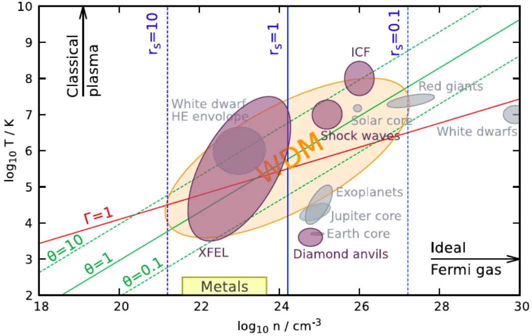
The Theory of Configuration Path Integral Monte Carlo

Kai Hunger

January 29, 2019

- Warm Dense Matter



Applications for calculations of the WDM state[1]

in a.u.: $r_s^3 = 3/(4\pi n)$, $\Theta = (k_B T/E_F)$, $\Gamma = (r_s k_B T)^{-1}$

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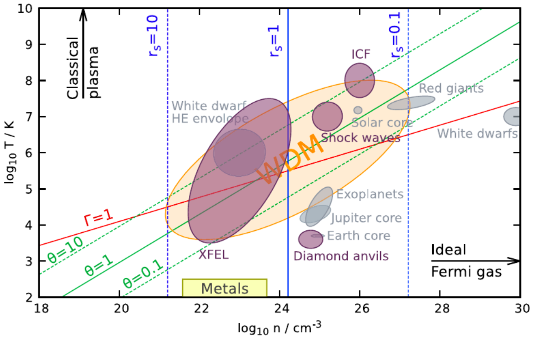
Motivation

- Warm Dense Matter
  - no exact large-scale ab initio approach
  - no "small" parameter allowing approximation
    - to interaction strength ($r_s \to 0, r_s \to \infty$)
    - by ground state ($\Theta \to 0$)
    - by classical methods ($\Gamma \to 0$)



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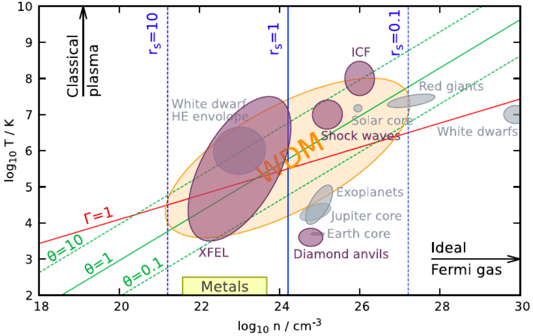

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[2]D. M. Ceperley, Rev. Mod. Phys. **67**, 279-355 (1995)

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  - CPIMC: Complementary behavior of FSP with r_s → no FSP at high densities

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Outline

Main Literature:

- S. Groth. *Strongly degenerate nonideal fermi systems: Configuration path integral monte carlo simulation.* Master's thesis, ITAP, CAU, 2014.
- T. Schoof. *Configuration Path Integral Monte Carlo: Ab initio simulations of fermions in the warm dense matter regime.* PhD thesis, ITAP, CAU, 2016.

Many-Particle System characterized by Canonical Ensemble[1] (N, β, V):

$$\hat{\rho} = \frac{1}{Z}\mathrm{e}^{-\beta \hat{H}}, \qquad Z = \mathrm{Tr}\,\mathrm{e}^{-\beta \hat{H}}$$

[1] N: number of particles, $T = 1/(k_\mathrm{B}\beta)$: temperature, V: volume

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Expectation Values of operator $\hat{O}$:

- from density operator:

$$\langle\hat{O}\rangle = \mathrm{Tr}\,\hat{\rho}\hat{O} = \frac{1}{Z}\,\mathrm{Tr}\,\hat{O}\mathrm{e}^{-\beta\hat{H}}$$

- from thermodynamic relations:

$$\langle\hat{H}\rangle = -\frac{\partial}{\partial\beta}\log(Z), \quad F = -T\log(Z),$$

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Time evolution operator:

$$\hat{U}(t := t_2 - t_1) = \mathrm{e}^{-\mathrm{i}\hat{H}t}$$
$$\Rightarrow \hat{\rho} = \hat{U}(-\mathrm{i}\beta)$$
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understand inverse temperature
as imaginary time
$\beta \leftrightarrow \tau := \mathrm{i}t$

[1] N: number of particles, $T = 1/(k_B\beta)$: temperature, V: volume

high temperature decomposition: $\tau \coloneqq (\beta/M)$

$$\hat{U}(-\mathrm{i}\beta) = \mathrm{e}^{-\beta\hat{H}} = \left[\mathrm{e}^{-\frac{\beta}{M}\hat{H}}\right]^{M} = \left[\hat{U}(-\mathrm{i}\tau)\right]^{M}$$

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- Tr with CONS[1] $|X\rangle = |x_1\rangle \ldots |x_N\rangle$

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$$\begin{aligned} Z = \mathrm{Tr}\,\hat{U}(-\mathrm{i}\beta, 0) &= \int \mathrm{d}X_1 \,\langle X_1|\hat{U}(-\mathrm{i}\tau)\hat{U}(-\mathrm{i}\tau)\dots\hat{U}(-\mathrm{i}\tau)|X_1\rangle \\ &= \underbrace{\int \mathrm{d}X_1 \int \mathrm{d}X_2 \dots \int \mathrm{d}X_M}_{\coloneqq\int_C} \underbrace{\langle X_1|\hat{U}(-\mathrm{i}\tau)|X_2\rangle \dots \langle X_M|\hat{U}(-\mathrm{i}\tau)|X_1\rangle}_{\coloneqq W(C)} \end{aligned}$$

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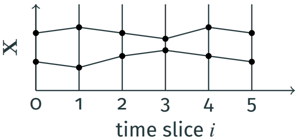
→ Interpretation:
Paths $C = (X, X_1, \dots, X_{M-1}, \tau_0, \tau_1, \dots, \tau_{M-1})$
Expectation Values: $\langle\hat{O}\rangle = \int_C O(C)W(C)$



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WHY USE
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DECOMPOSITION
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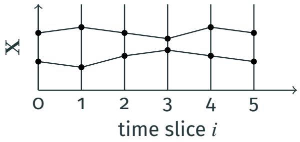

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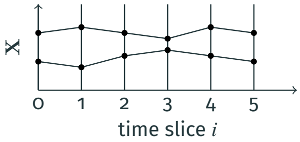

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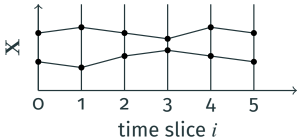
→ Use Monte Carlo Scheme to evaluate multidim. Integral



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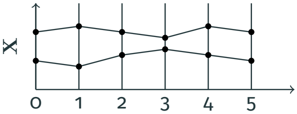
→ Sample Paths C using Metropolis-Hastings Algorithm



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[2]Landau, Binder. A Guide to Monte Carlo Simulations in Statistical Physics. Cambr. Univ. Press, 2000.

Introduction to PIMC — Metropolis Monte Carlo

Goal: Compute Expectation Values

$$\langle \hat{O} \rangle = \frac{1}{Z} \sum\!\!\!\!\!\!\int_C \underbrace{O(C)}_{\text{estimator}} \underbrace{W(C)}_{\text{weight}}$$

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- Approximate Expectation Value by

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  1. Start with initial Configuration C_0
  2. MC-Steps:

     for $1 \leq i \leq N_{\mathrm{MC}}$ **do**
     Propose C_i' with probability $Q(C_i \to C_i')$
     Accept $C_{i+1} \leftarrow C_i'$ with probability $A(C_i \to C_i')$
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  3. obtain *Markov-chain* $(C_0, C_1, \ldots, C_{N_{\mathrm{MC}}})$

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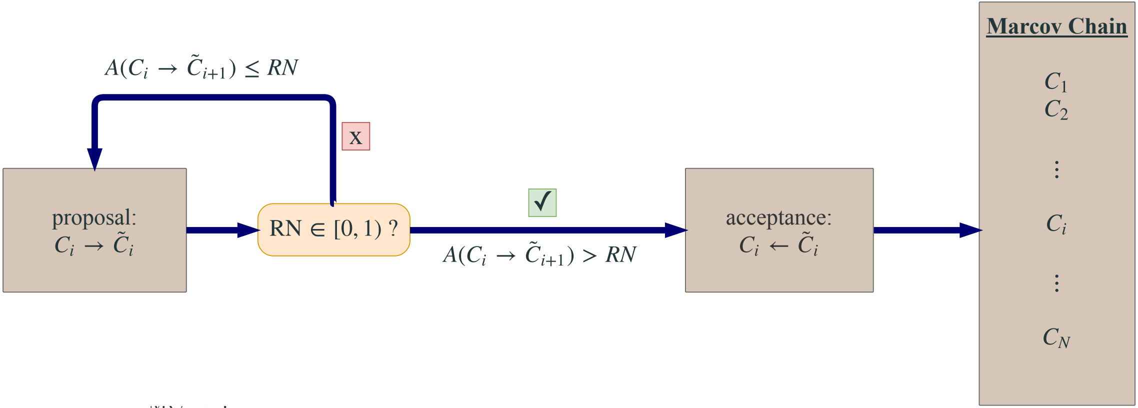

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- Approximate Expectation Value by

$$\langle \hat{O} \rangle = \frac{1}{N_{\mathrm{MC}}} \sum_{i=1}^{N_{\mathrm{MC}}} O(C_i) + \mathcal{O}(1/\sqrt{N_{\mathrm{MC}}})$$

- Metropolis-Hastings Algorithm:
  1. Start with initial Configuration C_0
  2. MC-Steps:

     for $1 \leq i \leq N_{\mathrm{MC}}$ **do**
     Propose C_i' with probability $Q(C_i \to C_i')$
     Accept $C_{i+1} \leftarrow C_i'$ with probability $A(C_i \to C_i')$
     end for
  3. obtain *Markov-chain* $(C_0, C_1, \dots, C_{N_{\mathrm{MC}}})$
- Conditions:
  - Detailed Balance:

$$A(C_i \to C_i') = \min\left[1, \frac{Q(C_i' \to C_i) W(C_i')}{Q(C_i \to C_i') W(C_i)}\right]$$

  - Ergodic MC Steps $C_i \to C_i'$

T. Müller-Gronbach, E. Novak, and K. Ritter. Monte Carlo-Algorithmen. Springer-Lehrbuch. Springer, Berlin, 2012.

Introduction to PIMC — Sign Problem

Fermions $\longrightarrow$ Antisymmetrize Productstates $|X\rangle = |x_1\rangle\,|x_2\rangle \ldots |x_N\rangle$

$$Z = \int \mathrm{d}X \int \mathrm{d}X_1 \ldots \int \mathrm{d}X_{M-1}\, \langle X|\hat{U}(-\mathrm{i}\tau)|X_1\rangle \ldots \langle X_{M-1}|\hat{U}(-\mathrm{i}\tau)|X\rangle$$

Schwabl. Quantenmechanik für Fortgeschrittene . Springer-Lehrbuch, Berlin, 2008. p.9
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Fermions $\longrightarrow$ Antisymmetrize Productstates $|X\rangle = \hat{S}_- |x_1\rangle |x_2\rangle \dots |x_N\rangle$

Antisymmetrization Operator:

$$\hat{S}_- := (1/\sqrt{N!}) \sum_{\pi \in S_N} (-1)^{\mathrm{sgn}(\pi)} \hat{\pi}, \quad [\hat{H}, \hat{S}_-] = 0, \quad \hat{S}_-^2 = \hat{S}_-$$

$$\Rightarrow Z = \sum_{\pi \in S_N} \int \mathrm{d}X \int \mathrm{d}X_1 \dots \int \mathrm{d}X_{M-1} \frac{1}{\sqrt{N!}} (-1)^{\mathrm{sgn}(\pi)} \langle X | \hat{U}(-\mathrm{i}\tau) | X_1 \rangle \dots \langle X_{M-1} | \hat{U}(-\mathrm{i}\tau) | \hat{\pi} X \rangle$$

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Sign-Conversion $\Rightarrow$ negative weight function W

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Solution: $W \to |W|$ and incorporate sign $\hat{s} = \mathrm{sgn}(W(C))$ in estimator:

$$\langle \hat{O} \rangle = \frac{\langle \hat{O}\hat{s} \rangle}{\langle \hat{s} \rangle}$$

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$(-1)^{\mathrm{sgn}(\pi)}$ $\Rightarrow$ cancellation in $\langle \hat{O}\hat{s} \rangle$ and $\langle \hat{s} \rangle$ $\longrightarrow$ Fermion Sign Problem: $\Delta \approx N_{\mathrm{MC}}^{-1/2} \mathrm{e}^{\beta N \Delta f}$

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2nd Quantization Fock-States already include correct particle statistics !

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CPIMC Formalism — 2nd Quantization

Fock states $|\{n^{()}\}\rangle$ defined by ONV[1] $\{n^{()}\} = \{\, n_i = 0, 1 \mid i \in \mathbb{N} \,\} = \{\, n_1, n_2, n_3, \dots \}$

[1]occupation number vector

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- One-particle excitation: $\{n^{()}\}^{p}_{q}$
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Calculating Matrix elements in ONV representation:

- one-particle operators

$$\hat{B}^{(1)} = \sum_{ij} b_{ij} \hat{a}^\dagger_i \hat{a}_j, \quad b_{ij} = \langle i|\hat{b}|j\rangle = \int !\mathrm{d}x \; \phi^*_i(x) b(x) \phi_j(x)$$

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- Two-particle excitation: $\{n^{()}\}_{r<s}^{p<q}$

Calculating Matrix elements in ONV representation:

- one-particle operators $\longrightarrow$ Slater-Condon rules

$$B_{12}^{(1)} = \begin{cases} \sum_k b_{kk} n_k & : \ \{n^{(1)}\} = \{n^{(2)}\} \\ (-1)^{\alpha_{1,p,q}} b_{pq} & : \ \{n^{(1)}\} = \{n^{(2)}\}_q^p \\ 0 & : \ \text{else} \end{cases}$$

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- pair-interaction operators: $w(x,y) = w(y,x) = w^*(y,x)$

$$\hat{W} = \sum_{ijkl} \tilde{w}_{ijkl} \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}_l \hat{a}_k, \quad \tilde{w}_{ijkl} = w_{ijkl} - w_{ijlk}$$

$$w_{ijkl} = \langle ij|\hat{w}|kl\rangle = \int \mathrm{d}x \int \mathrm{d}y \ \phi^*_i(x) \phi^*_j(y) w(x,y) \phi_k(x) \phi_l(y)$$

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$$W^{(2)}_{12} = \begin{cases} \sum_{i=0} \sum_{j=i+1} \tilde{w}_{ijij} n^1_i n^1_j & : \{n^{(1)}\} = \{n^{(2)}\} \\ \sum_{p,q \neq i=0} (-1)^{\alpha_{1,p,q}} \tilde{w}_{ipiq} n^1_i & : \{n^{(1)}\} = \{n^{(2)}\}^{p}_{q} \\ (-1)^{\alpha_{1,p,q} + \alpha_{2,r,s}} \tilde{w}_{pqrs} & : \{n^{(1)}\} = \{n^{(2)}\}^{p<q}_{r<s} \\ 0 & : \text{else} \end{cases}$$

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- arbitrary Hamiltonian $\hat{H} = \hat{B}^{(1)} + \hat{W}^{(2)}$ $\Rightarrow$ only 1- and 2-particle excitations !

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CPIMC Formalism — 2nd Quantization

- arbitrary Hamiltonian $\hat{H} = \hat{B}^{(1)} + \hat{W}^{(2)}$ $\Rightarrow$ only 1- and 2-particle excitations !

$\longrightarrow$ off-diagonal elements specified by T2 (p,q) and T4 (p,q,r,s)

Calculating Matrix elements in ONV representation:

- one-particle operators $\longrightarrow$ Slater-Condon rules

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Separate Hamiltonian: $\hat{H} =: \hat{D} + \hat{Y}$

$$H_{ij} := \langle \{n^{(i)}\} | \hat{H} | \{n^{(j)}\} \rangle = \begin{cases} D_i := \langle \{n^{(i)}\} | \hat{D} | \{n^{(i)}\} \rangle & : i = j \text{ diagonal} \\ Y_{i,j} := \langle \{n^{(i)}\} | \hat{Y} | \{n^{(i)}\} \rangle & : i \neq j \text{ off-diagonal} \end{cases} = \begin{pmatrix} D_1 & Y_{1,2} & Y_{1,3} & \cdots \\ Y_{2,1} & D_2 & Y_{2,3} & \cdots \\ Y_{3,1} & Y_{3,2} & D_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

CPIMC Formalism — Partition Function

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Separate Hamiltonian: $\hat{H} =: \hat{D} + \hat{Y} \longrightarrow$ Interaction Picture: $\hat{H}(t) = \hat{D} + \hat{Y}(t) = \hat{D} + \mathrm{e}^{\mathrm{i}\hat{D}t}\hat{Y}\mathrm{e}^{-\mathrm{i}\hat{D}t}$

- time evolution:

$$\hat{U}(t) = \mathrm{e}^{-\mathrm{i}\hat{D}t} \underbrace{\mathscr{T} \exp\left\{-\int_0^t \mathrm{d}t' \hat{Y}(t')\right\}}_{\text{time-ordered exponential}} = \mathrm{e}^{-\mathrm{i}\hat{D}t} \underbrace{\sum_{K=0}^{\infty} (-\mathrm{i})^K \int_0^t \mathrm{d}t_1 \int_{t_1}^t \mathrm{d}t_2 \ldots \int_{t_{K-1}}^t \mathrm{d}\, t_K \hat{Y}(t_K) \ldots \hat{Y}(t_2)\hat{Y}(t_1)}_{\text{Dyson series}}$$

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- perform trace:

$$Z = \mathrm{Tr}\,\hat{U}(-\mathrm{i}\beta) = \sum_{\{n^{(0)}\}} \langle\{n^{(0)}\}|\hat{U}(-\mathrm{i}\beta)|\{n^{(0)}\}\rangle$$

$$= \sum_{\{n^{(0)}\}} \sum_{K=0}^{\infty} \int_0^\beta \mathrm{d}\tau_1 \int_{\tau_1}^\beta \mathrm{d}\tau_2 \ldots \int_{\tau_{K-1}}^\beta \mathrm{d}\,\tau_K \langle\{n^{(0)}\}|(-1)^K \mathrm{e}^{-\mathrm{i}\hat{D}t}\hat{Y}(\tau_K)\ldots\hat{Y}(\tau_2)\hat{Y}(\tau_1)|\{n^{(0)}\}\rangle$$

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- perform trace, insert $\hat{\mathbb{1}} = \sum_{\{n^{(i)}\}} \langle\{n^{(i)}\}|\,|\{n^{(i)}\}\rangle$:

$$Z = \mathrm{Tr}\, \hat{U}(-\mathrm{i}\beta) = \sum_{\{n^{(0)}\}} \langle\{n^{(0)}\}|\hat{U}(-\mathrm{i}\beta)|\{n^{(0)}\}\rangle$$

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$$\times (-1)^K \exp\left(-\sum_{i=0}^{K} D_i(\tau_{i+1} - \tau_i)\right) \prod_{i=1}^{K} Y_{i,i-1}$$

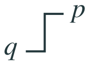
where is the path... ?

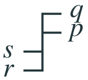
Define *Kinks*:

- type 2: $s_{\mathrm{T2}} := (p,q) \in \mathbb{N}^2$
- type 4: $s_{\mathrm{T4}} := (p,q,r,s) \in \mathbb{N}^4$
- General type: $s \in \mathbb{N}^2 \cup \mathbb{N}^4$

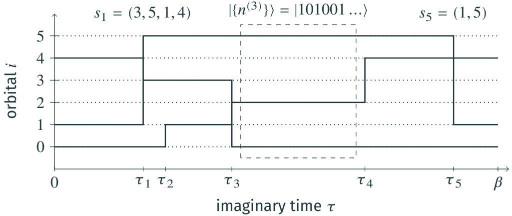
$$Z(N,V,\beta) = \overbrace{\sum_{\substack{K=0\\K\neq 1}}^{\infty} \sum_{\{n^{(k)}\}} \sum_{s_1} \ldots \sum_{s_{K-1}} \int_0^\beta \mathrm{d}\tau_1 \int_{\tau_1}^\beta \mathrm{d}\tau_2 \ldots \int_{\tau_{K-1}}^\beta \mathrm{d}\tau_K}^{:=\sum\!\!\!\!\!\!\int} \underbrace{(-1)^K \exp\left\{-\sum_{i=0}^{K} D_i(\tau_{i+1}-\tau_i)\right\} \prod_{i=1}^{K} Y_{i,i-1}(s_i)}_{:=W(C)}$$

Ingredients for β-periodic path:

- T2-kinks: 

- T4-kinks: 

- *stationary links*: ——



Example configuration Path $C := (\{n^{(\cdot)}\}s_1,\ldots,s_K,\tau_1,\ldots,\tau_K)$

CPIMC Algorithm

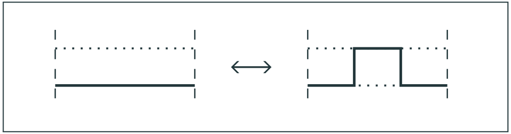
- Add/Remove 2 kinks

Detailed Balance:

$$p_{\mathrm{ap}} \frac{1}{2\beta N_0} p(\tau) |W(C)| \nu(C \to C')$$
$$= p_{\mathrm{rp}} \frac{1}{K+2} |W(C')| \nu(C' \to C)$$

CPIMC Algorithm

- Add/Remove 2 kinks
  - T2 kink

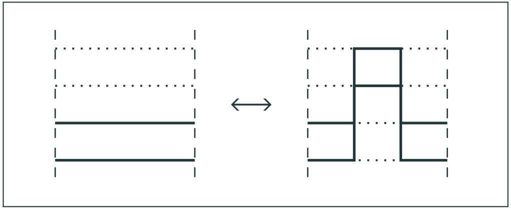


Detailed Balance:

$$
\begin{aligned}
& p_{\mathrm{ap}} \frac{1}{2\beta N_0} p(\tau) |W(C)| \nu(C \to C') \\
=& p_{\mathrm{rp}} \frac{1}{K+2} |W(C')| \nu(C' \to C)
\end{aligned}
$$

CPIMC Algorithm

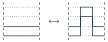
- Add/Remove 2 kinks
  - T2 kink • T4 kink



Detailed Balance:

$$p_{\mathrm{ap}} \frac{1}{2\beta N_o} p(\tau) |W(C)| \nu(C \rightarrow C')$$
$$= p_{\mathrm{rp}} \frac{1}{K+2} |W(C')| \nu(C' \rightarrow C)$$

CPIMC Algorithm

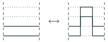
- Add/Remove 2 kinks
  - T2 kink  • T4 kink 
- Add/Remove 1 kink1

Detailed Balance:

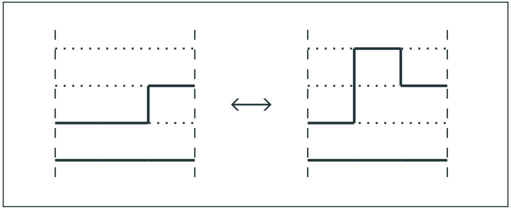
$$
\begin{aligned}
&p_{\mathrm{ak}}\frac{1}{4KN_0}p(\tau)|W(C)|\nu(C \to C') \\
=&p_{\mathrm{rk}}\frac{1}{K+1}\frac{1}{2N_K}|W(C')|\nu(C' \to C)
\end{aligned}
$$

CPIMC Algorithm

- Add/Remove 2 kinks
  - T2 kink • T4 kink



- Add/Remove 1 kink1
  - T2 kink

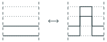


Detailed Balance:

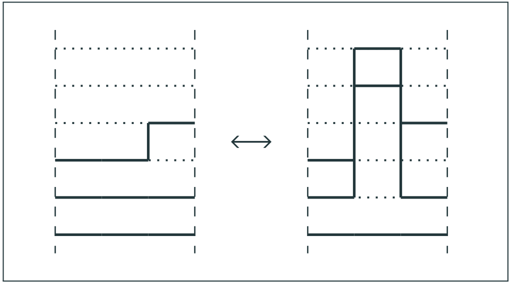
$$
\begin{aligned}
&p_{\mathrm{ak}}\frac{1}{4KN_0}p(\tau)|W(C)|v(C \to C') \\
=&p_{\mathrm{rk}}\frac{1}{K+1}\frac{1}{2N_K}|W(C')|v(C' \to C)
\end{aligned}
$$

CPIMC Algorithm

- Add/Remove 2 kinks
  - T2 kink • T4 kink



- Add/Remove 1 kink1
  - T2 kink • T4 kink



Detailed Balance:

$$
\begin{aligned}
&p_{\mathrm{ak}} \frac{1}{4KN_0} p(\tau) |W(C)| v(C \to C') \\
=&p_{\mathrm{rk}} \frac{1}{K+1} \frac{1}{2N_K} |W(C')| v(C' \to C)
\end{aligned}
$$

CPIMC Algorithm

- Add/Remove 2 kinks
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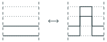
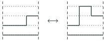
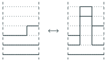


- Add/Remove 1 kink1
  - T2 kink • T4 kink

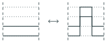



- Change 2 kinks

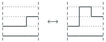
Detailed Balance:

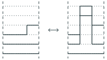
$$
\begin{aligned}
&p_{\mathrm{ck}} \frac{1}{2KN_0N_K} |W(C)| v(C \to C') \\
=&p_{\mathrm{ck}} \frac{1}{2KN_0N_{K'}} |W(C')| v(C' \to C)
\end{aligned}
$$

- Add/Remove 2 kinks
  - T2 kink • T4 kink

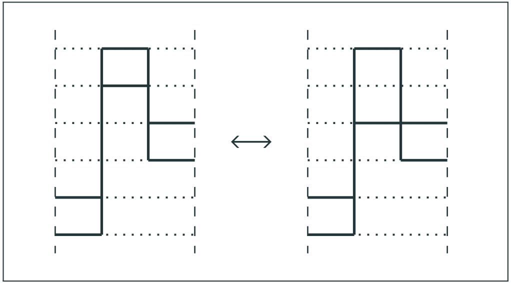


- Add/Remove 1 kink1
  - T2 kink • T4 kink





- Change 2 kinks
  - T2 kink

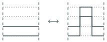


Detailed Balance:

$$p_{\text{ck}}\frac{1}{2KN_oN_K}|W(C)|v(C \to C') = p_{\text{ck}}\frac{1}{2KN_oN_{K'}}|W(C')|v(C' \to C)$$

CPIMC Algorithm

- Add/Remove 2 kinks
  - T2 kink • T4 kink



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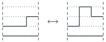
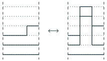
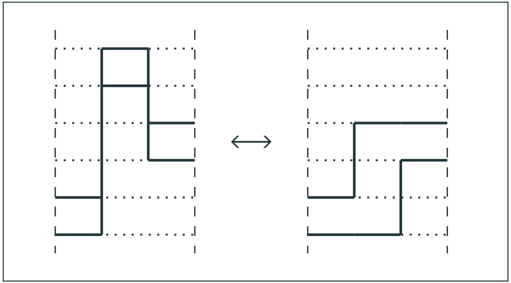




- Change 2 kinks
  - T2 kink • T4 kink



Detailed Balance:

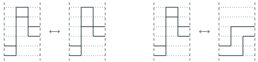
$$p_{\mathrm{ck}}\frac{1}{2KN_{\mathrm{o}}N_K}|W(C)|\nu(C\to C')$$
$$=p_{\mathrm{ck}}\frac{1}{2KN_{\mathrm{o}}N_{K'}}|W(C')|\nu(C'\to C)$$

CPIMC Algorithm

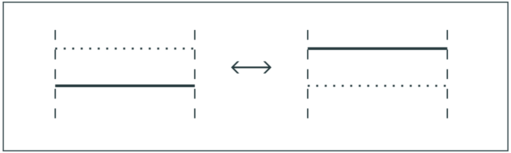
- Add/Remove 2 kinks
  - T2 kink • T4 kink

- Add/Remove 1 kink1
  - T2 kink • T4 kink

- Change 2 kinks
  - T2 kink • T4 kink



- Excite stationary orbital



Detailed Balance:

$$
\begin{aligned}
&p_{\mathrm{eo}} \frac{1}{\tilde{N}_p \tilde{N}_q} |W(C)| v(C \to C') \\
=&p_{\mathrm{eo}} \frac{1}{\tilde{N}_p \tilde{N}_q} |W(C')| v(C' \to C)
\end{aligned}
$$

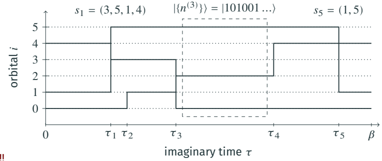
CPIMC Algorithm

- Add/Remove 2 kinks
  - T2 kink • T4 kink

- Add/Remove 1 kink1
  - T2 kink • T4 kink

- Change 2 kinks
  - T2 kink • T4 kink

- Excite stationary orbital



wrong figure!!!

- N electrons located in a finite volume $V = L^3$ of cubic shape
- ions ↔ *uniform* background (*jellium*) ⇒ overall charge-neutrality
- single-particle CONS: plane waves $\langle \boldsymbol{r}|\boldsymbol{k}\sigma\rangle = \frac{1}{\sqrt{V}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$
- periodic boundary conditions $\Rightarrow \boldsymbol{k} = \frac{2\pi}{L}(n_1, n_2, n_3)$ with $n_1, n_2, n_3 \in \mathbb{Z}$
- Hamiltonian:

  - in thermodynamic limit:

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{\boldsymbol{p}}_i^2}{2} + \frac{1}{2L^3} \sum_{i,j=1}^{N} \sum_{\boldsymbol{q}\neq 0} v_{\boldsymbol{q}} \left[\mathrm{e}^{\mathrm{i}\boldsymbol{q}(\hat{\boldsymbol{r}}_i - \hat{\boldsymbol{r}}_j)} - \hat{N}\right]$$

  - for finite systems:

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hat{\boldsymbol{p}}_i^2}{2} + \frac{1}{2} \sum_{i\neq j=1}^{N} \underbrace{U(\hat{\boldsymbol{r}}_i, \hat{\boldsymbol{r}}_j)}_{\substack{\text{Ewald} \\ \text{pair potential}}} + \underbrace{E_{\mathrm{M}}}_{\substack{\text{PBC} \\ \text{self-interaction}}}$$

  - in ONV representation:

$$\hat{H} = \sum_{i,j} \varepsilon_{ij} \hat{a}_i^\dagger \hat{a}_j + \sum_{\substack{i<j,k<l \\ i\neq k, j\neq l}} \tilde{w}_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k, \qquad \tilde{w} = w_{ijkl} - w_{ijlk}$$

$$\varepsilon_{ij} = \frac{\boldsymbol{k}_i^2}{2}\delta_{ij}, \qquad w_{ijkl} = \frac{4\pi}{v(\boldsymbol{k}_i - \boldsymbol{k}_k)} \delta_{(\boldsymbol{k}_i + \boldsymbol{k}_j)(\boldsymbol{k}_k + \boldsymbol{k}_l)} \delta_{\sigma_i \sigma_k} \delta_{\sigma_j \sigma_l}$$

CPIMC for the HEG — MC Steps

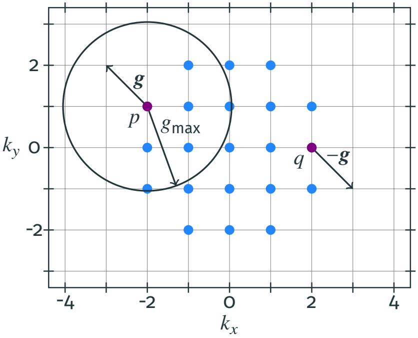
Momentum Conservation ⇒ no single-particle excitations (T2)

[1] $|\boldsymbol{g}| < g_{\mathsf{max}}$, e.g. $g_{\mathsf{max}} = 2$

Momentum Conservation ⇒ no single-particle excitations (T2)

- MC-Steps 1,2: Add/Remove kink:

  choose 2 occupied $n_i(\tau)$



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Momentum Conservation ⇒ no single-particle excitations (T2)

- MC-Steps 1,2: Add/Remove kink:

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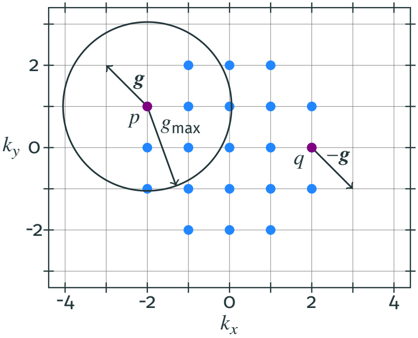
  → randomly choose *excitation vector*[1] $\boldsymbol{g} \in \mathbb{Z}^3$



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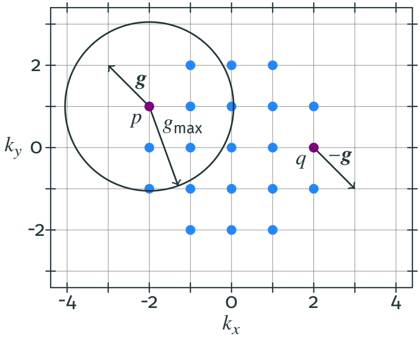
Momentum Conservation ⇒ no single-particle excitations (T2)

- MC-Steps 1,2: Add/Remove kink:

  choose 2 occupied $n_i(\tau)$

  → randomly choose *excitation vector*[1] $\boldsymbol{g} \in \mathbb{Z}^3$

  → propose $\boldsymbol{k}_{r/s} = \boldsymbol{k}_{p/q} \pm \boldsymbol{g}$



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Momentum Conservation ⇒ no single-particle excitations (T2)

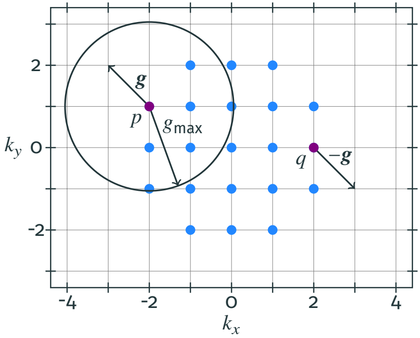
- MC-Steps 1,2: Add/Remove kink:

  choose 2 occupied $n_i(\tau)$

  → randomly choose *excitation vector*[1] $\boldsymbol{g} \in \mathbb{Z}^3$

  → propose $\boldsymbol{k}_{r/s} = \boldsymbol{k}_{p/q} \pm \boldsymbol{g}$
- MC-Step 4: excite stationary orbital

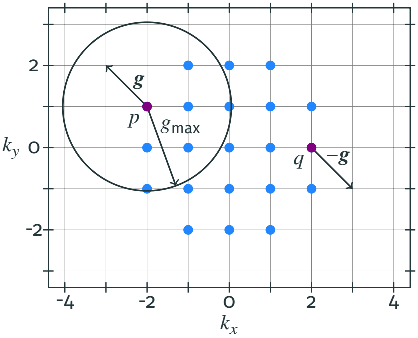
  randomly choose stationary orbital within *shell* i of energy $\varepsilon_{\boldsymbol{k}} \in [i\Delta_\varepsilon, i+1\Delta_\varepsilon)$



[1] $|\boldsymbol{g}| < g_{\max}$, e.g. $g_{\max} = 2$

Momentum Conservation $\Rightarrow$ no single-particle excitations (T2)

- MC-Steps 1,2: Add/Remove kink:
  - choose 2 occupied $n_i(\tau)$
  - $\rightarrow$ randomly choose *excitation vector*[1] $\boldsymbol{g} \in \mathbb{Z}^3$
  - $\rightarrow$ propose $\boldsymbol{k}_{r/s} = \boldsymbol{k}_{p/q} \pm \boldsymbol{g}$
- MC-Step 4: excite stationary orbital
  - randomly choose stationary orbital within *shell* i of energy $\varepsilon_{\boldsymbol{k}} \in [i\Delta_\varepsilon, i+1\Delta_\varepsilon)$



[1] $|\boldsymbol{g}| < g_{\text{max}}$, e.g. $g_{\text{max}} = 2$

Momentum Conservation ⇒ no single-particle excitations (T2)

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  choose 2 occupied $n_i(\tau)$

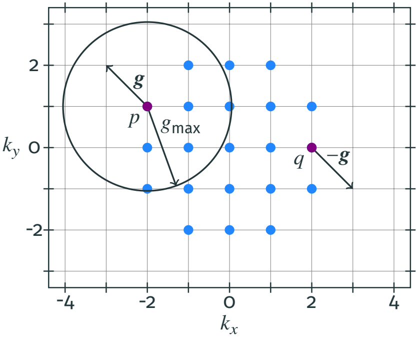
  → randomly choose *excitation vector*[1] $\boldsymbol{g} \in \mathbb{Z}^3$

  → propose $\boldsymbol{k}_{r/s} = \boldsymbol{k}_{p/q} \pm \boldsymbol{g}$

- MC-Step 4: excite stationary orbital

  randomly choose stationary orbital within *shell* i of energy $\varepsilon_{\boldsymbol{k}} \in [i\Delta_\varepsilon, i+1\Delta_\varepsilon)$

  → propose target orbital from adjacent shells $[i-1, i, i+1]$



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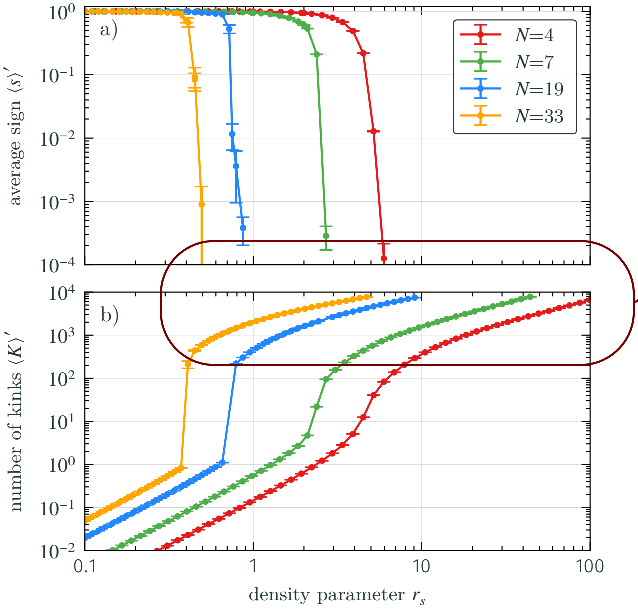
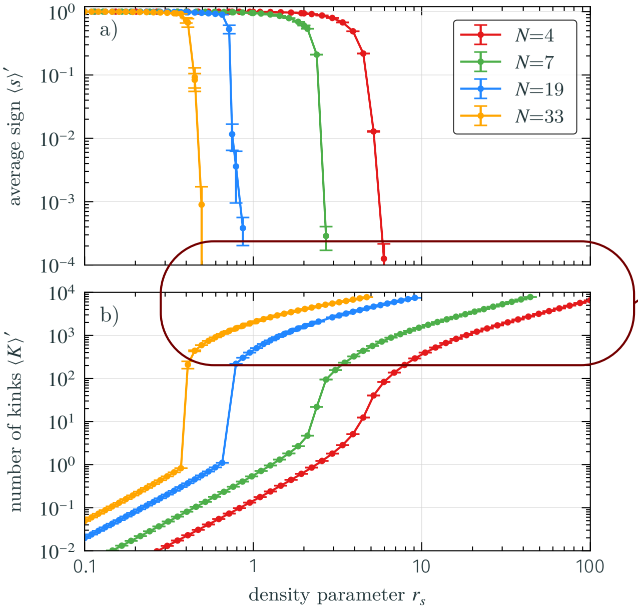


Kink-Explosion:
physical or due to
$W(C) \to |W(C)|$
???

figure: $\Theta = 0.125$,
from: T. Schoof. PhD thesis, ITAP, CAU, 2016. p. 115

CPIMC for the HEG — Sign Problem



Kink-Explosion:
physical or due to
$W(C) \to |W(C)|$
???

Observation:
Contributions from large K
cancel within errorbars.

figure: $\Theta = 0.125$,
from: T. Schoof. PhD thesis, ITAP, CAU, 2016. p. 115

introduce factor $V_K(\kappa, \delta)$ to partition sum: $Z \to Z(\kappa, \delta) = \sum\!\!\!\!\!\!\int_{C_K} W(C_K) \cdot V_K(\kappa, \delta)$

figure from: T. Schoof. PhD thesis, ITAP, CAU, 2016. p. 119

introduce factor $V_K(\kappa,\delta)$ to partition sum: $Z \to Z(\kappa,\delta) = \sum_{C_K} W(C_K)\cdot V_K(\kappa,\delta)$

Property:

- convergence parameter κ:
  $\lim_{\kappa\to\infty} V_K(\kappa,\delta) = 1$

Fermi-like function:

$$V_K(\kappa,\delta) = \left[\mathrm{e}^{-\delta(\kappa-K+\frac{1}{2})} + 1\right]^{-1}$$

Procedure:

- choose convenient δ (e.g.$=1$)
- simulate for various κ
- extrapolate estimates
  to the limit $\kappa \to \infty$

figure from: T. Schoof. PhD thesis, ITAP, CAU, 2016. p. 119

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Property:

- convergence parameter κ: $\lim_{\kappa \to \infty} V_K(\kappa, \delta) = 1$

Fermi-like function:

$$V_K(\kappa, \delta) = \left[e^{-\delta(\kappa - K + \frac{1}{2})} + 1 \right]^{-1}$$

Procedure:

- choose convenient δ (e.g.$= 1$)
- simulate for various κ
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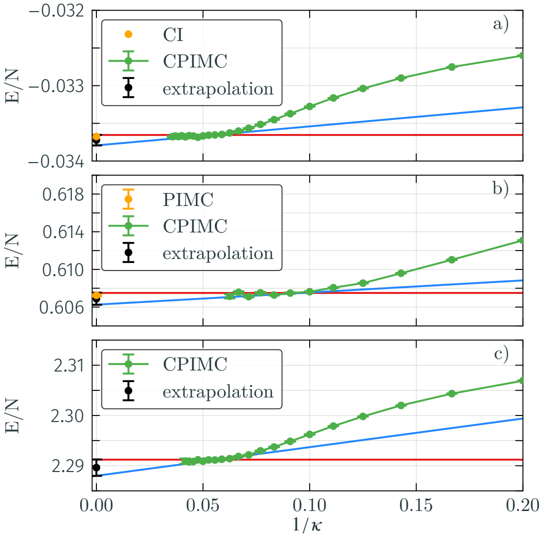
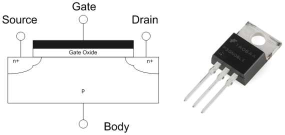


figure from: T. Schoof. PhD thesis, ITAP, CAU, 2016. p. 119

Outlook

- implemented and tested for qm. coupled harmonic oscillators
- HEG solved at finite temperatures
- exact data for WDM regime
- x include relativistic effects for $r_s \to 0$, $\beta > 1$
- x 2D Electron Gas



MOSFET realize 2DEG in inversion mode[1]

[1] https://en.wikipedia.org/wiki/Two-dimensional_electron_gas


MUSE
三难困境
SIMULATION
Theory