The Uniform Electron Gas at Warm Dense Matter Conditions

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in collaboration with Travis Sjostrom[2], Fionn D. Malone[3], and W.M.C. Foulkes[3]

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Introduction: warm dense matter

Warm dense matter (WDM):

- Nearly classical ions
- Degenerate non-ideal electrons
- Coupling parameter:

$$r_s = \frac{\bar{r}}{a_B} \sim 0.1 \ldots 10$$

- Degeneracy parameter:

$$\theta = k_B T / E_F \sim 0.1 \ldots 10$$

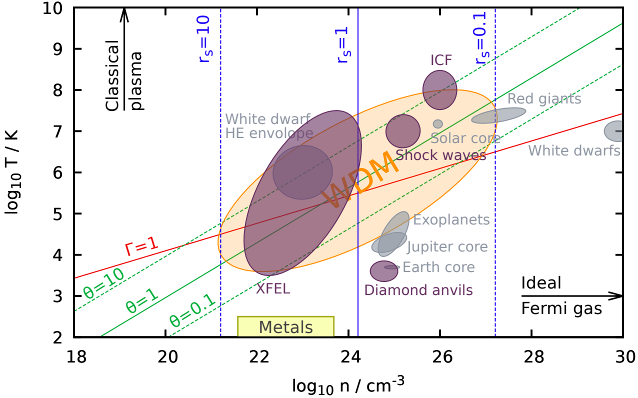

Figure: From T. Dornheim, S. Groth, and M. Bonitz, *Phys. Rep.* (2018), arXiv:1801.05783

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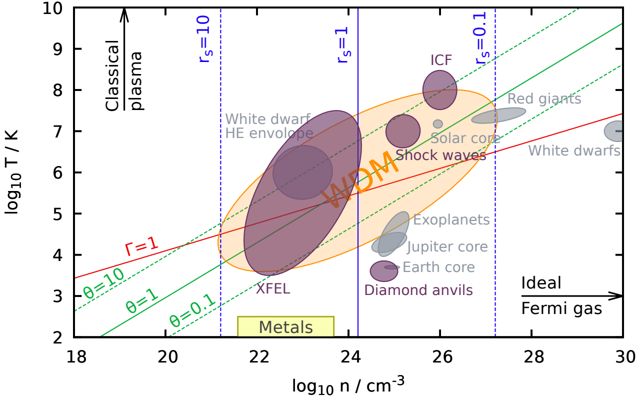
- Temperature, degeneracy and coupling effects equally important
  $\rightarrow$ No small parameters



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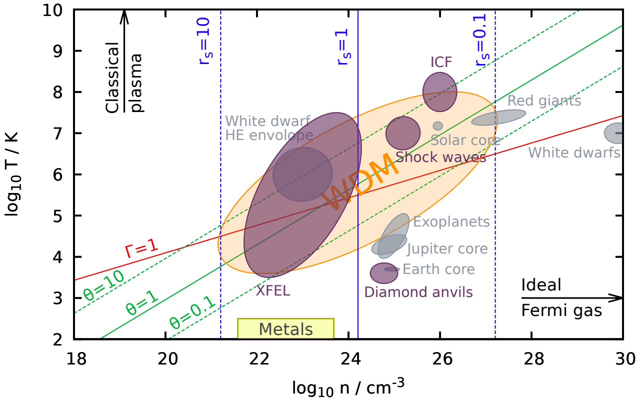

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Perturbation theory and ground-state approaches (DFT etc.) fail

The uniform electron gas - Coulomb interacting electrons in a uniform positive background

Ground state:

- Model description of metals
- **Input for density functional theory (DFT)**
- Accurate parametrization of XC-energy[1] for all r_s from ground state Monte Carlo data[2]
  $\rightarrow$ DFT simulations of real materials

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  $\rightarrow$ **Thermal DFT**[4]
  $\rightarrow$ **Requires finite-T XC-functional**[3]
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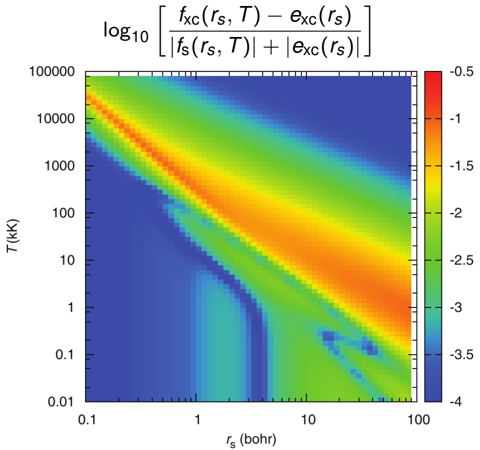

Figure: Relative importance of finite-T XC-functional[3] (diagonal corresponds to $\theta \sim 0.5$)

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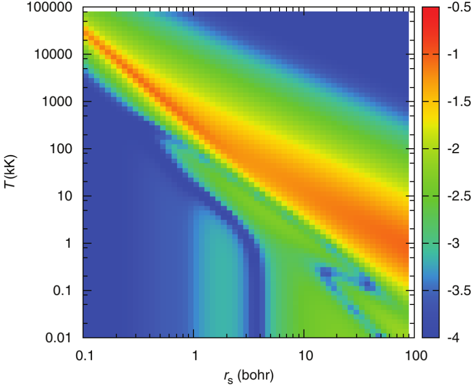
- Finite-T XC-functional directly incorporated into
  - **EOS models** of astrophysical objects[5]
  - **approximations in QHD**[6]

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



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Reliability of these approaches crucially depends on accurate parametrization of $f_{xc}(r_s, \theta)$

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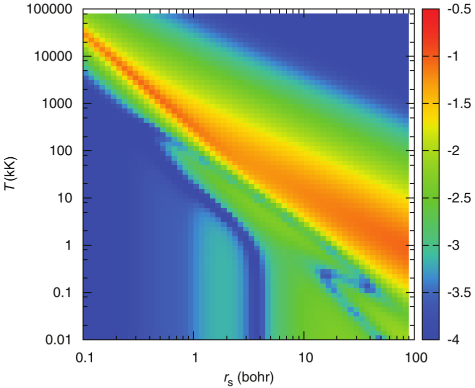

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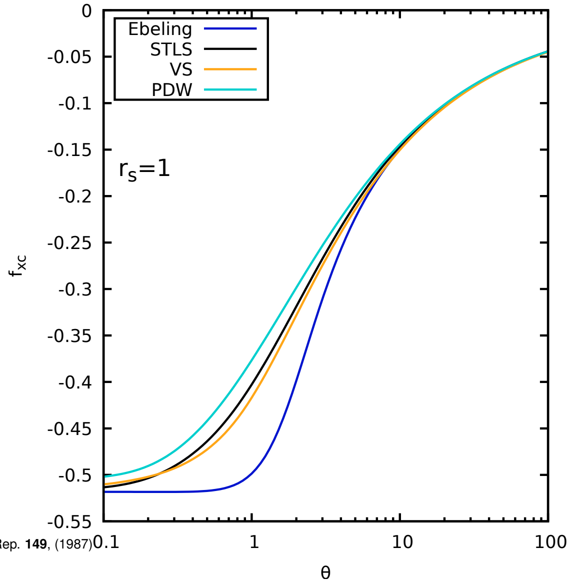
Many parametrizations for f_{xc} based on different approximate approaches:

- Semi-analytical approaches by **Ebeling**[1]
- Dielectric methods, e.g. Singwi-Tosi-Land-Sjölander[2] (**STLS**) and Vashista-Singwi[3] (**VS**)
- Quantum-classical mappings, e.g. Perrot and Dharma-wardana[4] (**PDW**)



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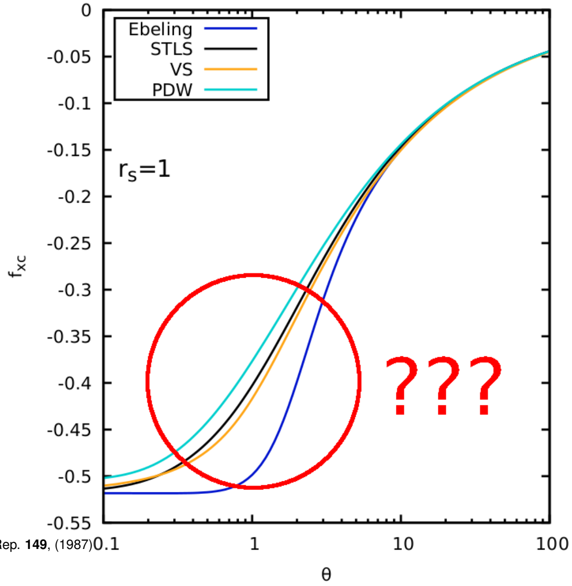

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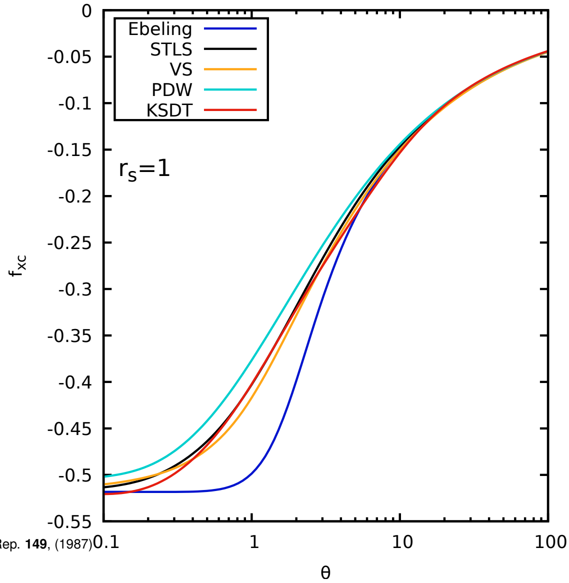
  But: RPIMC invokes *fixed node approximation* $\rightarrow$ induces **uncontrolled systematic errors**[7]



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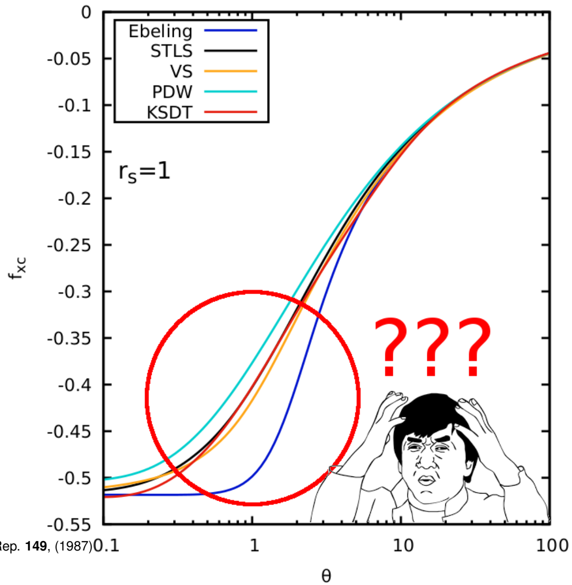

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***Ab initio* description of the warm dense UEG highly needed**

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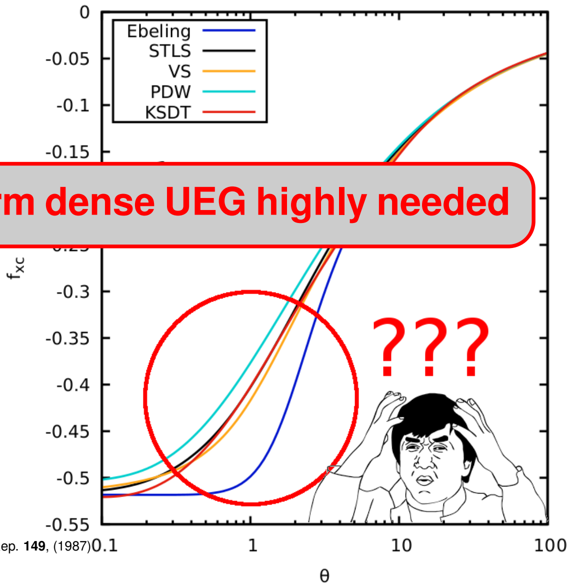

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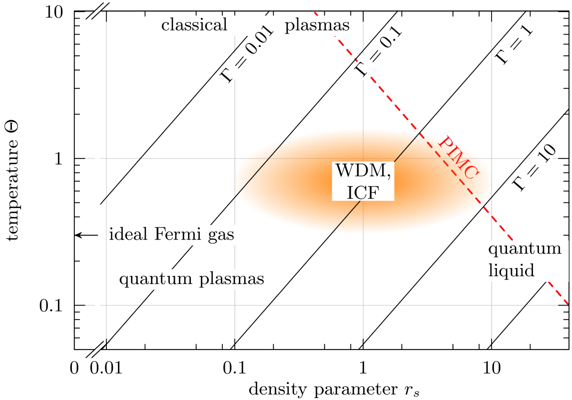

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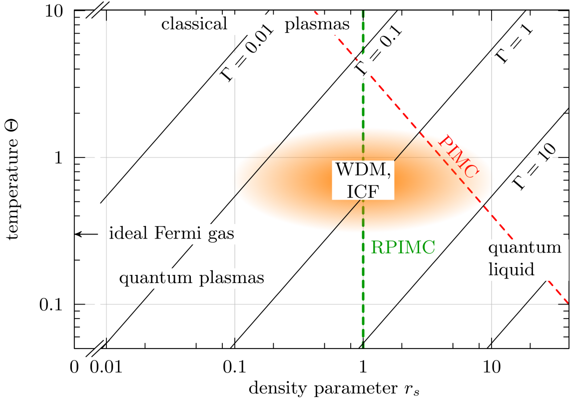

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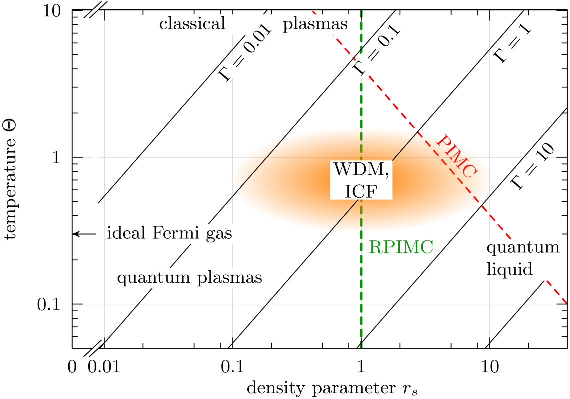
Avoid fermion sign problem by combining two novel exact and complementary QMC methods:



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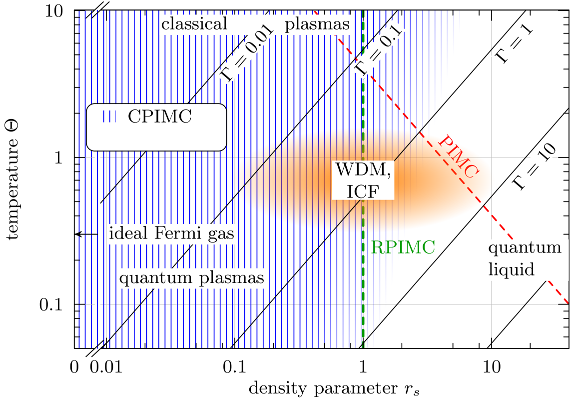
   → Excels at high density $r_s \lesssim 1$ and strong degeneracy



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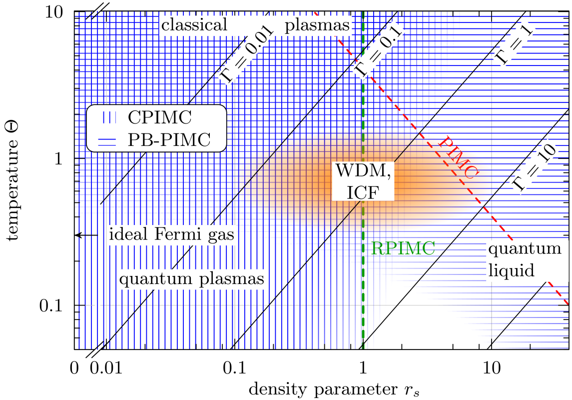

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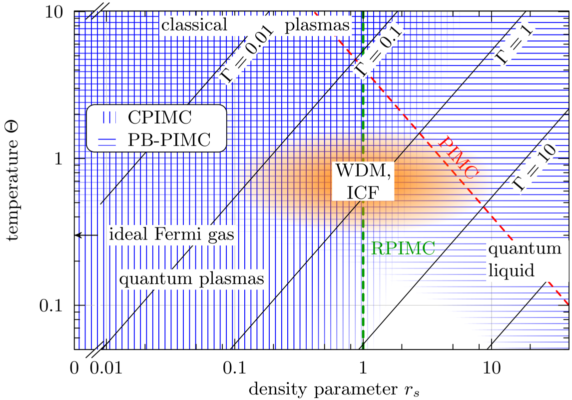

Exact *ab initio* simulations over broad range of parameters

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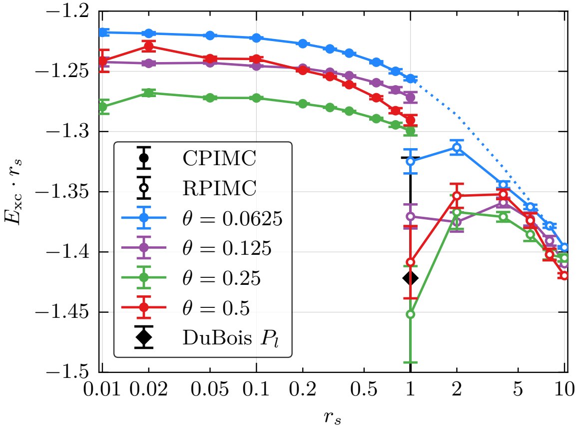
Exact exchange-correlation energy $E_{xc} = E - E_0$ (E_0 : ideal energy) ($N = 33$ spin-polarized electrons, $\theta \leq 0.5$, $r_s \leq 1$)

T. Schoof, S. Groth, J. Vorberger, and M. Bonitz, PRL **115**, 130402 (2015)



RPIMC: E.W. Brown *et al.*, PRL **110**, 146405 (2013) **DuBois:** ($\theta = 0.0625$) J.L. DuBois *et al.*, arXiv:1409.3262 (2014)

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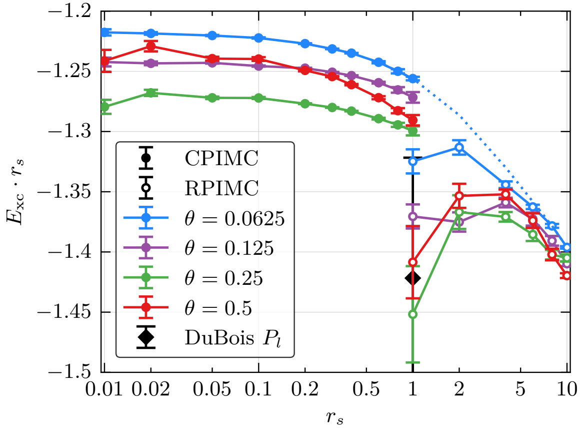

RPIMC carries systematic errors exceeding 10%

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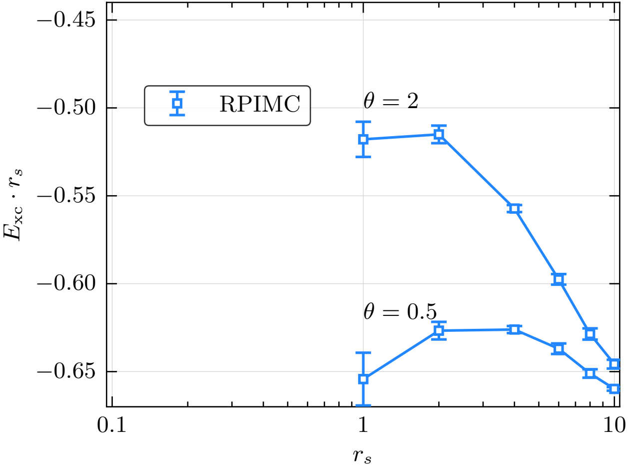

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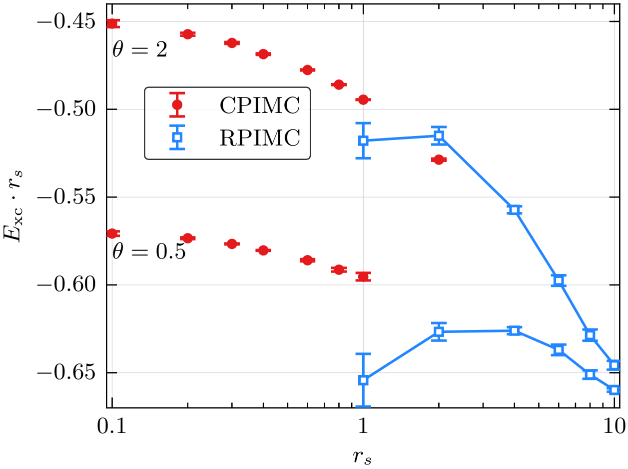
- **CPIMC** excels at high density



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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 $r_s \geq 1$
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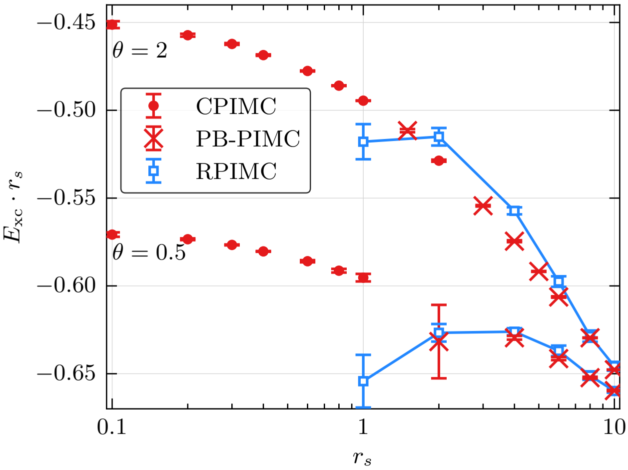

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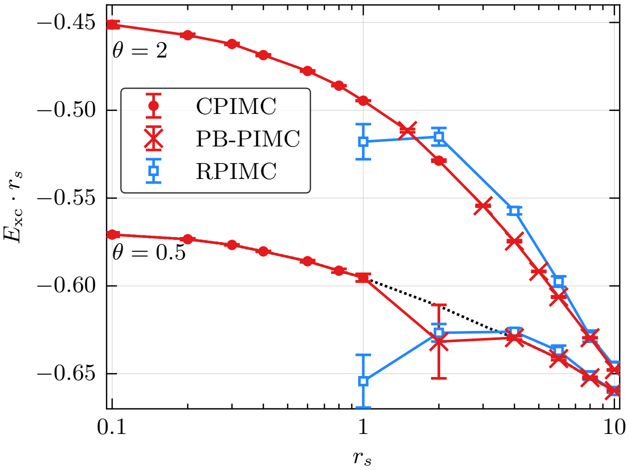

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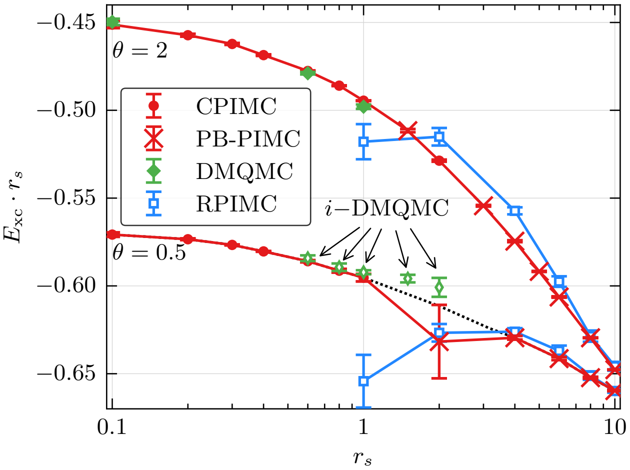

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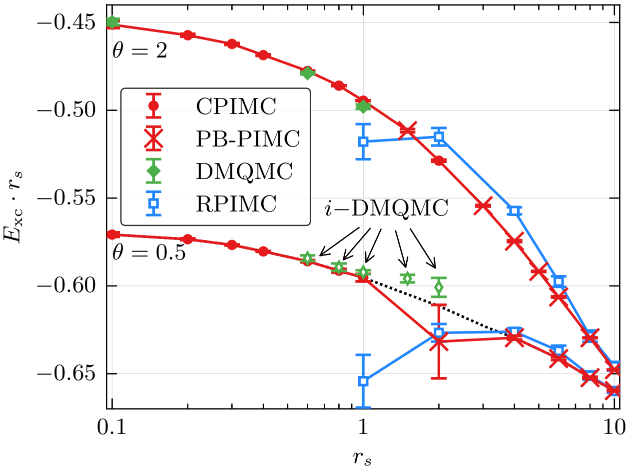
UEG well understood[4] for finite N

How to extend the simulations to the thermodynamic limit ($N \to \infty$) ???



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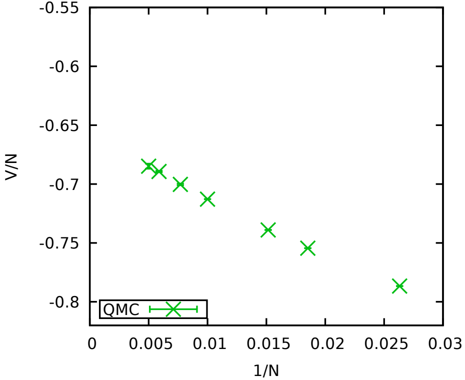
Extension of the QMC results to the TD limit[1]

- QMC results are afflicted with a finite-size error $\Delta V(N)$

$$\nu = \frac{V_N}{N} + \Delta V(N)$$



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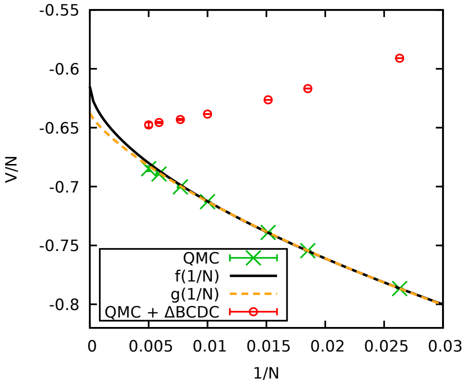

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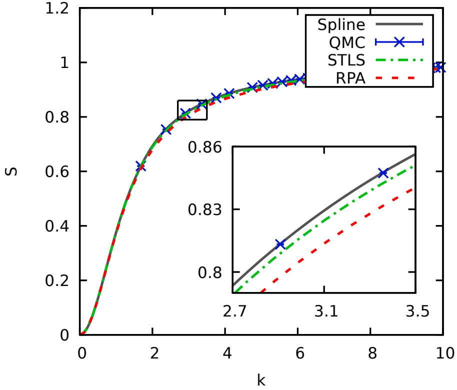

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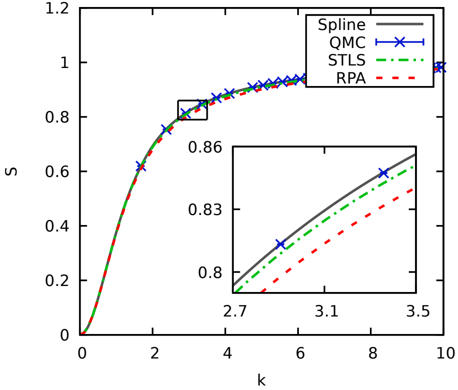
Accurate $S(k)$ over entire k-range in TDL

$$\nu = \frac{V_N}{N} + \Delta V(N)$$



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Improved finite-size correction for all WDM parameters!

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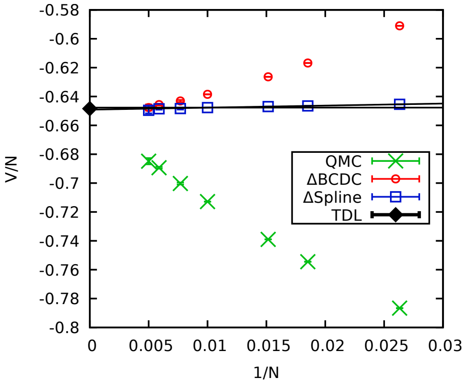

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- Exchange-correlation free energy f_{xc} linked to potential energy via

$$2 f_{\text{xc}}(r_s, \theta) + r_s \left. \frac{\partial f_{\text{xc}}(r_s, \theta)}{\partial r_s} \right|_\theta = v(r_s, \theta)$$

- Use suitable parametrization for f_{xc} and fit l.h.s. to r.h.s.

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Paramatrization of f_{xc} in the entire r_s-θ-plane

- Padé interpolation for r_s-θ−dependence[1,2]

$$f_{xc}(r_s,\theta) = -\frac{1}{r_s}\frac{a(\theta)+b(\theta)\sqrt{r_s}+c(\theta)r_s}{1+d(\theta)\sqrt{r_s}+e(\theta)r_s}$$

$$b(\theta) = \tanh\left(\frac{1}{\sqrt{\theta}}\right)\frac{b_1 + b_2\theta^2 + b_3\theta^4}{1+b_4\theta^2+b_5\theta^4}$$

$$c(\theta) = \left[c_1 + c_2 e^{-\frac{1}{\theta}}\right] e(\theta)$$

$$d(\theta) = \tanh\left(\frac{1}{\sqrt{\theta}}\right)\frac{d_1 + d_2\theta^2 + d_3\theta^4}{1+d_4\theta^2+d_5\theta^4}$$

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$$f_{xc}(r_s, \theta) = -\frac{1}{r_s} \frac{a(\theta) + b(\theta)\sqrt{r_s} + c(\theta) r_s}{1 + d(\theta)\sqrt{r_s} + e(\theta) r_s}$$

Build in known asymptotics:

- **High-density limit:**

$$\lim_{r_s \to 0} f_{xc}(r_s, \theta) = f_x^{HF} = -\frac{1}{r_s} a(\theta) \quad \text{[Known Hartree-Fock limit]}$$

- **High-T limit:**

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

Fulfilled by setting $b_5 = (3/2)^{1/2} \left(\frac{9\pi}{4}\right)^{1/3} b_3$

- **Low-T limit:**

$$\lim_{T \to 0} f_{xc}(r_s, \theta) = e_{xc}(r_s) = -\frac{1}{r_s} \frac{a_0^{HF} + b_1\sqrt{r_s} + c_1 e_1 r_s}{1 + d_1\sqrt{r_s} + e_1 r_s}$$

Fulfilled by fitting e_{xc} to $T = 0$ QMC data[3] (fixes b_1, c_1, e_1, d_1)

- **Remaining 13 parameters fitted to our exact finite-T QMC data**

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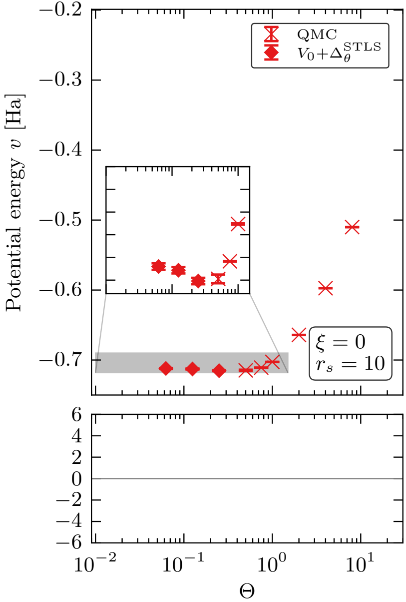
Construct finite-T XC-functional:

- Temperature-corrected ground state data smoothly connects to exact finite-T QMC data (over entire WDM regime)



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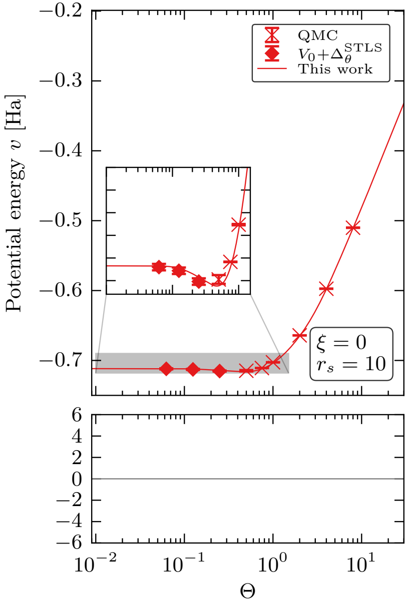

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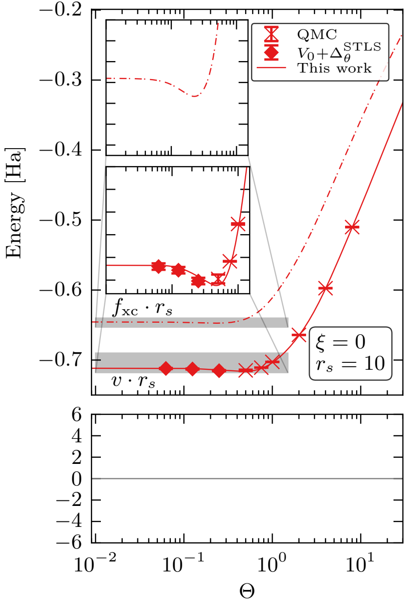

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S. Groth, T. Dornheim, T. Sjostrom, F.D. Malone, W.M.C. Foulkes, and M. Bonitz, *PRL* 119, 135001 (2017)

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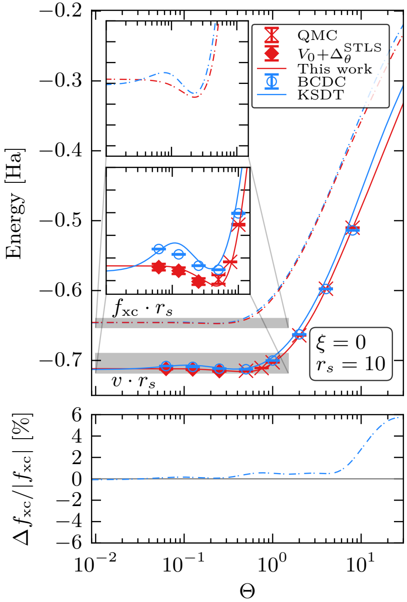
Comparison to other parametrizations (large r_s):

- **KSDT:**[1] small relative deviations but artificial bump at low T
  $\rightarrow$ Induces unphysical negative entropy[2]



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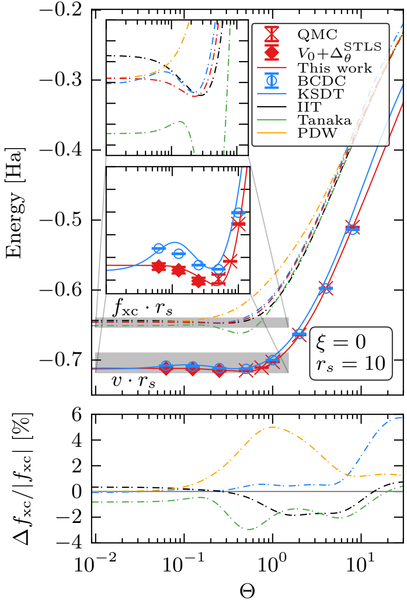
- **IIT**[3], **Tanaka**[4], **PDW**[5]: systematic errors of $\sim 2-6\%$



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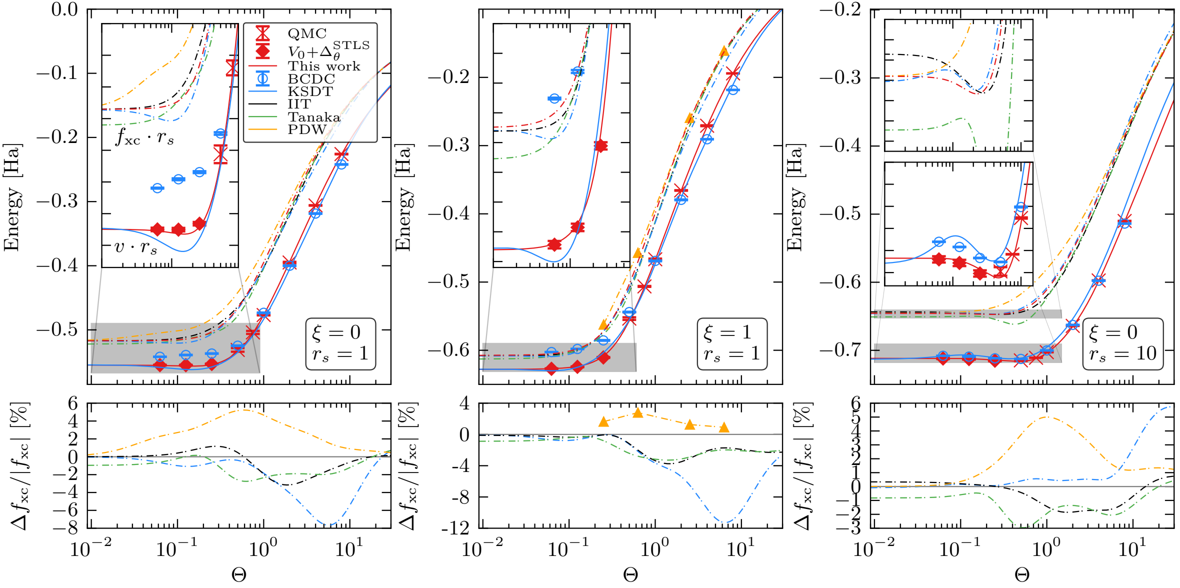

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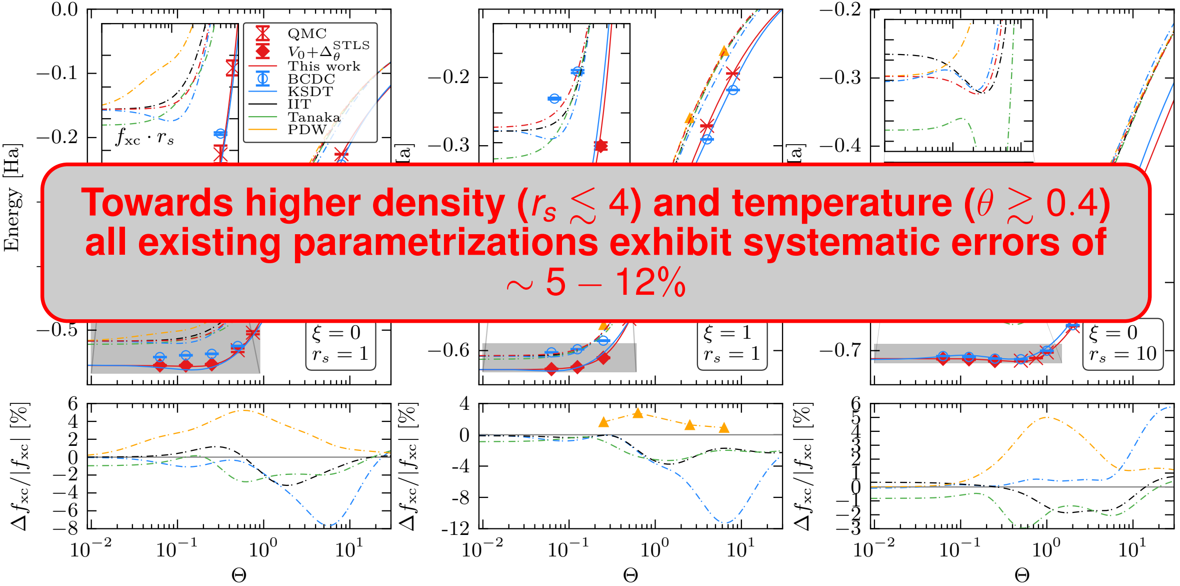

Towards higher density ($r_s \lesssim 4$) and temperature ($\theta \gtrsim 0.4$) all existing parametrizations exhibit systematic errors of $\sim 5-12\%$

XC-functional at arbitrary spin-polarization:

- DFT in local spin-density approximation requires $f_{\text{xc}}(r_s, \theta)$ at arbitrary $\xi = (N_\uparrow - N_\downarrow)/(N_\uparrow + N_\downarrow)$

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- Extensive new QMC data for $\xi = 0, 1/3, 0.6$, and 1

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XC-functional at arbitrary spin-polarization:

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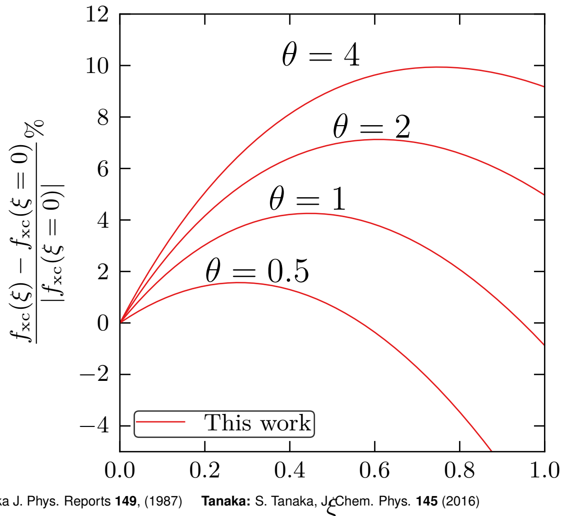
Relative spin-dependency of f_{xc} at $r_s = 1$



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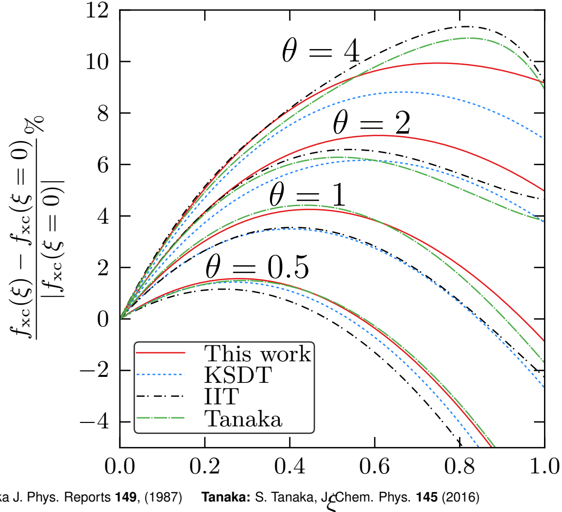

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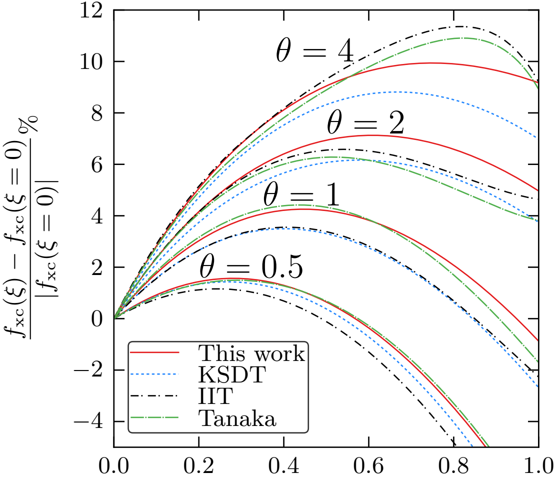

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- **First benchmarks of previous parametrizations**[7]
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  - Unsatisfactory description of spin-dependency

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Concluding remarks:

- Use our new f_{xc}-functional as input for
  - DFT calculations
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  - Equation of state models of astrophysical objects
- Functional available online (C++, Fortran, Python) at https://github.com/agbonitz/xc_functional
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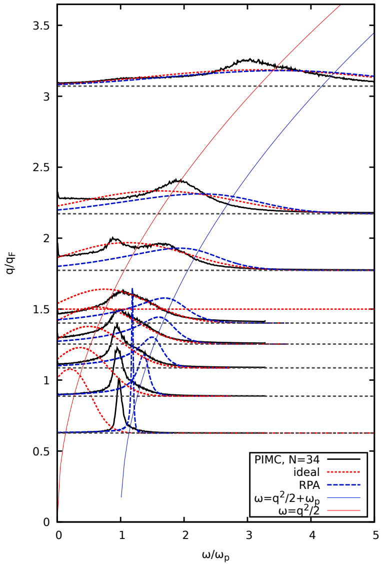
Outlook:

- *inhomogeneous* UEG
  $\rightarrow$ Access to static local field correction
- *ab initio* results for imaginary-time correlation functions
  $\rightarrow$ Reconstruction of dynamic structure factor $S(\mathbf{q},\omega)$[1]

$S(\mathbf{q},\omega)$ for $\theta = 1$, $r_s = 10$



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Thank you for your attention!