Ab Initio Quantum Monte Carlo Simulation of Warm Dense Electrons

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Christian-Albrechts-Universität zu Kiel

38th International Workshop on High Energy Density Physics with Intense Ion and Laser Beams

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- **Warm dense matter**: $r_s = \bar{r}/a_\mathrm{B} \sim 1$, $\theta = k_\mathrm{B}T/E_\mathrm{F} \sim 1 \Rightarrow$ nontrivial interplay of coupling, temperature and quantum degeneracy effects
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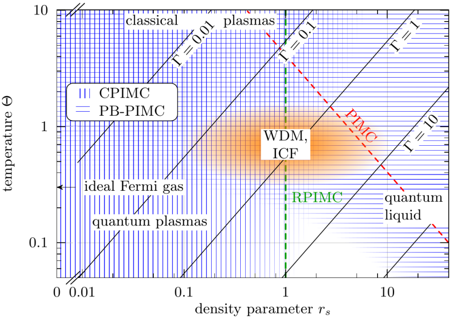

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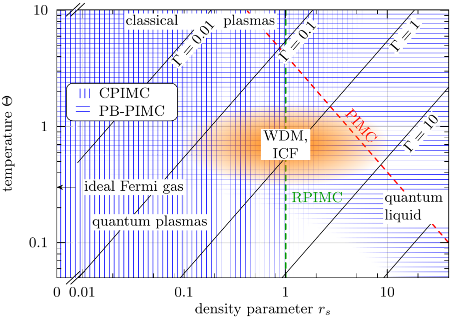
- **Our solution:** Combination of two complementary QMC methods
  $\rightarrow$ **Permutation Blocking PIMC (PB-PIMC)**
  $\rightarrow$ **Configuration PIMC (CPIMC)**



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   → The Fermion Sign Problem
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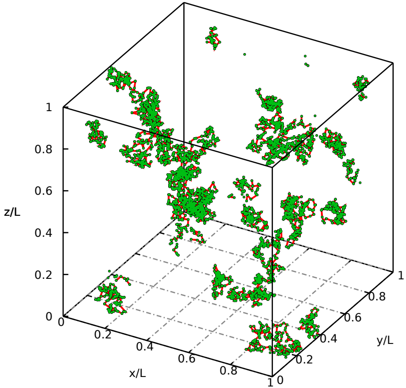

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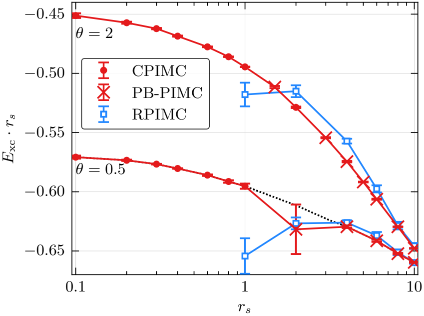

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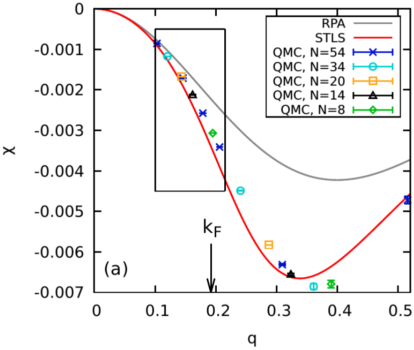

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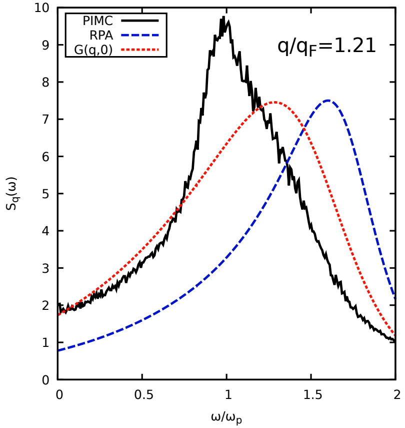
4. **Reconstruction of the Dynamic Structure Factor $S(\mathbf{q}, \omega)$ from QMC data**



Theory of PIMC[8]

- Canonical partition function for N spin-polarized fermions in coordinate space, $\beta = 1/k_\mathrm{B}T$ and $\mathbf{R} = \{\mathbf{r}_1, \ldots, \mathbf{r}_N\}$

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

- Express the density matrix as a path over P sets of particle coordinates at P times higher temperature

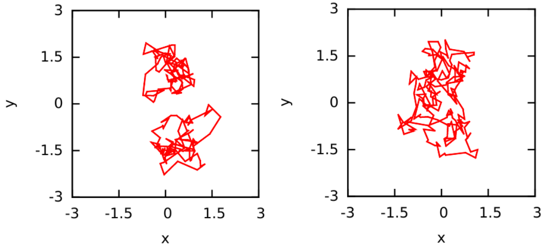
$$Z = \frac{1}{N!} \sum_{\sigma \in S_N} \mathrm{sgn}(\sigma) \int \mathrm{d}\mathbf{X} \ \langle \mathbf{R}_0 | \, e^{-\epsilon \hat{H}} \, | \mathbf{R}_1 \rangle \ldots \langle \mathbf{R}_{P-1} | \, e^{-\epsilon \hat{H}} \, | \hat{\pi}_\sigma \mathbf{R}_0 \rangle$$

- Primitive factorization $e^{-\epsilon \hat{H}} \approx e^{-\epsilon \hat{K}} e^{-\epsilon \hat{V}}$, $\epsilon = \beta / P$, with the commutator error $\mathcal{O}(\epsilon^2)$
- The partition function is the sum over all closed paths $\mathbf{X} = \{\mathbf{R}_0, \ldots, \mathbf{R}_{P-1}\}$ in imaginary time, with P “time slices”

$$Z = \sum_{\mathbf{X}} W(\mathbf{X}) \quad , \quad W(\mathbf{X}) \text{: configuration weight of path } \mathbf{X}$$

[8] D. Ceperley, Rev. Mod. Phys. **67**, 279 (1995)

Fermion Sign Problem of PIMC



- Sample all permutations/ exchange cycles
- For every exchange, the sign of $W(\mathbf{X})$ changes
- $W(\mathbf{X})$ cannot be interpreted as a probability distribution

$\Rightarrow$ Calculate fermionic observables using the **Metropolis algorithm**[9] via

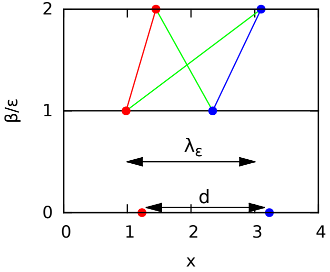
$$\langle O \rangle_{\mathrm{f}} = \frac{\langle OS \rangle'}{\langle S \rangle'} \,, \quad Z' = \int \mathrm{d}\mathbf{X}\, |W(\mathbf{X})| \,, \quad \langle S \rangle' = \frac{1}{Z'} \int \mathrm{d}\mathbf{X}\, |W(\mathbf{X})| \mathrm{sign}(\mathbf{X}) = e^{-\beta N (f - f')}$$

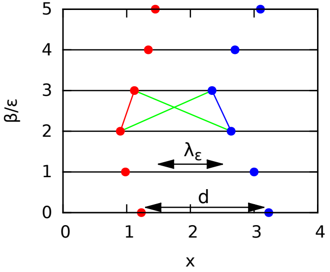
$\Rightarrow$ The statistical error increases exponentially with N and β

$$\Delta O \propto \frac{1}{\langle S \rangle'} \propto e^{\beta N (f - f')}$$

[9] N. Metropolis *et al.*, J. Chem. Phys. **21**, 1087 (1953)

Idea of Permutation Blocking PIMC[12]





- **Blocking**: Combine positive with negative terms to perform the cancellation (at least partly) analytically
- Use antisymmetric propagators (determinants)[10,11] to combine positive and negative permutations into a single configuration weight
  $\Rightarrow$ permutation blocking
- With increasing number of propagators P, the effect of the blocking decreases
  $\Rightarrow$ Use higher order factorization of $e^{-\epsilon\hat{H}}$

[10] M. Takahashi and M. Imada, J. Phys. Soc. Jpn. **53**, 963-974 (1984)
[11] A.P. Lyubartsev, J. Phys. A: Math. Gen. **38**, 6659 (2005)
[12] T. Dornheim *et al.*, New J. Phys. **17**, 073017 (2015)

Configuration PIMC

- **Basic idea:**[13,14] Use antisymmetric states (i.e., Slater determinants)

$$\langle O \rangle_f = \mathrm{Tr}\left(\hat{O}\hat{\rho}^-\right) = \mathrm{Tr}^-\left(\hat{O}\hat{\rho}\right)$$

- Hamiltonian (arbitrary one particle basis $\{|i\rangle\}$)

$$\hat{H} = \sum_{i,j} h_{ij}\hat{a}_i^\dagger \hat{a}_j + \sum_{i<j,k<l} w_{ijkl}^- \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k$$

- Split Hamiltonian into diagonal and off-diagonal part:[15] $\hat{H} = \hat{D} + \hat{Y}$
- Switch to interaction picture in imaginary time with respect to $\hat{D}$

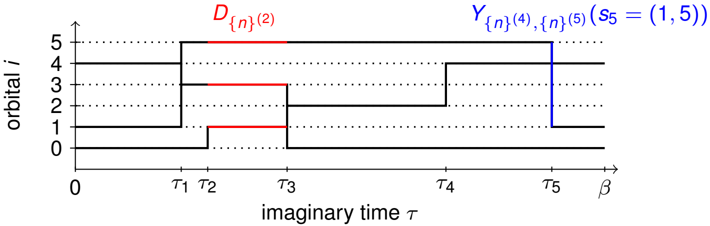
$$e^{-\beta\hat{H}} = e^{-\beta\hat{D}}\hat{T}_\tau e^{-\int_0^\beta \hat{Y}(\tau)\mathrm{d}\tau} \quad \text{with} \quad \hat{Y}(\tau) = e^{\tau\hat{D}}\hat{Y}e^{-\tau\hat{D}}, \quad \tau \in (0,\beta)$$

13 T. Schoof *et al.*, Contrib. Plasma Phys. **51**, 687-697 (2011)
14 T. Schoof *et al.*, Phys. Rev. Lett. **115**, 130402 (2015)
15 N.V. Prokof'ev, B.V. Svistunov and I.S. Tupitsyn, JETP Lett., **64**, 911 (1996)

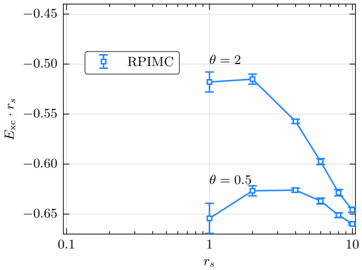
CPIMC - Partition function

$$Z_{\mathrm{CP}} = \sum_{\substack{K=0\\K\neq 1}}^{\infty} \sum_{\{n\}} \sum_{s_1} \cdots \sum_{s_{K-1}} \int_0^\beta \mathrm{d}\tau_1 \int_{\tau_1}^\beta \mathrm{d}\tau_2 \ldots \int_{\tau_{K-1}}^\beta \mathrm{d}\tau_K$$
$$(-1)^K \exp\left\{ -\sum_{i=0}^{K} D_{\{n^{(i)}\}}(\tau_{i+1}-\tau_i) \right\} \prod_{i=1}^{K} Y_{\{n^{(i-1)}\},\{n^{(i)}\}}(s_i) = \sum_{c_{\mathrm{CP}}} W(c_{\mathrm{CP}})$$

$\Rightarrow$ Generate all closed paths $c_{\mathrm{CP}} = \left\{(K), \{n\}, \tau_1, \ldots, \tau_K, s_1, \ldots, s_{K-1}\right\}$ acc. to the configuration weight $W(c_{\mathrm{CP}})$



- Density dependence of $N = 33$ spin-polarized electrons[16]
- Exchange-correlation (XC) energy: $E_{xc} = E - E_0$ (E_0: non-interacting UEG)



- **RPIMC**[17] simulations are limited to $r_s \geq 1$

[16] T. Dornheim *et al.*, arXiv 1611.02658 (submitted to Phys. Plasmas), [17] E.W. Brown *et al.*, Phys. Rev. Lett. **110**, 146405 (2013)
[18] S. Groth *et al.*, Phys. Rev. B **93**, 085102 (2016), [19] T. Dornheim *et al.*, J. Chem. Phys. **143**, 204101 (2015)
[20] F.D. Malone *et al.*, J. Chem. Phys. **143**, 044116 (2015), [21] F.D. Malone *et al.*, Phys. Rev. Lett. **117**, 115701 (2016)

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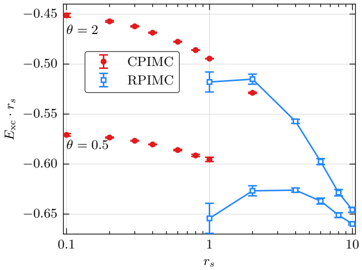

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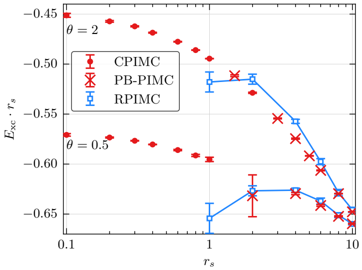

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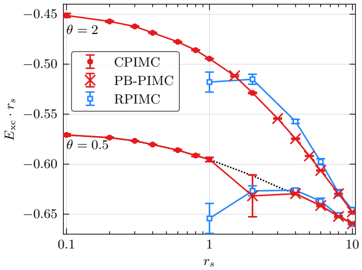

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Combination of **PB-PIMC** and **CPIMC** allows for accurate results over broad parameter range[18,19]

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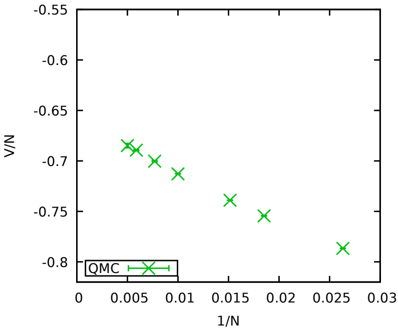

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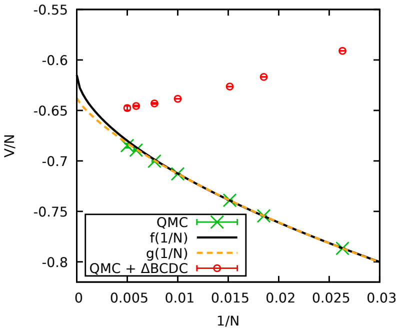

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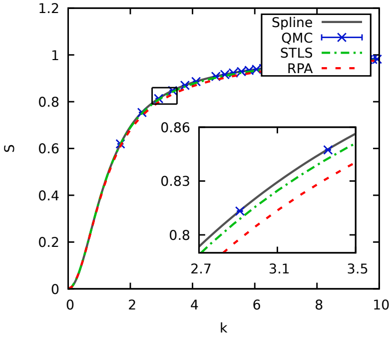

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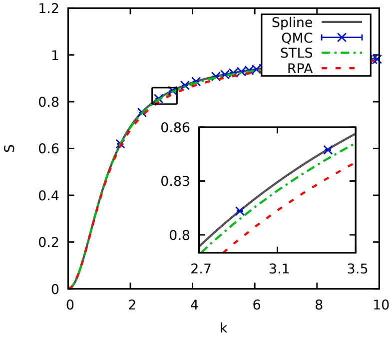
Accurate $S(k)$ over entire k-range in TDL



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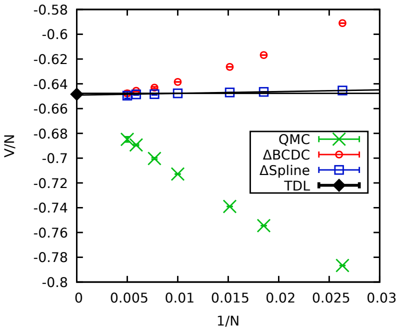
Improved finite-size correction for all WDM parameters!

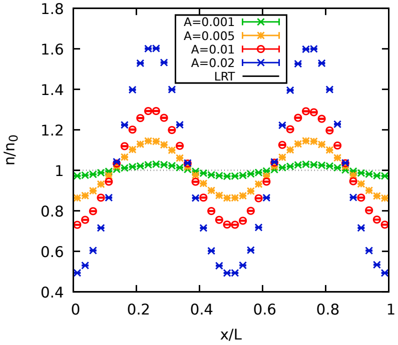


- Unprecedented accuracy, $\Delta V/V \sim 0.3\%$ $\rightarrow$ Input for parametrization of $f_{xc}(r_s, \theta, \xi)$ [PRL **119**, 135001 (2017)]

$\rightarrow$ **See poster by S. Groth**

The inhomogeneous electron gas: $\hat{H} = \hat{H}_0 + 2A\sum_k \cos(\mathbf{q}\cdot\mathbf{r}_k)$

- **Basic idea:** Apply small external harmonic perturbation of wave vector **q**, amplitude A



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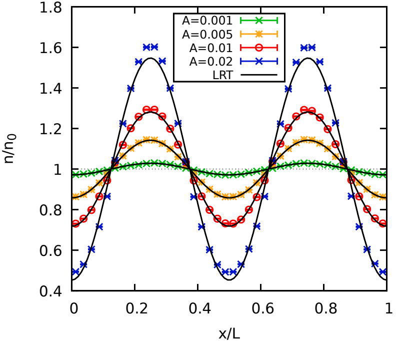

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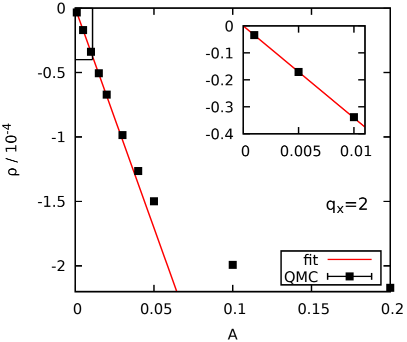
$$\rho_{\text{ind}}(\mathbf{q}) = \frac{1}{V}\left\langle \sum_{k=1}^{N} e^{-i\mathbf{q}\cdot\mathbf{r}_k} \right\rangle_A = \chi(\mathbf{q})A \quad ,$$

with the density–density response function $\chi(\mathbf{q})$



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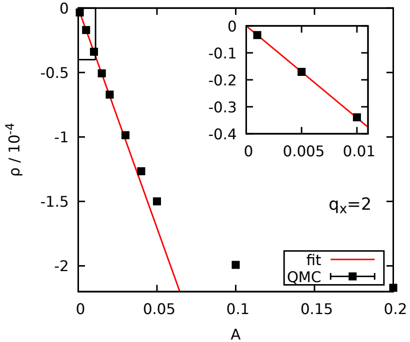
QMC simulations for multiple *A*-values for each wave vector q allows us to obtain $\chi(\mathbf{q})$.



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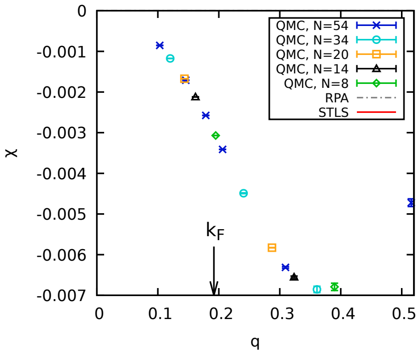
Results: Electron Gas at $r_s = 10$, $\theta = 1$ [PRE 96, 023203 (2017)]



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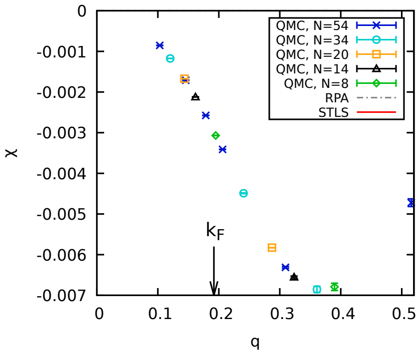

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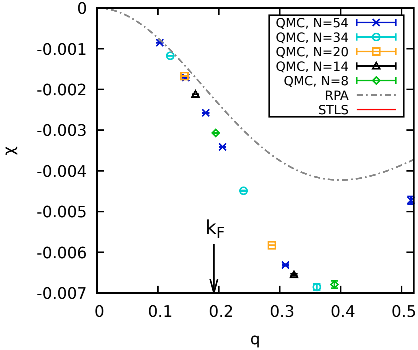

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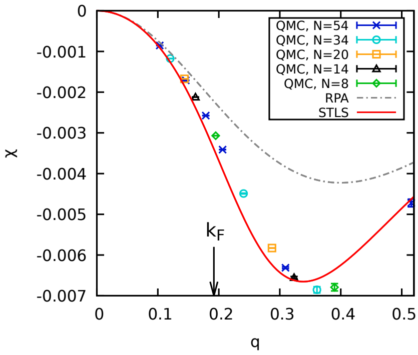

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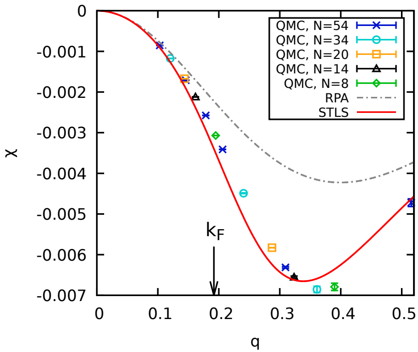

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Ab initio **QMC results for the static density response of the warm dense UEG possible!**

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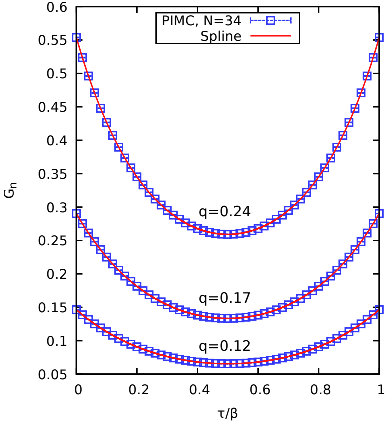
preliminary, unpublished
($r_s = 10, \theta = 1$)



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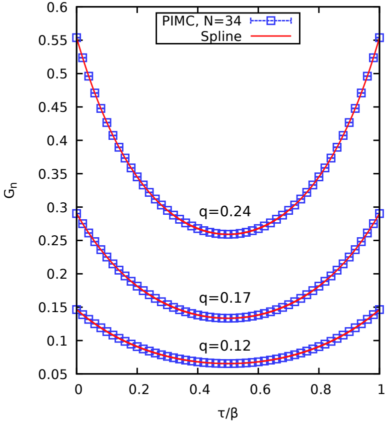

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We need to perform an inverse Laplace transform

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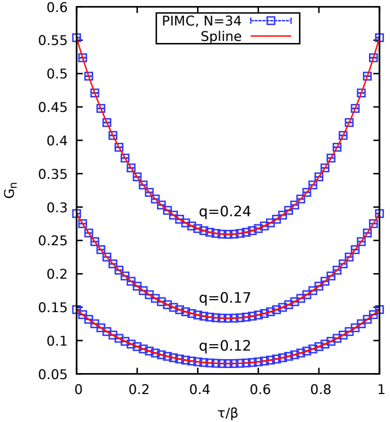

QMC Results for the Dynamic Structure Factor

- **Reconstruction:** Find a model function $S_\mathrm{M}(\mathbf{q},\omega)$ which reproduces the QMC data for $G_n(\mathbf{q},\tau)$

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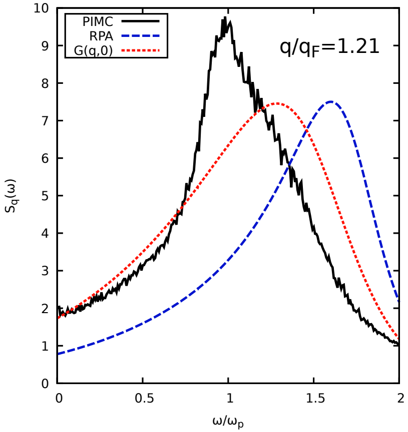

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Ab initio QMC results for $S(\mathbf{q}, \omega)$ possible for some parameters!

preliminary, unpublished
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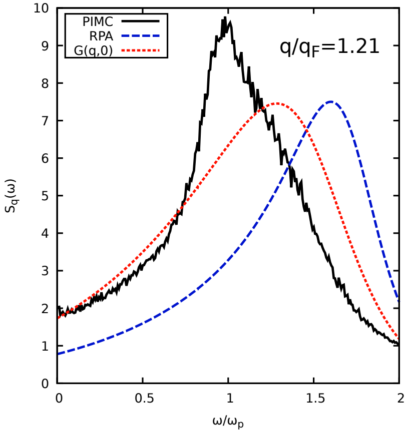

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Summary and outlook

- QMC simulations of WDM are severely hampered by the **fermion sign problem**
- Solution: Combine the complementary **CPIMC** and **PB-PIMC** approaches

$\rightarrow$ New FSC allows for accurate results of the warm dense UEG in the TDL with $\Delta V/V \sim 10^{-3}$ $\Rightarrow$ Parametrization of $f_{\mathbf{xc}}(r_s, \theta, \xi)$

- Simulation of the inhomogeneous electron gas

***Ab initio* results for static density response $\chi(\mathbf{q})$, $G(\mathbf{q})$ of warm dense UEG**

- QMC allows to compute imaginary-time correlation functions

Reconstruction of the dynamic structure factor $S(\mathbf{q}, \omega)$ possible!

New Review: arXiv:1801.05783 (2018)