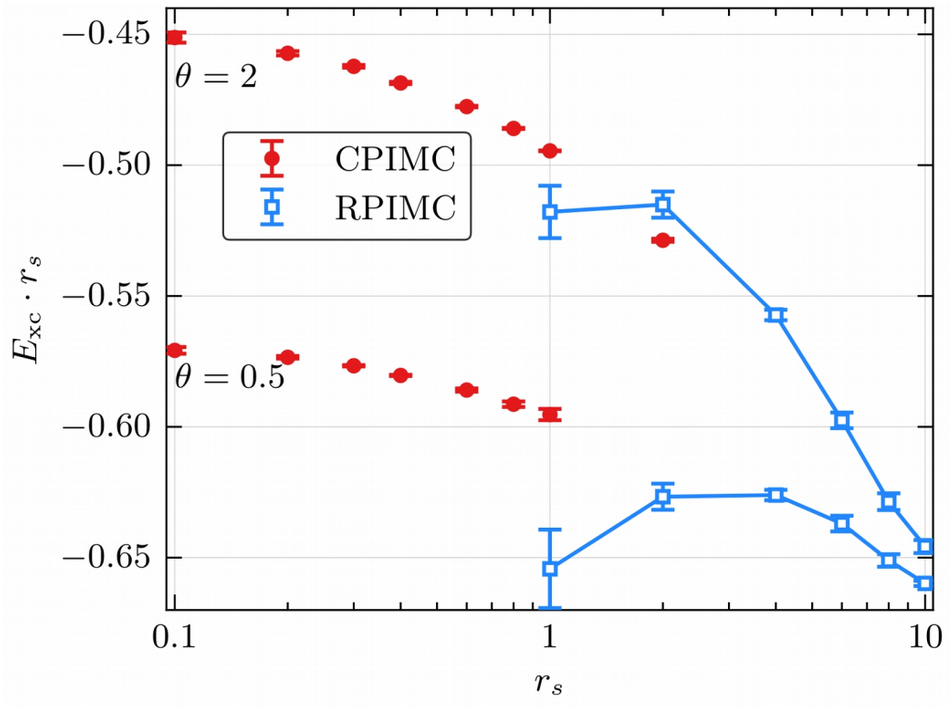

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[3] S. Groth *et al.*, PRB **93,** 085102 (2016)

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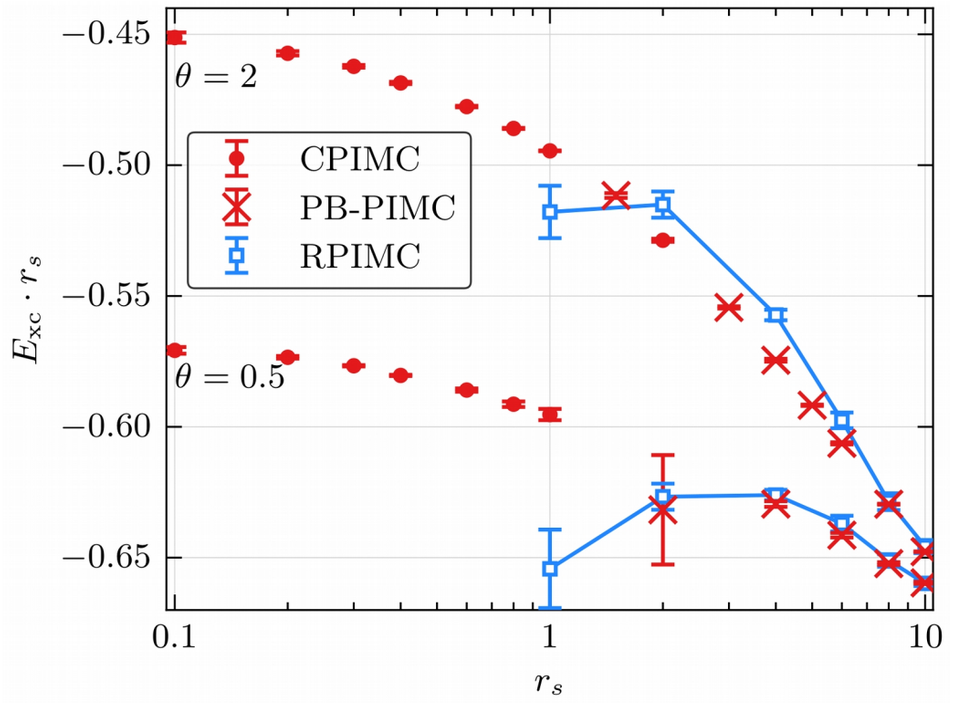

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Combination of PB-PIMC and CPIMC allows for accurate results over broad parameter range

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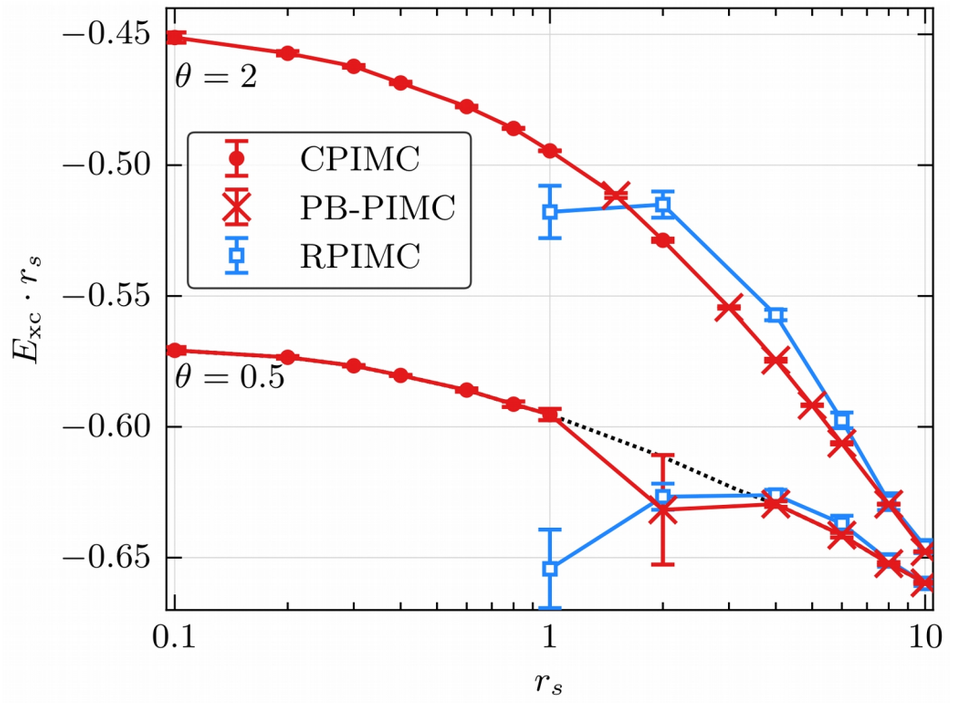

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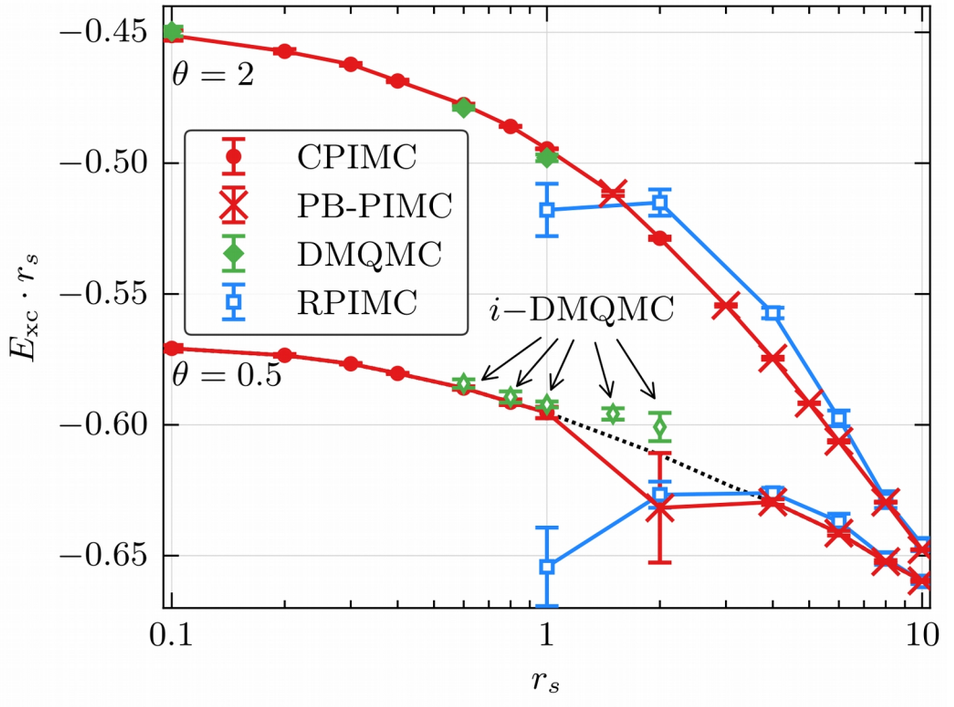
Recent development:
Density matrix QMC confirms our results

→ Sample thermal density matrix expanded in a basis of Slater determinants [5,6]

$$\hat{\rho} = \sum_{\{n\},\{n'\}} \rho_{\{n\},\{n'\}} |\{n\}\rangle\langle\{n'\}|$$

→ efficient at small rs, eventually fails with increasing coupling
→ initiator approximation [7] allows to significantly extend the rs-range

N=33 spin-polarized electrons



Accurate QMC simulations of the electron gas with *finite N* are possible without fixed nodes!

[1] E.W. Brown *et al.*, PRL **110**, 146405 (2013)
[2] T. Schoof *et al.*, PRL **115**, 130402 (2015)
[3] S. Groth *et al.*, PRB **93,** 085102 (2016)
[4] T. Dornheim *et al.,* J. Chem. Phys. **143**, 204101 (2015)
[5] N.S. Blunt *et al.,* PRB **89,** 245124 (2014)
[6] F.D. Malone *et al.*, J. Chem. Phys. **143**, 044116 (2015)
[7] F.D. Malone *et al.*, PRL **117**, 115701 (2016)

5. Removing finite-size errors in QMC simulations of the warm dense electron gas

QMC simulations possible for finite N=30...200
→ Direct QMC results are afflicted with finite-size error

$$v = \frac{V_N}{N} + \frac{\Delta V_N}{N}$$

How to obtain results for the thermodynamic limit?

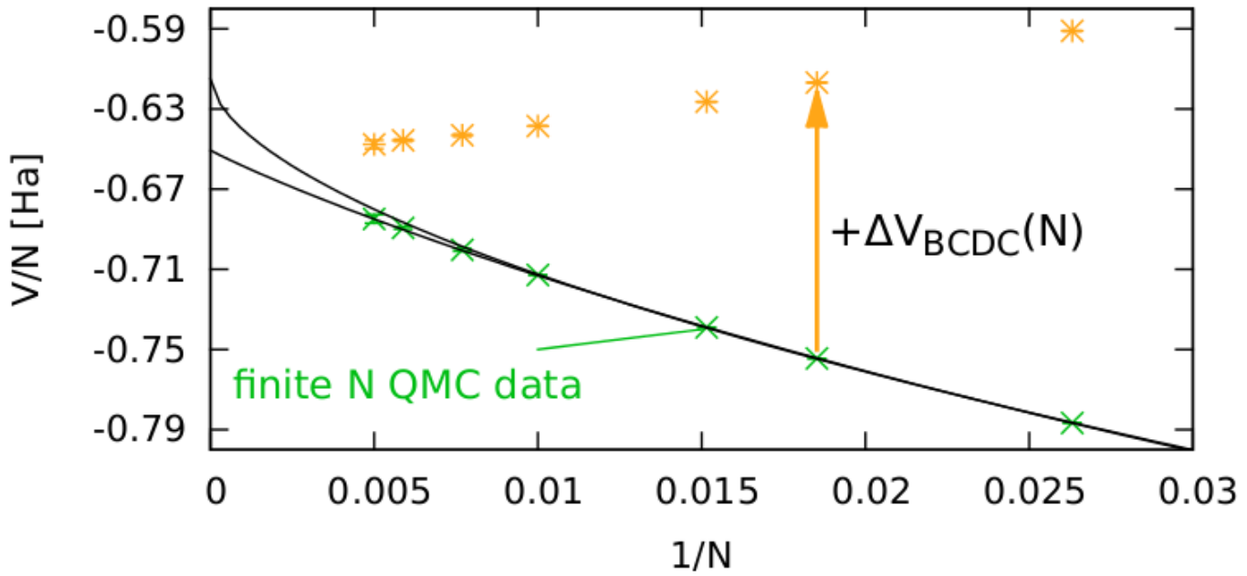
a) Direct extrapolation of the QMC data over system size N
→ unreliable if the exact functional form V(N) is not known

b) Add a finite-size correction (FSC) to the finite-N QMC results
→ Brown *et al.* [2] suggested finite-T extension of Chiesa *et al.* formula [3]

$$\Delta V_{\mathrm{BCDC}}(N) = \frac{\omega_p}{4N} \coth\left(\frac{\beta\omega_p}{2}\right)$$

→ **Problem:** The BCDC FSC is only appropriate in parts of the warm dense regime

Interaction energy for rs=0.5, T/T_F=2 [1]



We need an improved finite-size correction that is valid for all warm dense matter parameters!

[1] T. Dornheim, S. Groth *et al.*, PRL **117**, 156403 (2016)
[2] E.W. Brown *et al.*, PRL **110**, 146405 (2013)
[3] S. Chiesa *et al.*, PRL **97**, 076404 (2006)

Novel finite-size corrections for QMC simulations of the warm dense electron gas

QMC simulations possible for finite N=30...200
→ Direct QMC results are afflicted with finite-size error

$$v = \frac{V_N}{N} + \frac{\Delta V_N}{N}$$

Estimation of finite-size errors [1,2,3]:

$$\frac{V_N}{N} = \frac{1}{2\Omega} \sum_{\mathbf{G}\neq\mathbf{0}} \left[S_N(\mathbf{G}) - 1\right] \frac{4\pi}{G^2} + \frac{\xi_M}{2} \qquad \text{(i)}$$

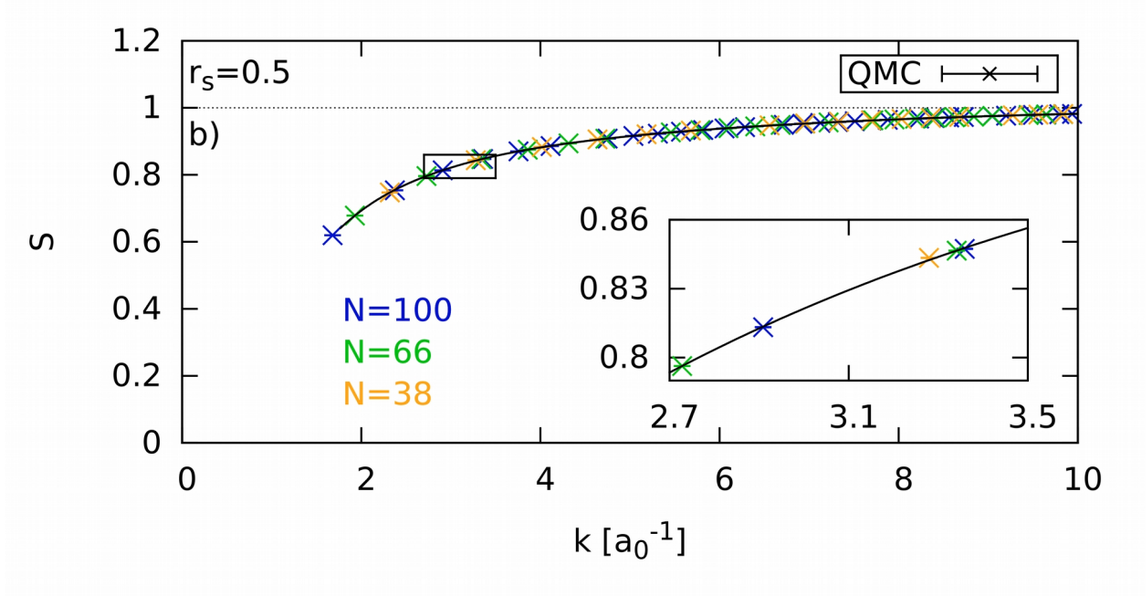
$$v = \frac{1}{2} \int_{k<\infty} \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3} \left[S(k) - 1\right] \frac{4\pi}{k^2} \qquad \text{(ii)}$$

Two possible sources for the finite-size error:

1) Replacing $S(k)$ by its finite-size pendant $S_N(k)$
→ Not the dominating issue

2) Approximation of the integral in (ii) by a discrete sum over lattice vectors ***G*** (momentum quantization)

Static structure factors $S(k)$ of the unpolarized UEG with rs=0.5, T/T_F=2 [3]



The finite-size effects are (mainly) due to momentum discretization in a finite simulation cell!

[1] S. Chiesa *et al.*, PRL **97**, 076404 (2006)
[2] N.D. Drummond *et al.*, PRB **78**, 125106 (2008)
[3] T. Dornheim, S. Groth *et al.*, PRL **117**, 156403 (2016)

Novel finite-size corrections for QMC simulations of the warm dense electron gas

Estimation of finite-size errors [1-3]:

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2) Approximation of the integral in (ii) by discrete sum over lattice vectors ***G*** (momentum quantization)

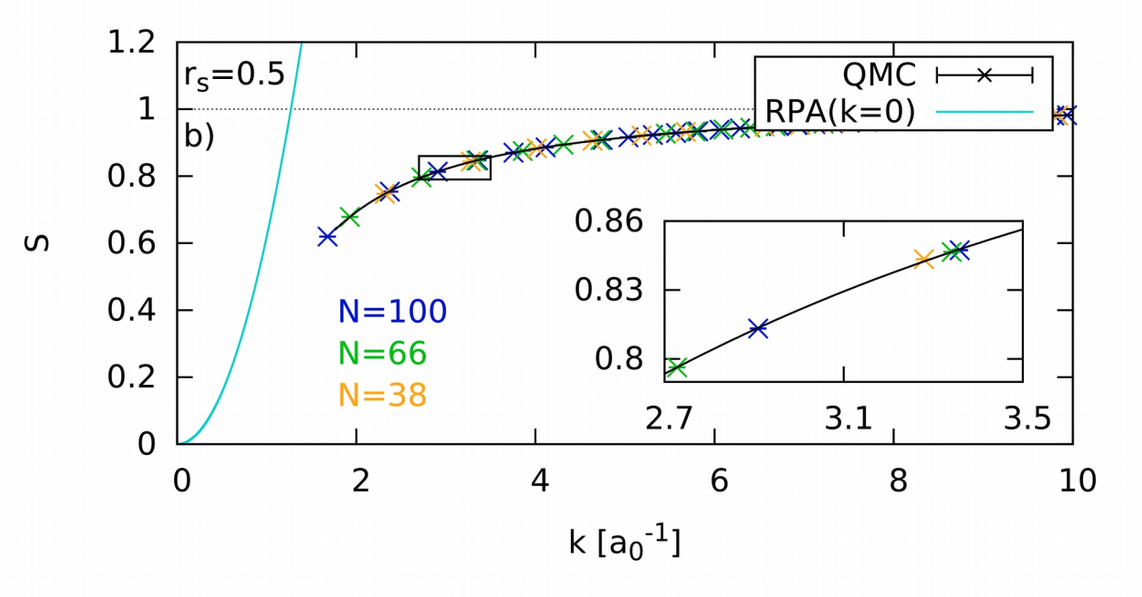
→ Chiesa *et al.*[1]: Main contribution to difference (i)-(ii) is due to missing ***G*=0** term
→ use RPA-expansion around *k*=0

$$S_0^{\mathrm{RPA}}(k) = \frac{k^2}{2\omega_p} \coth\left(\frac{\beta\omega_p}{2}\right)$$

→ this gives the finite-size correction used by Brown *et al.* [4]

$$\Delta V_{\mathrm{BCDC}}(N) = \frac{\omega_p}{4N} \coth\left(\frac{\beta\omega_p}{2}\right)$$

Static structure factors *S*(*k*) of the unpolarized UEG with rs=0.5, T/T_F=2 [3]



→ RPA expansion does not connect to QMC data
→ not sufficient for finite-size correction

We need improved data for *S*(*k*) !

[1] S. Chiesa *et al.*, PRL **97**, 076404 (2006)
[2] N.D. Drummond *et al.*, PRB **78**, 125106 (2008)
[3] T. Dornheim, S. Groth *et al.*, PRL **117**, 156403 (2016)
[4] E.W. Brown *et al.*, PRL **110**, 146405 (2013)

Novel finite-size corrections for QMC simulations of the warm dense electron gas

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2) Approximation of the integral in (ii) by a discrete sum over lattice vectors ***G*** (momentum quantization)

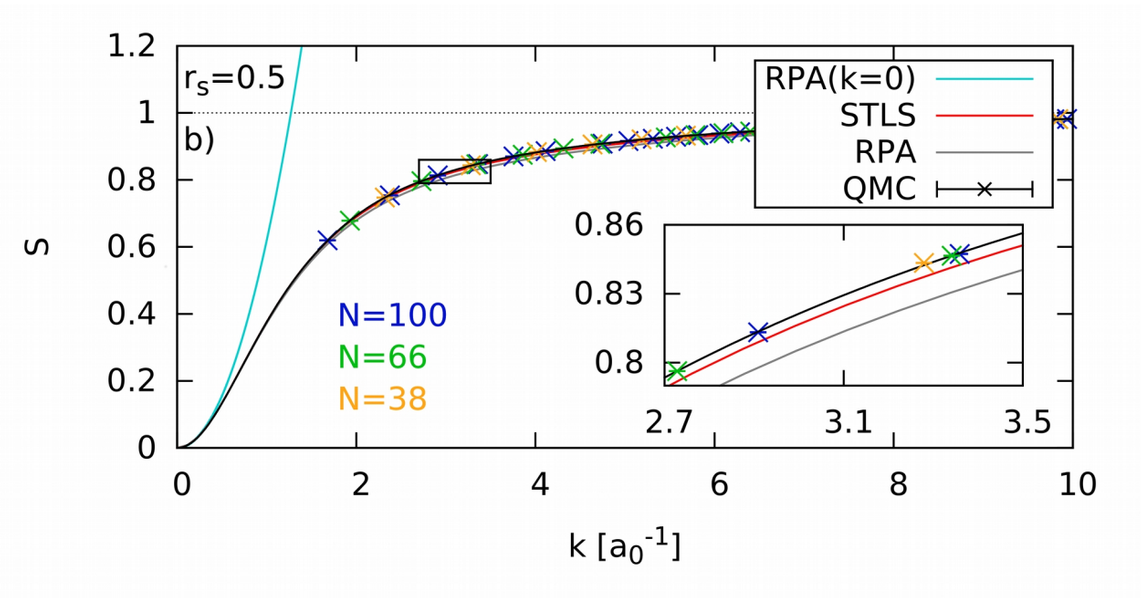
→ **Better:** Use STLS (or full RPA) data [4] for *S*(*k*)

- STLS smoothly connects to the QMC data
- Combination of *S*(*k*) from STLS and QMC (e.g. with spline) allows for accurate structure factors for all ***k***

Improved finite-size correction [3]:

→ Use the spline to explicitly compute the difference between (i) and (ii) for all ***k*** up to *S*(*k*)=1

Static structure factors *S*(*k*) of the unpolarized UEG with rs=0.5, T/T_F=2 [3]



[1] S. Chiesa *et al.*, PRL **97**, 076404 (2006)
[2] N.D. Drummond *et al.*, PRB **78**, 125106 (2008)
[3] T. Dornheim, S. Groth *et al.*, PRL **117**, 156403 (2016)
[4] T. Sjostrom and J. Dufty, PRB **88**, 115123 (2013)

Novel finite-size corrections for QMC simulations of the warm dense electron gas

Estimation of finite-size errors [1-3]:

$$\frac{V_N}{N} = \frac{1}{2\Omega} \sum_{\mathbf{G}\neq\mathbf{0}} \left[S_N(\mathbf{G}) - 1\right] \frac{4\pi}{G^2} + \frac{\xi_M}{2} \qquad \text{(i)}$$

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Improved finite-size correction [3]:

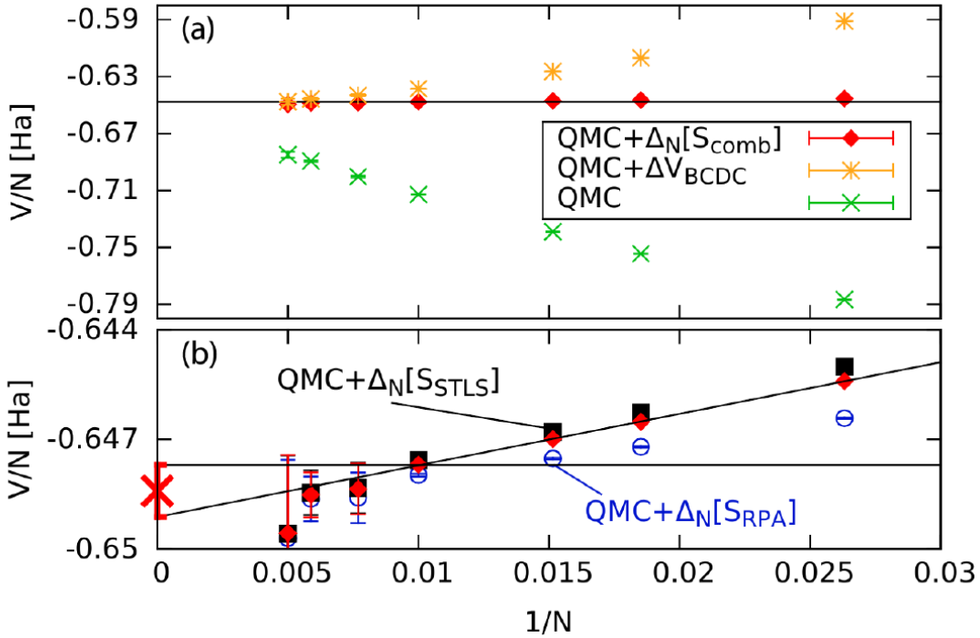
→ use the spline to explicitly compute the difference between (i) and (ii) for all ***k*** until $S(k)=1$

→ The new finite-size correction improves accuracy by two orders of magnitude

→ The residual finite-size error comes from the small N-dependence of $S_N(k)$ itself and are removed by an additional extrapolation

→ using the *full STLS or RPA results only* is sufficient to compute the discretization error (ii)-(i)

Interaction energy of the unpolarized UEG with rs=0.5, T/T_F=2 [3]



Our new finite-size correction works for all warm dense matter parameters (even rs=0.1, T/T_F=8)

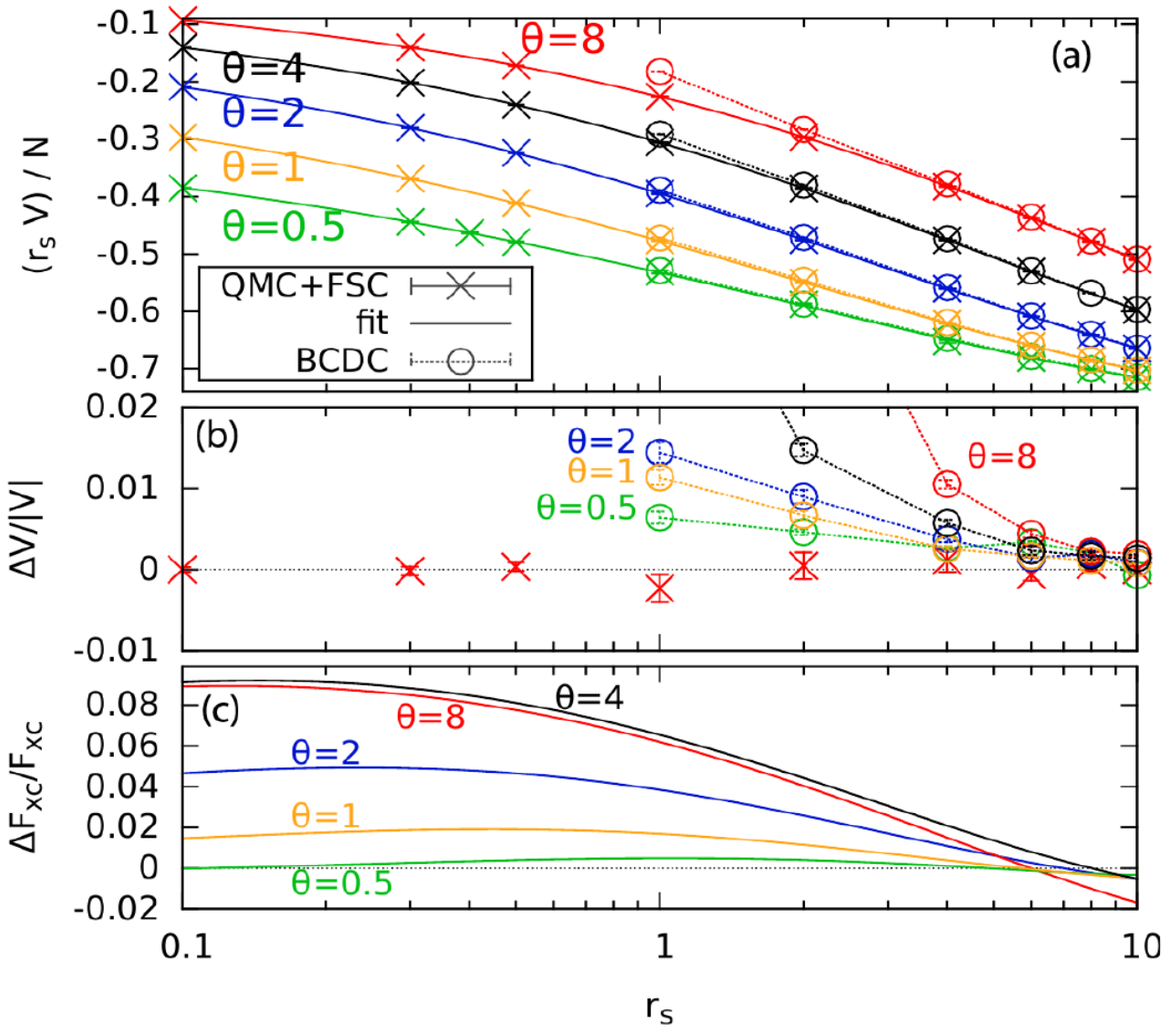
[1] S. Chiesa *et al.*, PRL **97**, 076404 (2006)
[2] N.D. Drummond *et al.*, PRB **78**, 125106 (2008)
[3] T. Dornheim, S. Groth *et al.*, PRL **117**, 156403 (2016)
[4] T. Sjostrom and J. Dufty, PRB **88**, 115123 (2013)

Finally: first *ab initio* QMC results for the warm dense electron gas in the thermodynamic limit

Interaction energy
of the unpolarized UEG
in the thermodynamic limit [1]

interaction energy:
Relative error of
Previous data [2]

xc free energy:
Relative error of
Previous data [3]



[1] T. Dornheim, S. Groth, T. Sjostrom, F. Malone, M. Foulkes, and M. Bonitz, PRL **117**, 156403 (2016)
[2] E.W. Brown *et al.*, PRL **110**, 146405 (2013)
[3] V.V. Karasiev *et al.*, PRL **112**, 076403 (2014)

Finally: first *ab initio* QMC results for the warm dense electron gas in the thermodynamic limit

New Results for the macroscopic electron gas:

→ Extensive new QMC results for up to *N*=1000 electrons enable us to compute *V* in the macroscopic limit with an unprecedented accuracy ~0.1%

→ A comparison of the RPIMC data with the Brown finite-size correction [2] reveals deviations of ~20%, at high density and temperature

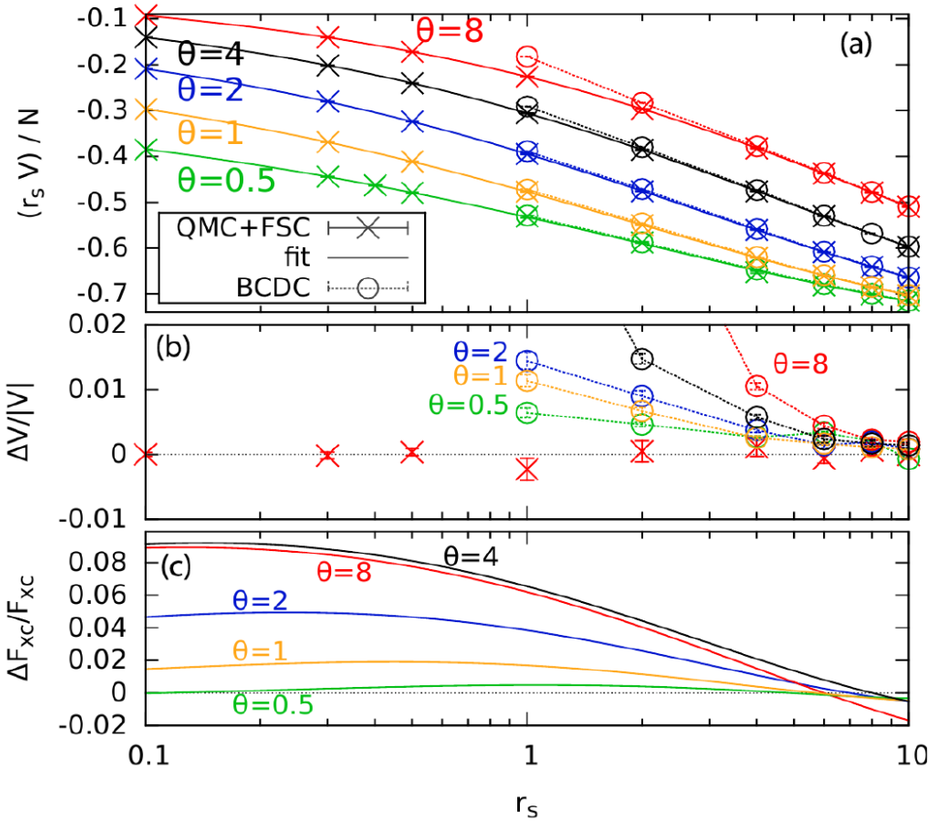
→ Having *V* allows us to obtain f_{xc}

$$f_{xc}(r_s,\theta) = \frac{1}{r_s^2}\int_0^{r_s} \mathrm{d}\bar{r}_s\, \bar{r}_s V(\bar{r}_s,\theta)$$

and, thus, *all thermodynamic observables*

→ The f_{xc} parametrization by Karasiev *et al.* [3] (KSDT) exhibits significant deviations of up to 9% (at high *T*)

Interaction and free XC-energy of the unpolarized UEG in the thermodynamic limit [1]



[1] T. Dornheim, S. Groth, T. Sjostrom, F. Malone, M. Foulkes and M. Bonitz, PRL **117**, 156403 (2016)
[2] E.W. Brown *et al.*, PRL **110**, 146405 (2013) [3] V.V. Karasiev *et al.*, PRL **112**, 076403 (2014)

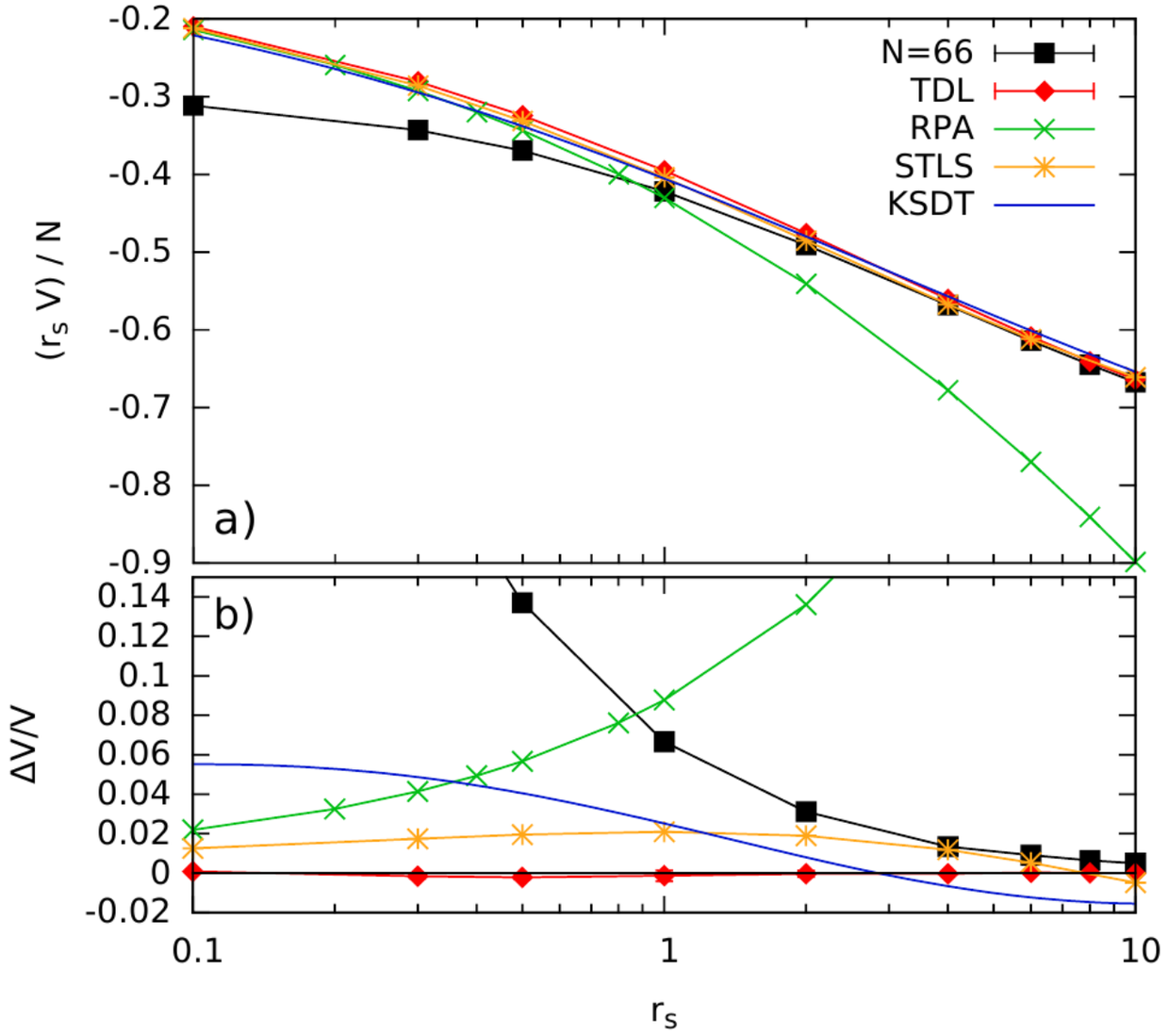
Testing analytical models: interaction energy

Isotherm, Θ=2

RPA: Random phase approximation

STLS: Singwi-Tosi-Land-Sjölander

KSDT: fit by Karasiev et al. (2014)



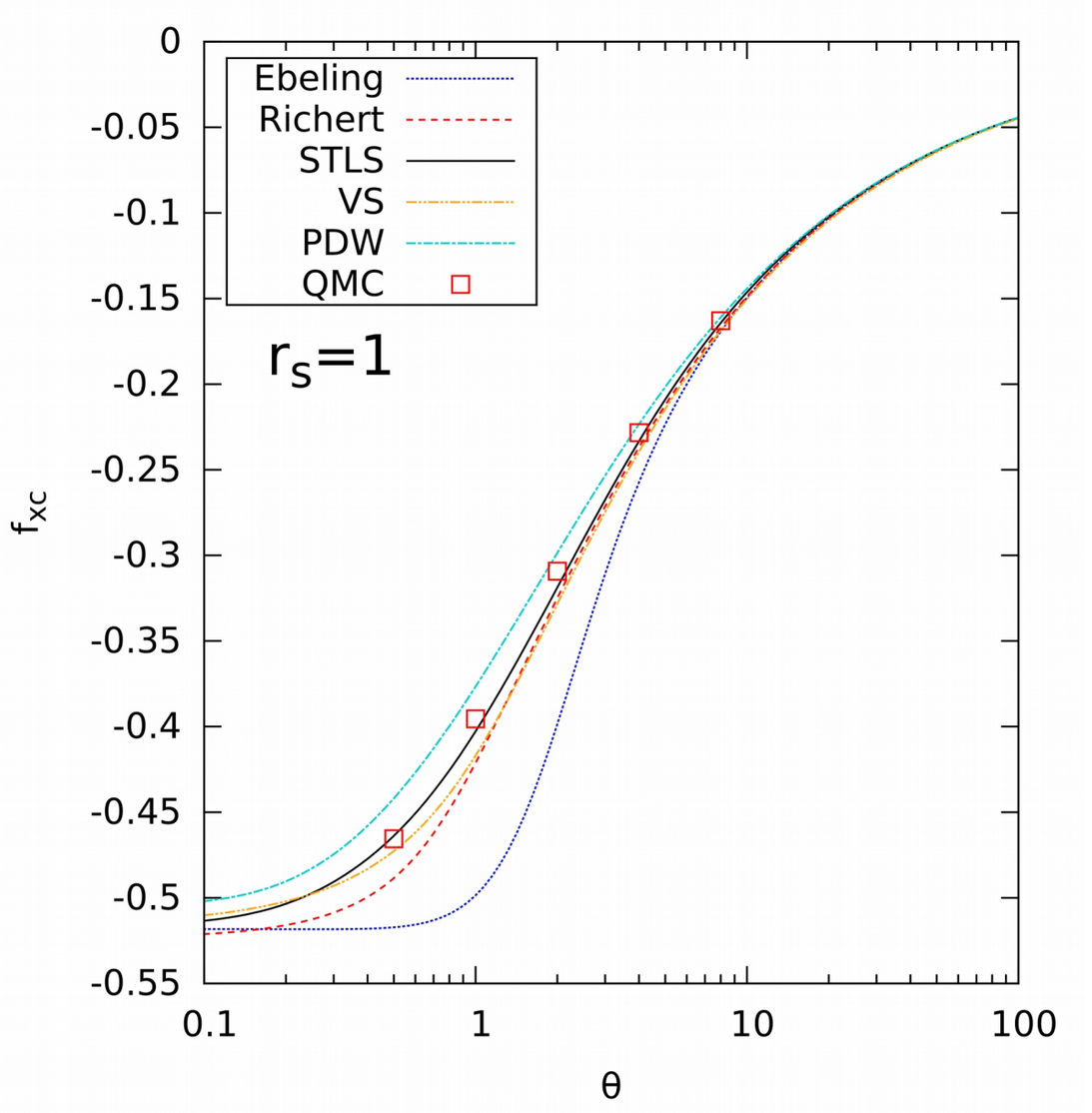
Testing analytical models: xc-free energy

Richert, Ebeling: Padé approximations

STLS: Singwi-Tosi-Land-Sjölander

VS: Vashista-Singwi

PDW:Quantum-Classical mapping of
Perrot and Dharma-wardana

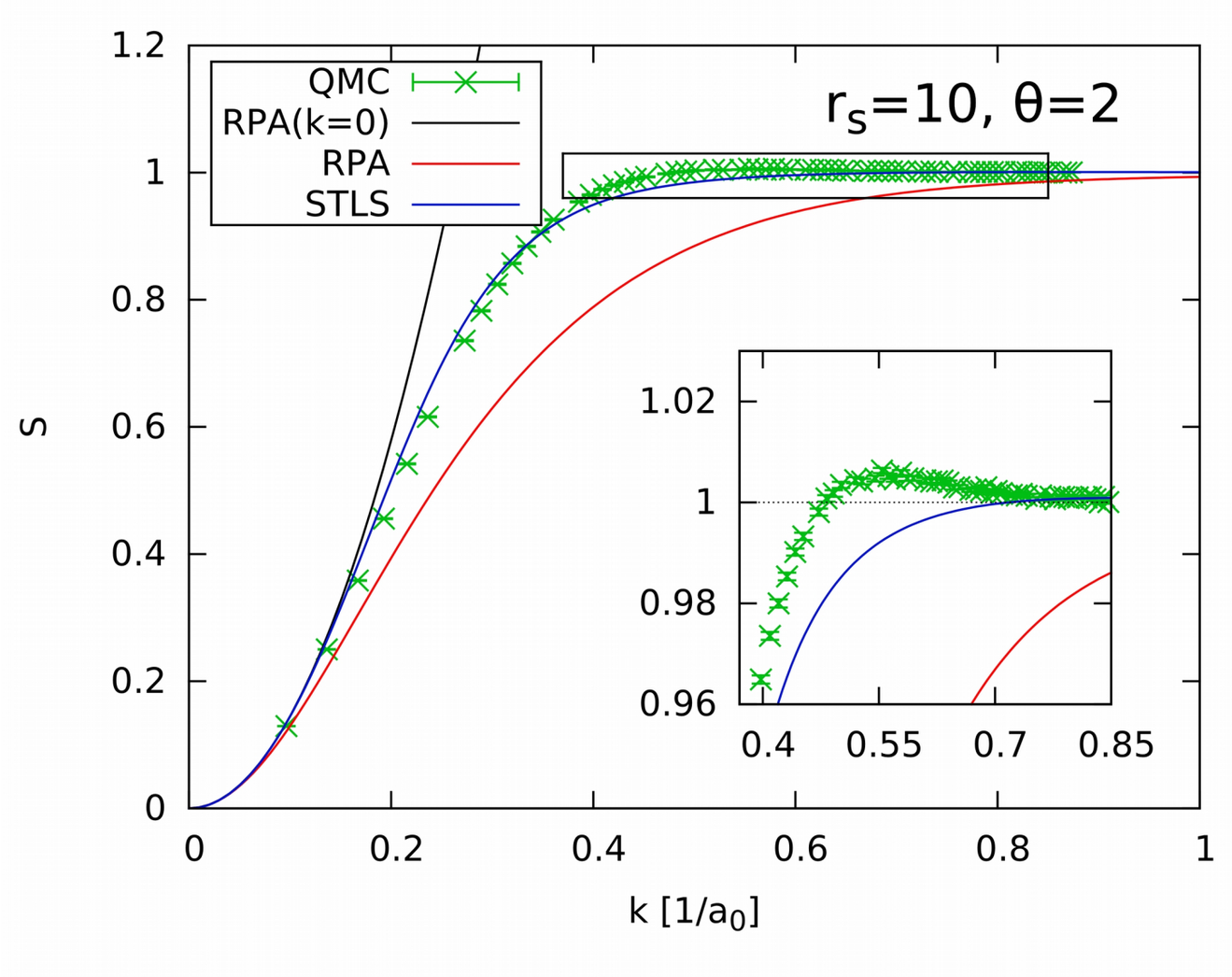


Testing analytical models: structure factors

STLS: Singwi-Tosi-Land-Sjölander

RPA: Random phase approximation

RPA (k=0): long wavelength limit



Summary

1. Warm dense matter: no small parameters → analytical models fail

2. Quantum Monte Carlo severely hampered by the fermion sign problem (FSP)

3. novel Path integral Monte Carlo approaches: CPIMC, PB-PIMC, DM-QMC:
   Combination allows to avoid the FSP

4. Novel highly accurate PIMC results for the electron gas (finite N)

5. Novel finite size correction extends finite-N-results to thermodynamic limit
   with unprecedented accuracy of ~ 0.1%

6. New data important for finite-T DFT simulations of WDM and for testing
   And improving alternative models and simulations

Open questions. Outlook

1. Present thermodynamic data should be transformed to accurate analytical fit

2. Warm dense matter: two-component system → electron gas results need to be Incorporated in DFT simulations via fit for fxc.
   Requires data for arbitrary spin polarizations (*in progress*)

3. Quantum Monte Carlo still severely hampered by the fermion sign problem (FSP)
   Need to extend simulations below Θ=0.5. Requires
   - method development,
   - smart additional approximations
   - combination with known T=0 results

4. Extend QMC simulations to dynamic quantities such as spectral function and dynamic structure factor. Ill-posed problem (analytical continuation);
   novel concepts: stochastic reconstruction [Filinov, Bonitz, PRA **86**, 043628 (2012)]

5. many additional applications:
   - 2D warm dense electron gas
   - ultra-high density matter (relativistic effects). Straightforward with CPIMC

Updates. Progress made in 2016-2017

Comparisons with previous models have been published in Refs. 1, 2 below

The open questions of the connection with the present finite T data to the ground state results has been solved and published in Ref. 3.

An analytical parametrization of *ab initio* data for the free energy of the uniform electron gas for the entire density-temperature-spin polarization range is now available at this link:

https://github.com/agbonitz/xc_functional

Additional *ab initio* thermodynamic data for the warm dense electron gas are being produced. In particular, results for the static density response are published in Refs. 4, 5

For further updates, check our web page:

http://www.itap.uni-kiel.de/theo-physik/bonitz/

[1] T. Dornheim *et al*., Physics of Plasmas **24**, 056303 (2017);
[2] S. Groth *et al.,* Contrib. Plasma Phys. **57**, 137-146 (2017);
[3] S. Groth *et al.*, Physical Review Letters **119**, 135001 (2017)
[4] T. Dornheim et al., Physical Review E **96**, 023203 (2017)
[5] S. Groth et al., J. Chem. Phys., in press (2017), arXiv:1708.03934