Application of Quantum Monte Carlo to the Hubbard Model

Huy Nguyen

Advisor: Darrell Schroeter (Reed)
Collaborator: Shiwei Zhang (W&M)

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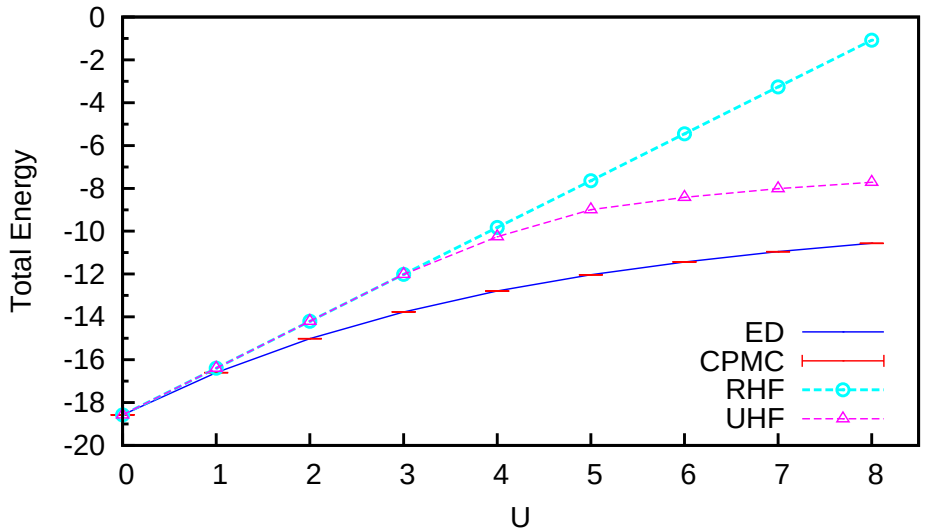
Layout

- Strongly correlated systems.
- The Hubbard model.
- QMC basics.
- `CPMC-Lab`.
- Imaginary-time Green's functions.
  - Benchmarks.
  - Applications.

Strongly correlated systems

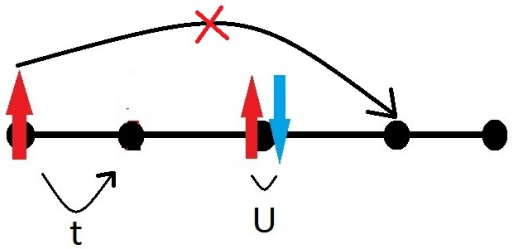
- Frontier in physics, exotic and exciting properties:
  - High-T_c, colossal magnetoresistance, heavy-fermion metals etc.
- Particles interact strongly and cannot be treated individually.

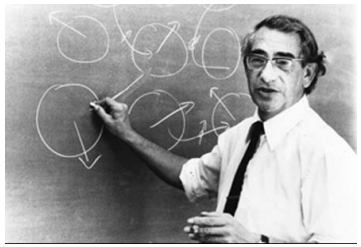


Failure of traditional methods (16×1 Hubbard $5 \uparrow 7 \downarrow$).

[Nguyen, Shi, Xu and Zhang, CPC (in press)]

Hamiltonian of Hubbard model





- Hamiltonian (2^{nd} quantization)

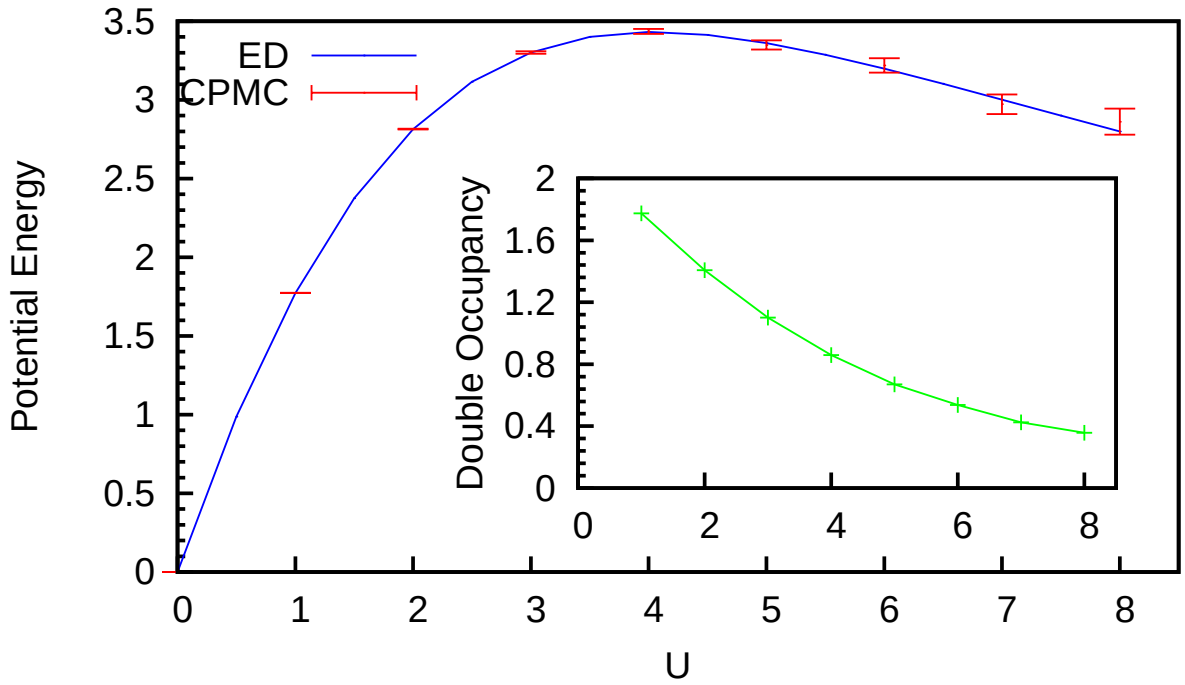
$$\widehat{H} = \widehat{K} + \widehat{V} = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \text{H.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

[John Hubbard, *Proc. R. Soc. A* (1963)]

- Simplest model to capture both band structure and electron-electron interactions.
- Minimal model for cuprate superconductors.

Parameters of Hubbard model

- 2 parameters: correlation strength U/t and filling $N_{\text{electrons}}/N_{\text{sites}}$.



[Nguyen *et al.*, CPC (in press)]

Potential energy & double occupancy (16×1 Hubbard $5\uparrow 7\downarrow$).

Challenges of Hubbard model

- No analytic formulas for energy and equal-time correlations in more than 1-D.
  - No analytic formulas for unequal-time correlations in 1-D.
- Exact numerical methods: computational cost increases exponentially with N_{sites}.
- Largest 2-D Hubbard lattice solved exactly: 20 sites at half-filling.
  - 34 billion basis states.
  - A vector in this basis takes 254GB of memory.

Quantum Monte Carlo (QMC)

- Class of stochastic algorithms.
  - Constrained Path Monte Carlo (CPMC) [Zhang, Carlson & Gubernatis, PRB (1997)].
- Ground state projection:

$$|\Psi_0\rangle = \lim_{\tau\to\infty} \mathrm{e}^{-\tau(\widehat{H}-E_0)}\,|\Psi_\mathrm{T}\rangle$$

- Hubbard-Stratonovich transformation:

$$\mathrm{e}^{-U n_{i\uparrow} n_{i\downarrow}} \propto \sum_{x_i=\pm 1} \mathrm{e}^{x_i (n_{i\uparrow}-n_{i\downarrow})\times\mathrm{const}}$$

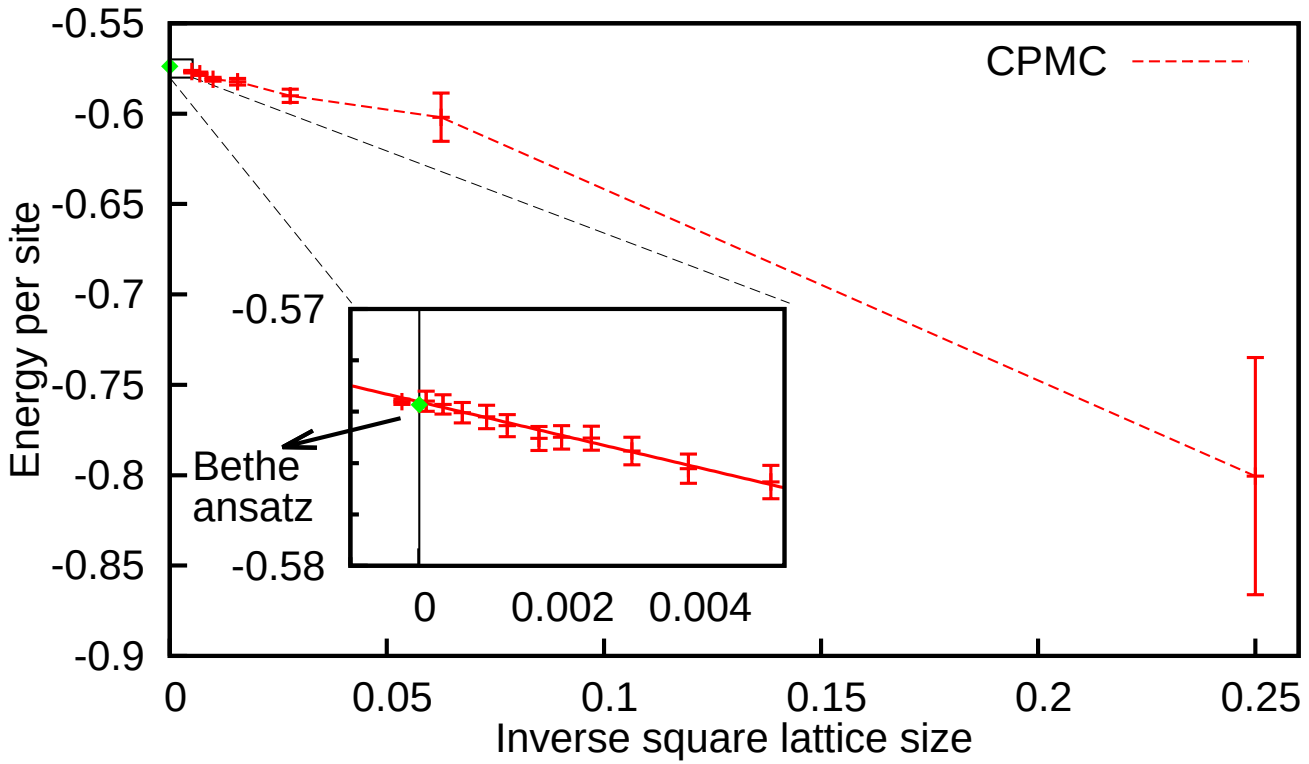
- Suzuki-Trotter decomposition

$$\mathrm{e}^{-\Delta\tau\widehat{H}} = (\mathrm{e}^{-\tau\widehat{K}}\mathrm{e}^{-\tau\widehat{V}}) + \mathcal{O}(\Delta\tau^2)$$

QMC basics

- Works in one-particle Hilbert spaces (subject to external fields).
  - Much smaller matrices.
- Computational cost increases polynomially: $(N_{\text{sites}})^3$ to $(N_{\text{sites}})^4$.
  - Can reach very large system sizes.
  - Accurate extrapolation to thermodynamic limit.

QMC extrapolation

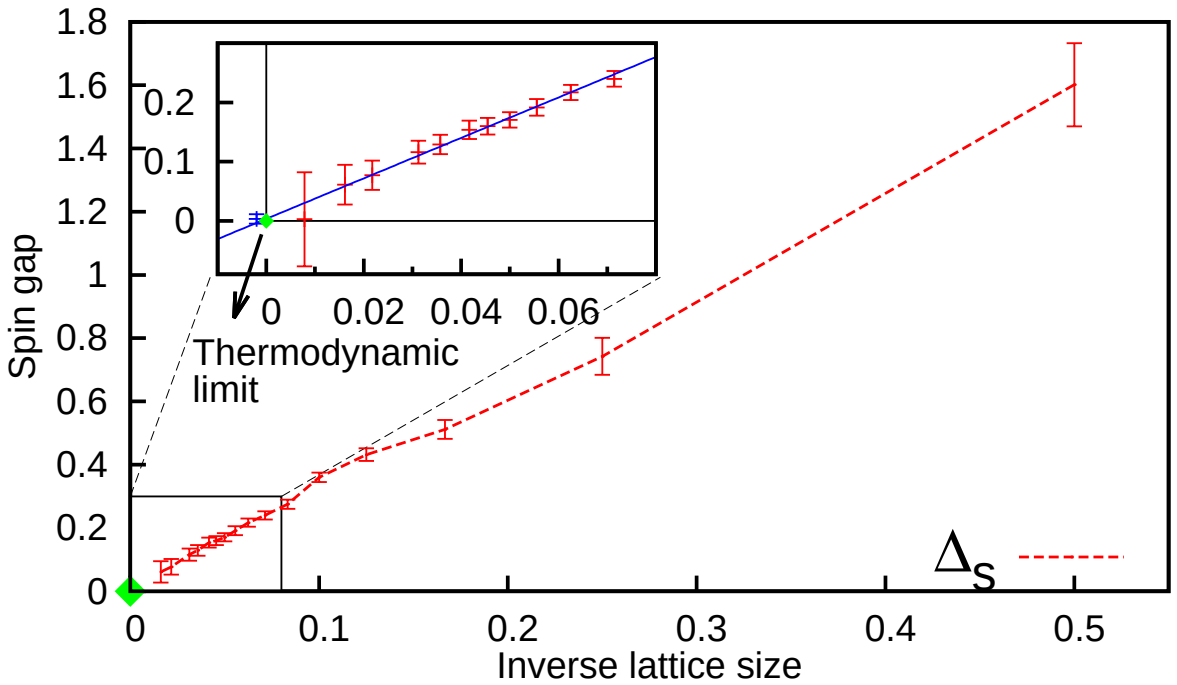


[Nguyen *et al.*, CPC (in press)]

Energy/site of 1-D Hubbard at half-filling, $U = 4$ (2 to 128 sites).

QMC extrapolation

$$\text{Spin gap} = E_0(N_\uparrow + 1, N_\downarrow - 1) - E_0(N_\uparrow, N_\downarrow)$$

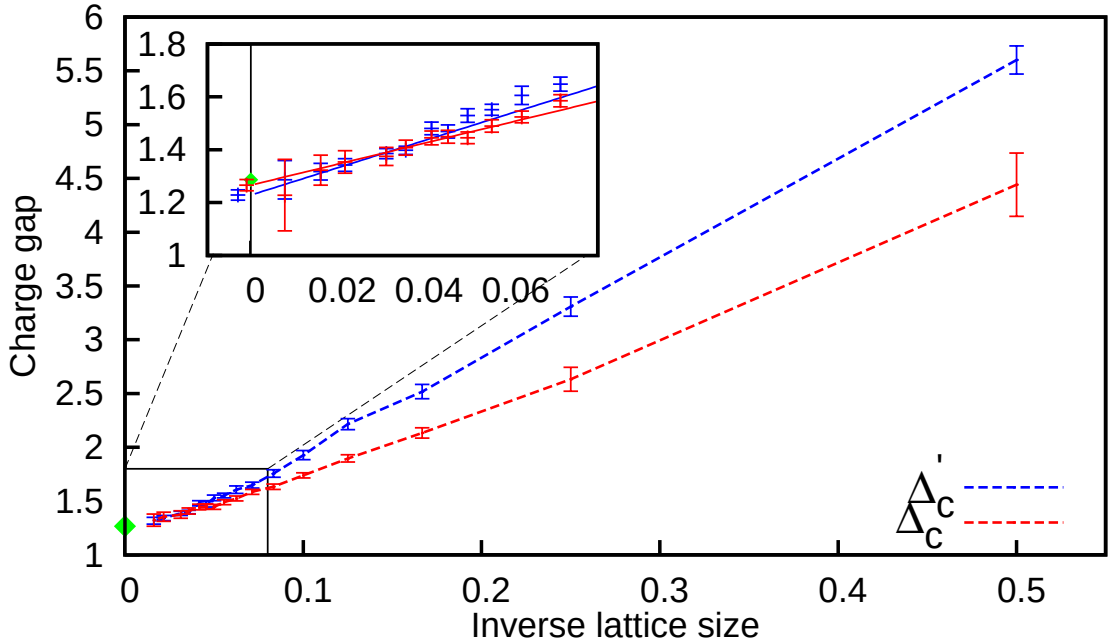


[Nguyen *et al.*, CPC (in press)]

Spin gap of 1-D Hubbard at half-filling, $U = 4$ (2 to 128 sites).

QMC extrapolation

$$\text{Charge gap} = E_0(N_\uparrow + 1, N_\downarrow) + E_0(N_\uparrow - 1, N_\downarrow) - 2E_0(N_\uparrow, N_\downarrow)$$



[Nguyen *et al.*, CPC (in press)]

Charge gap of 1-D Hubbard at half-filling, $U = 4$ (2 to 128 sites).

CPMC-Lab

- Written in MATLAB.
  - Only use built-in MATLAB functions.
  - Interactive development and Graphical User Interface.
- Allow further method development.
  - Other model Hamiltonians besides Hubbard.
  - Real materials.

Equal-time Green's function

- Equal-time Green's function

$$G_{ij} = \langle c_i c_j^\dagger \rangle = \langle \Psi_{\mathrm{T}} | \mathrm{e}^{-\Delta\tau \widehat{H}} \dots \mathrm{e}^{-\Delta\tau \widehat{H}} \; c_i c_j^\dagger \; \mathrm{e}^{-\Delta\tau \widehat{H}} \dots \mathrm{e}^{-\Delta\tau \widehat{H}} | \Psi_{\mathrm{T}} \rangle$$

[Zhang *et al.*, PRB (1997)]

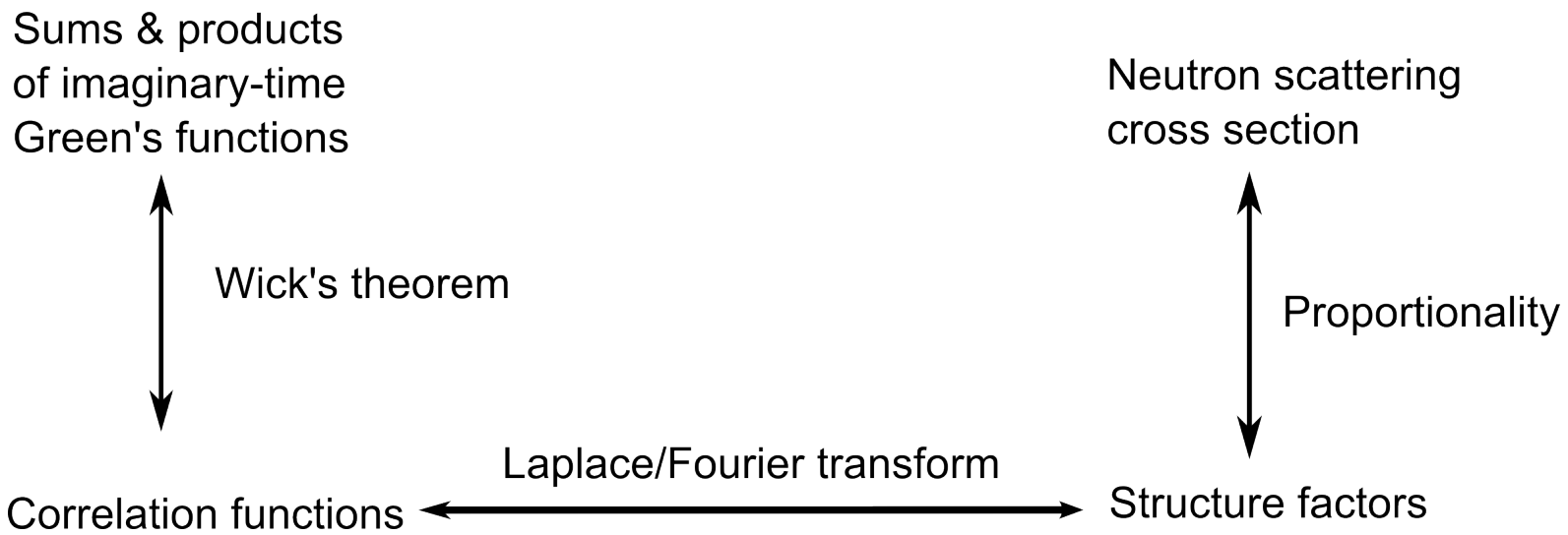
- Unequal-time Green's function

$$\begin{aligned}
\langle c_i(\tau_1) c_j^\dagger(\tau_2) \rangle &= \langle \Psi_{\mathrm{T}} | \mathrm{e}^{-\Delta\tau \widehat{H}} \dots c_i \; \mathrm{e}^{-\Delta\tau \widehat{H}} \dots \mathrm{e}^{-\Delta\tau \widehat{H}} c_j^\dagger \dots \mathrm{e}^{-\Delta\tau \widehat{H}} | \Psi_{\mathrm{T}} \rangle \\
&= \left[B \dots B \langle \Psi_{\mathrm{T}} | \mathrm{e}^{-\Delta\tau \widehat{H}} \dots \; c c^\dagger \dots \mathrm{e}^{-\Delta\tau \widehat{H}} | \Psi_{\mathrm{T}} \rangle \right]_{ij} \\
&= [B(\tau_1, \tau_2) G(\tau_2)]_{ij}
\end{aligned}$$

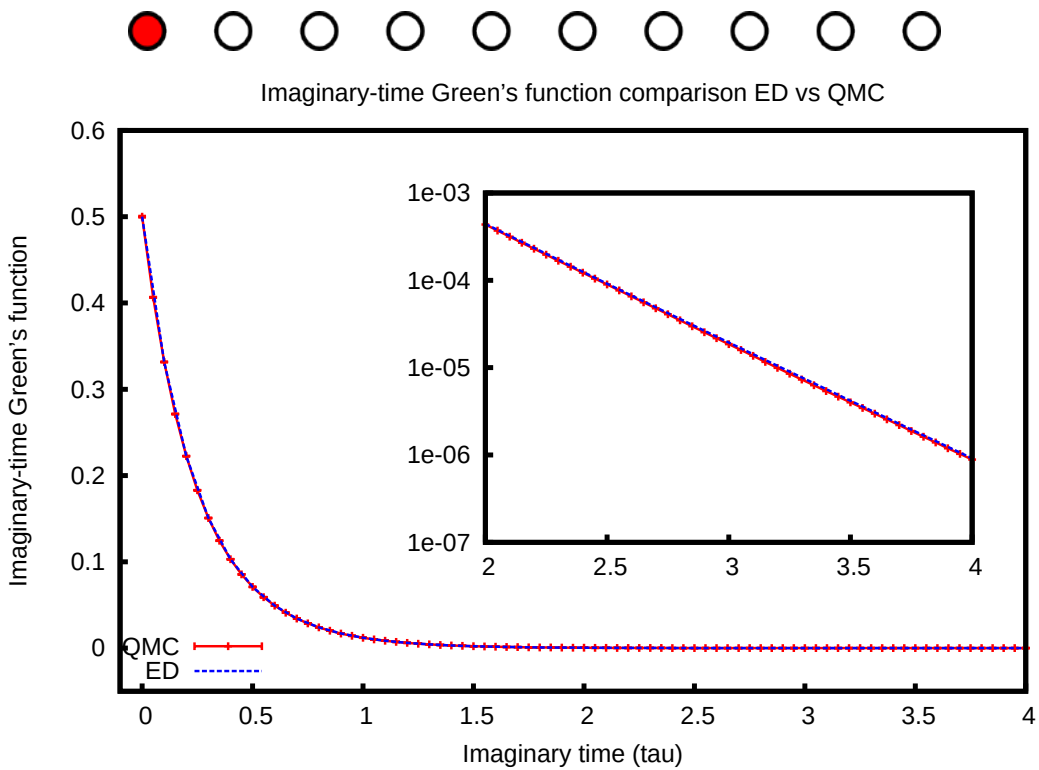
[Feldbacher & Assaad, PRB (2001)]

Unequal-time Green's function

- Connect theory to experiments.



Benchmark 1-D



Benchmark: 10×1 lattice, $5 \uparrow 5 \downarrow$, $U = 4$

Chemical potential

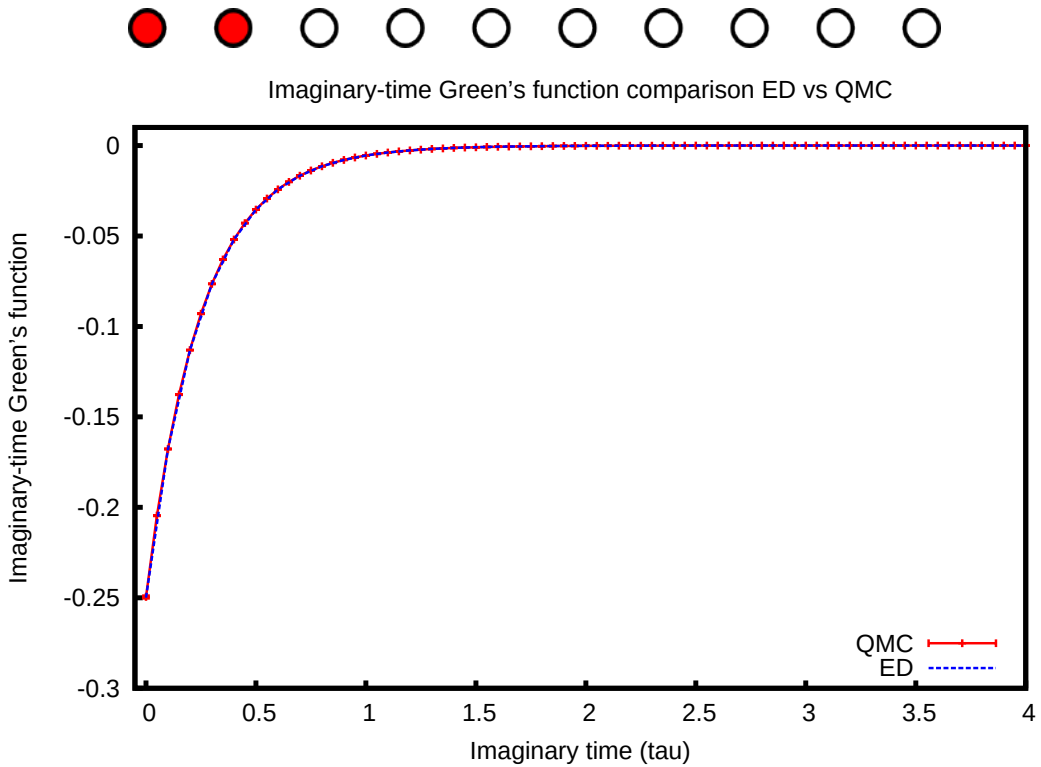
$$\langle c_i(\tau) c_j^\dagger \rangle = \sum_k a_k \, \mathrm{e}^{-\tau (E_k^{N+1} - E_0^N)}$$

$$\underset{\tau \to \infty}{=} \text{constant} \times \mathrm{e}^{-\tau (E_0^{N+1} - E_0^N)}$$

$$\implies \text{slope} = -\,\text{chemical potential}$$

- Exact chemical potential: 2.981.
- Slope of log plot: 3.01(3) (for $\tau = 3$ to 4).

Benchmark 1-D



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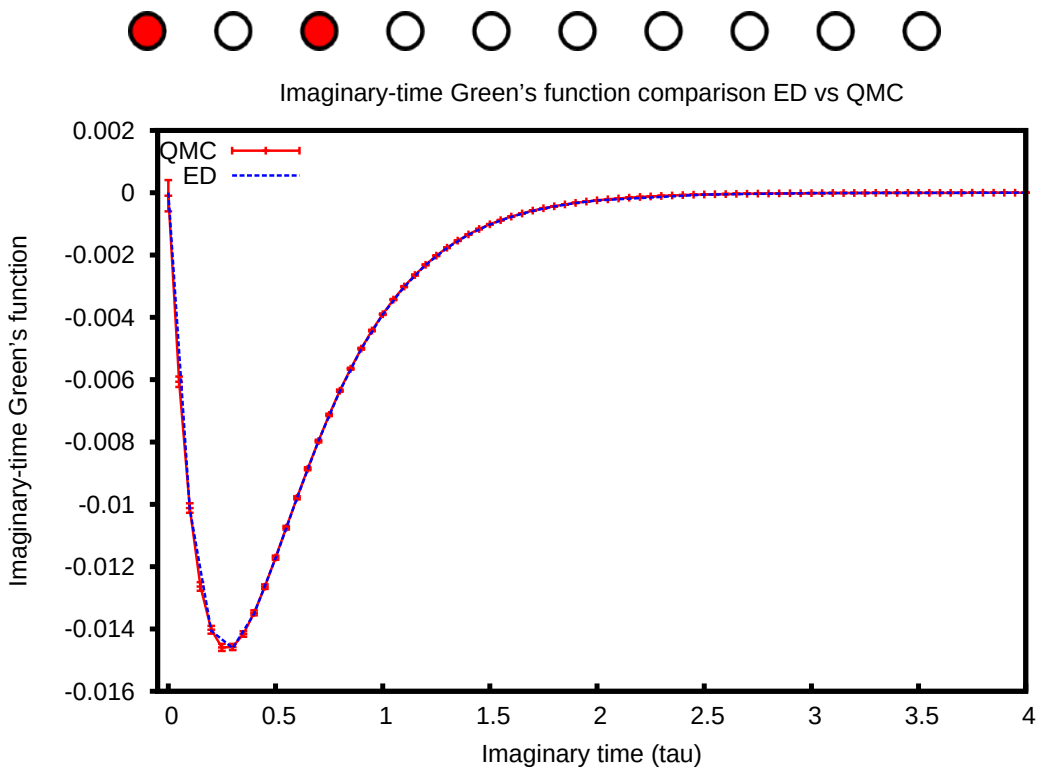

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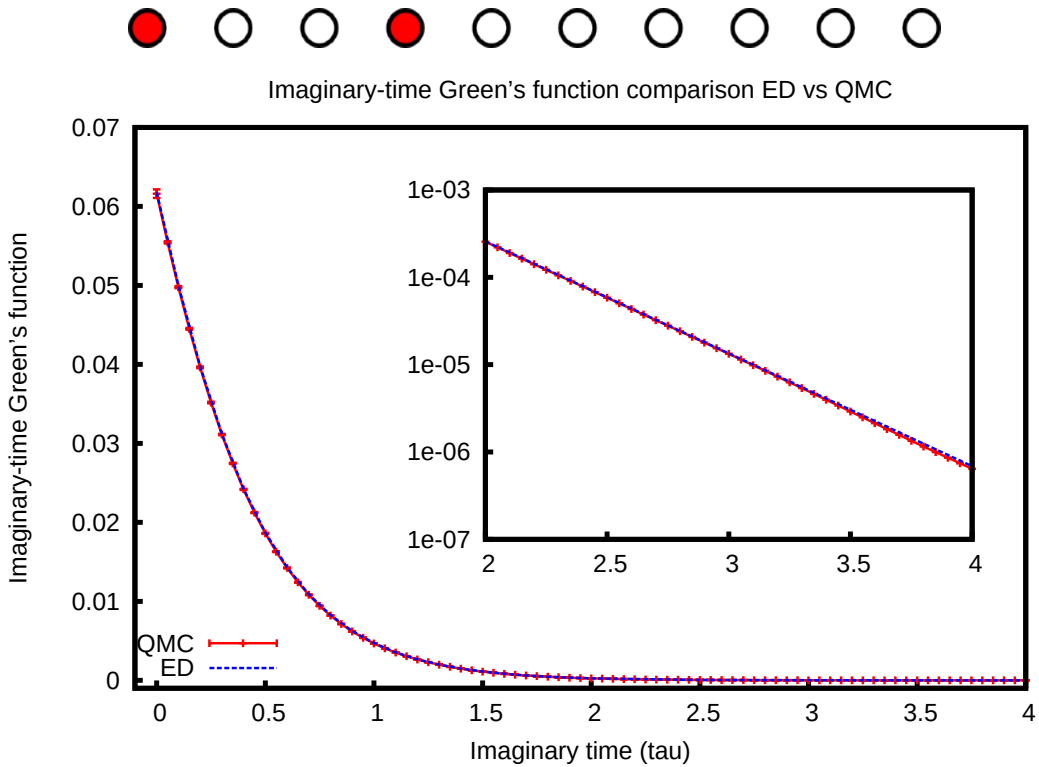

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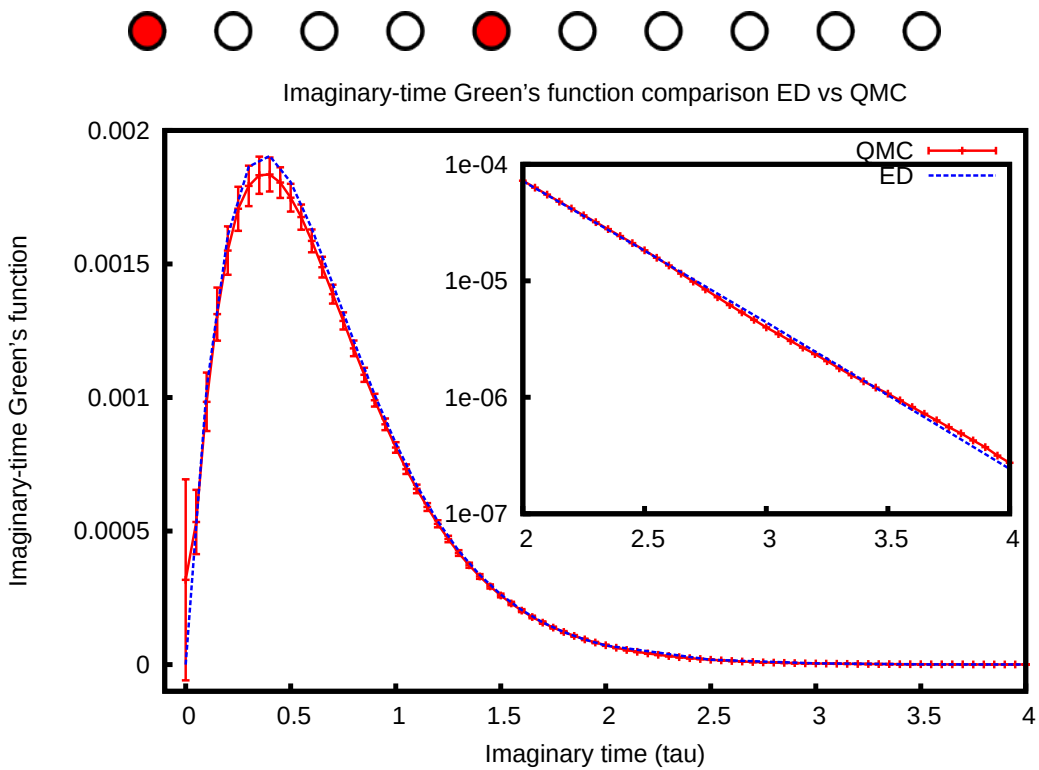

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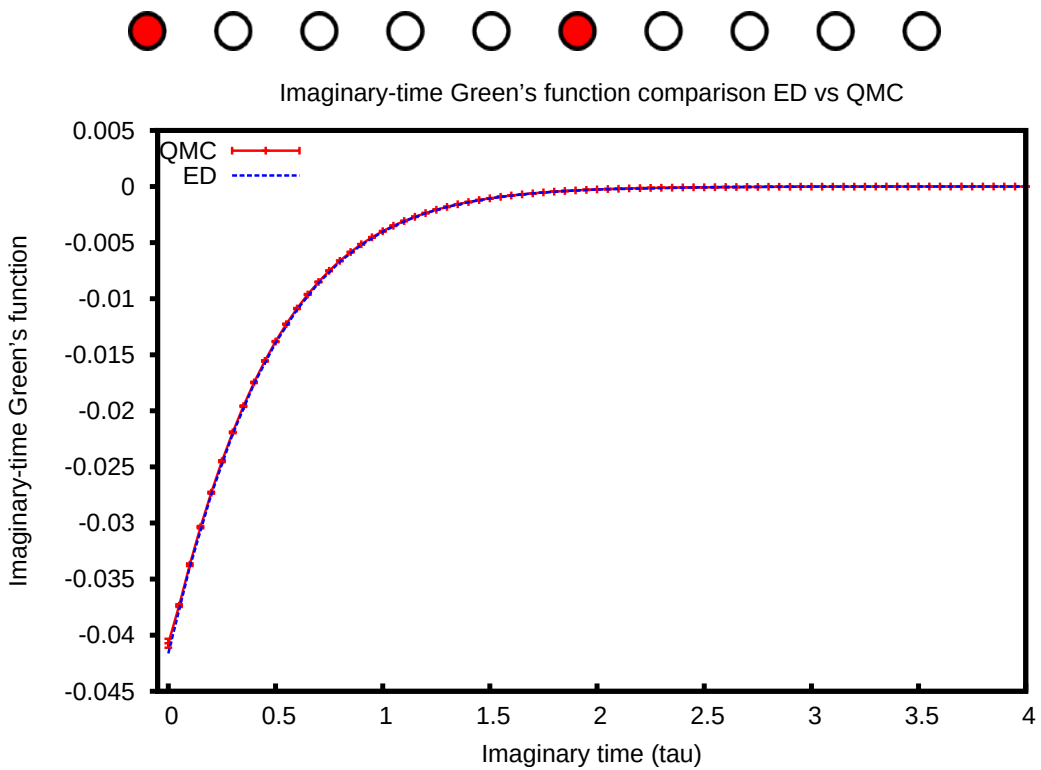
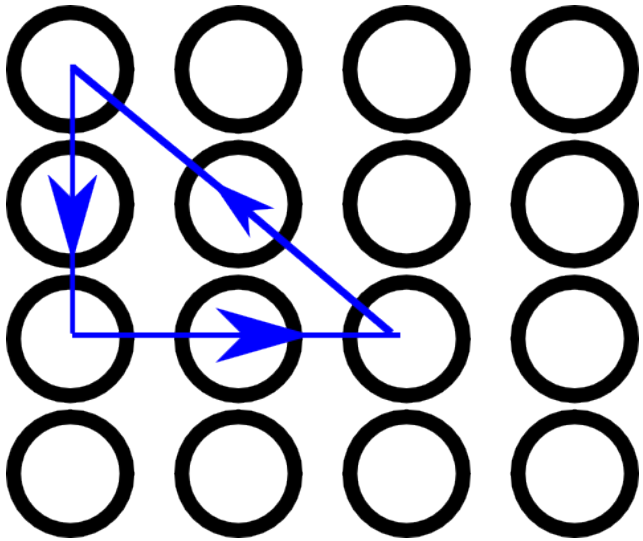


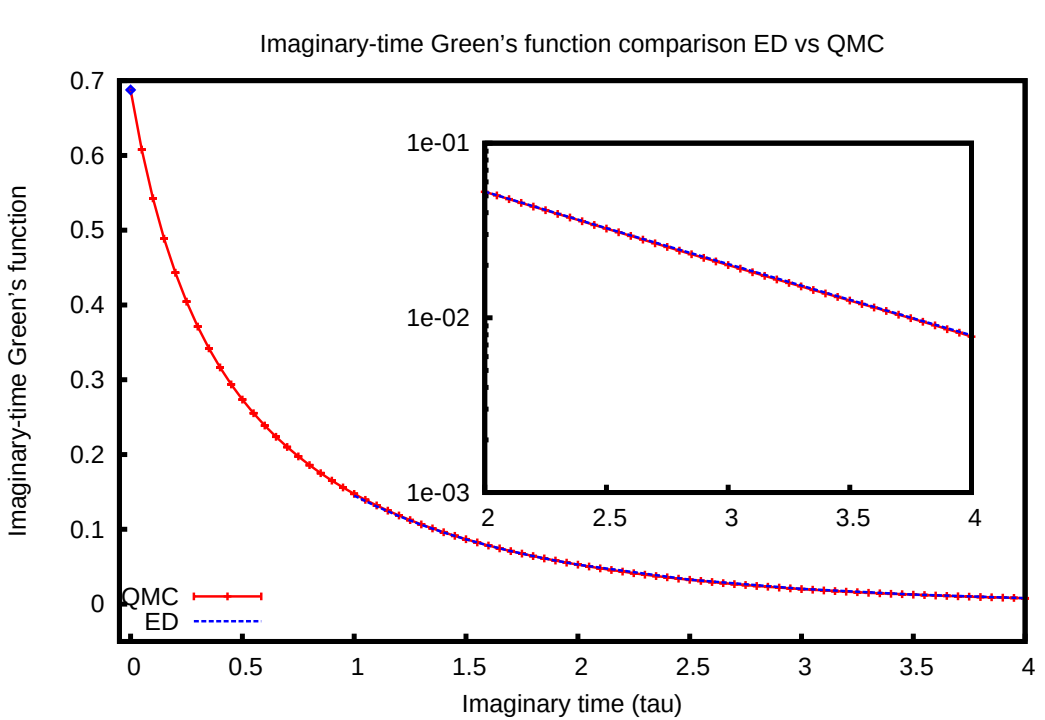
Benchmark: 10×1 lattice, $5 \uparrow 5 \downarrow$, $U = 4$

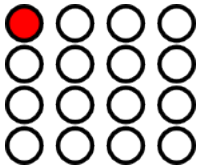
Benchmark 2-D



4×4 lattice, periodic boundary condition.

Benchmark 2-D

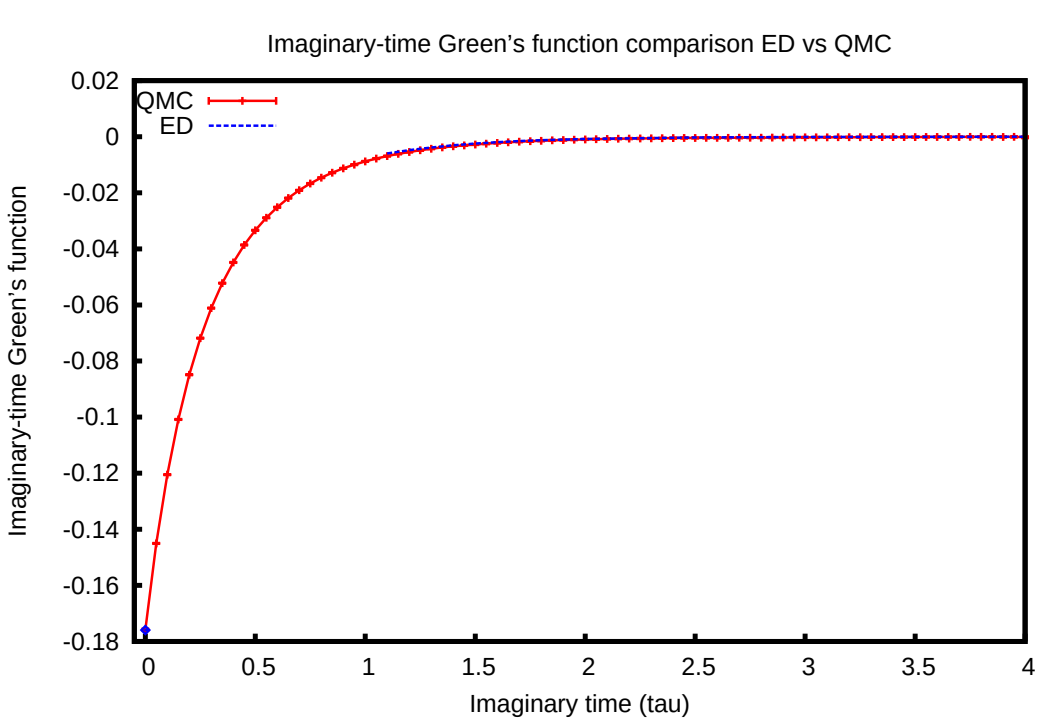


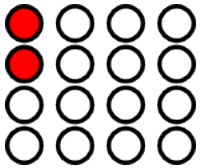


Benchmark: 4×4 lattice, $5 \uparrow 5 \downarrow$, $U = 4$

Exact chemical potential: 0.933. Slope: 0.935(6) for $\tau = 3$ to 4.

Benchmark 2-D





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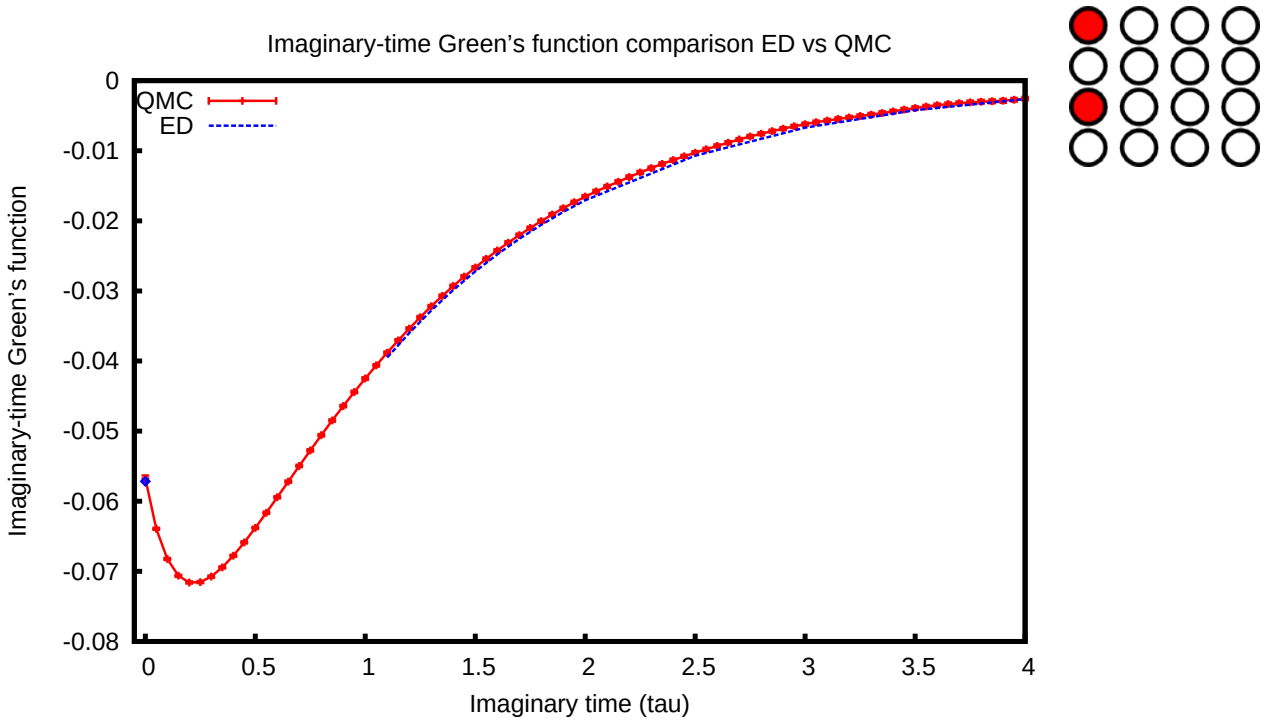

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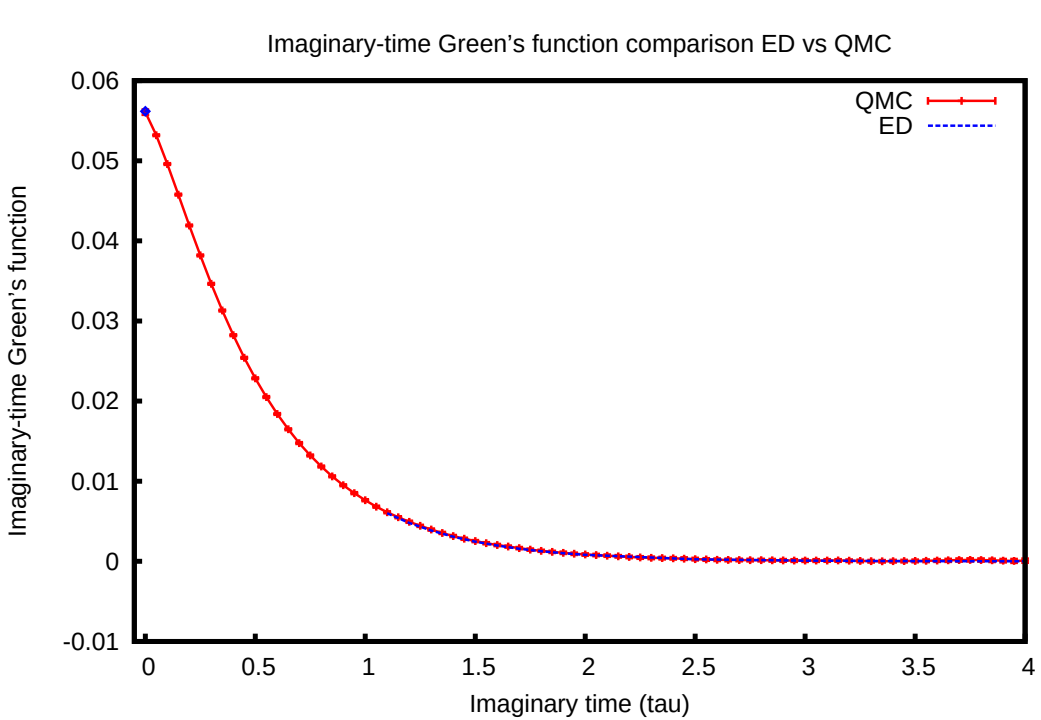

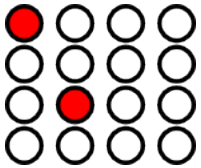

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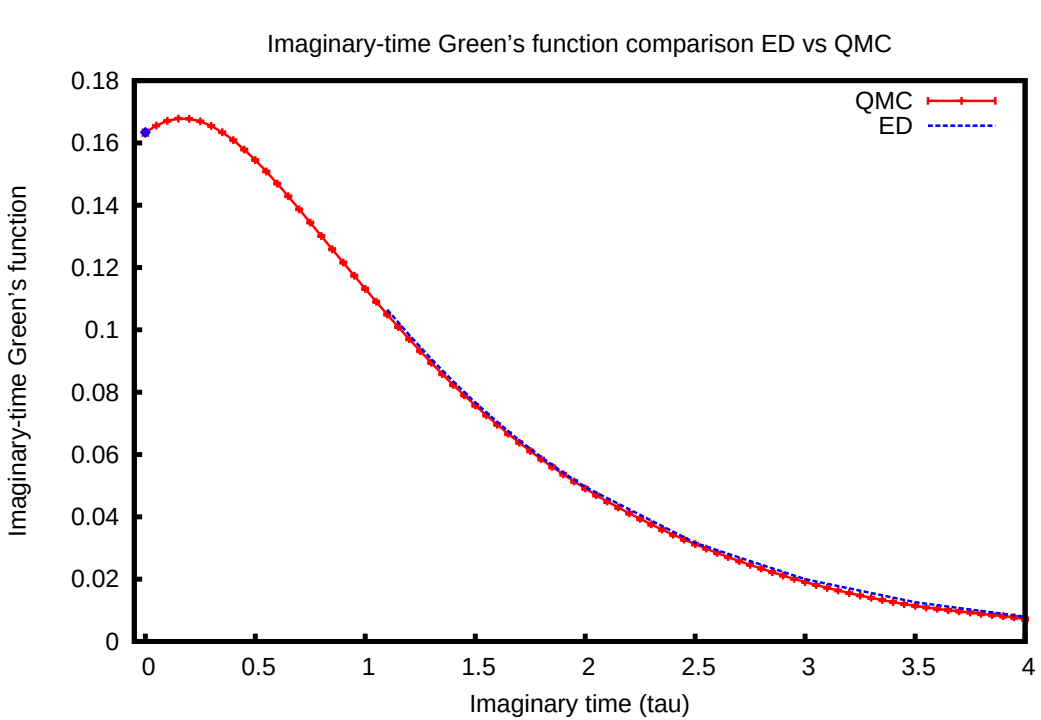

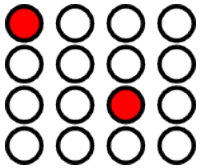

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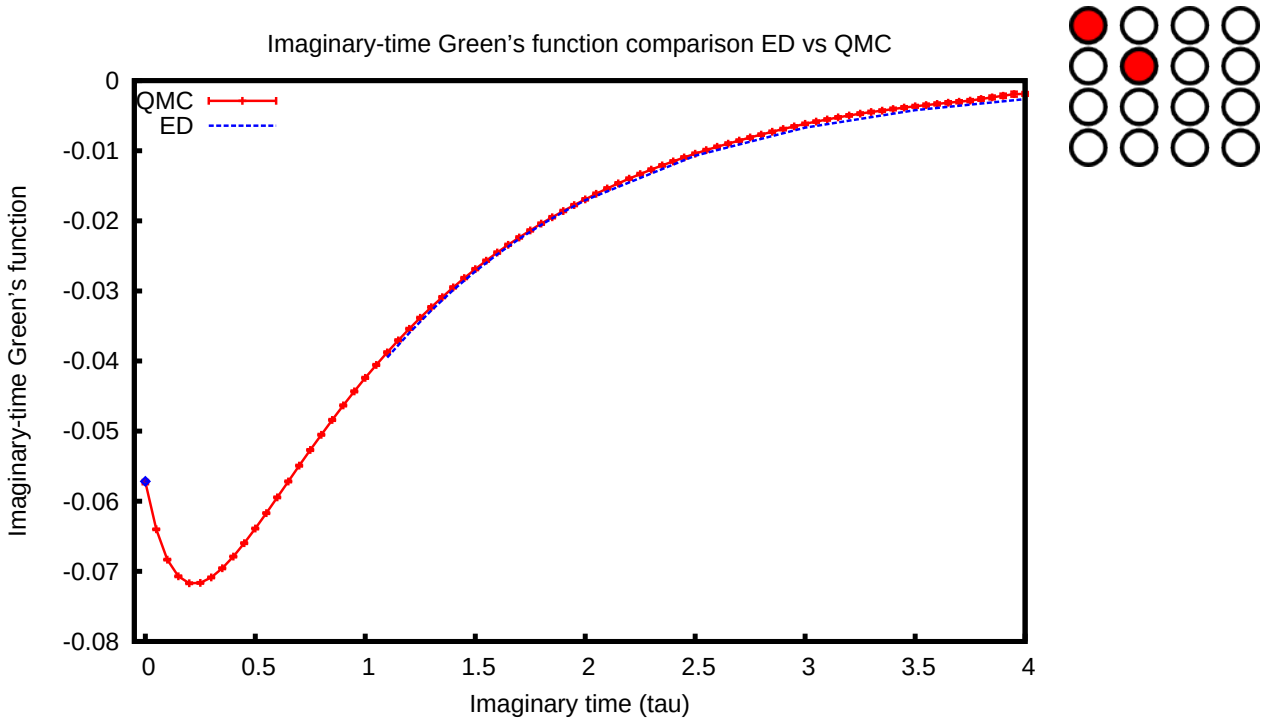
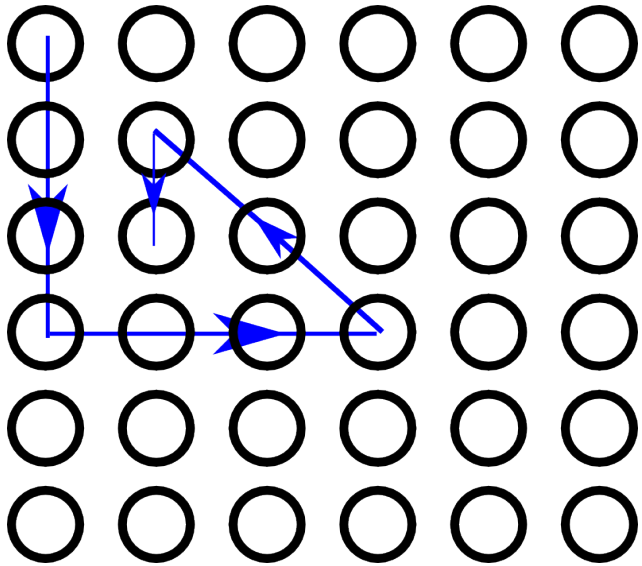


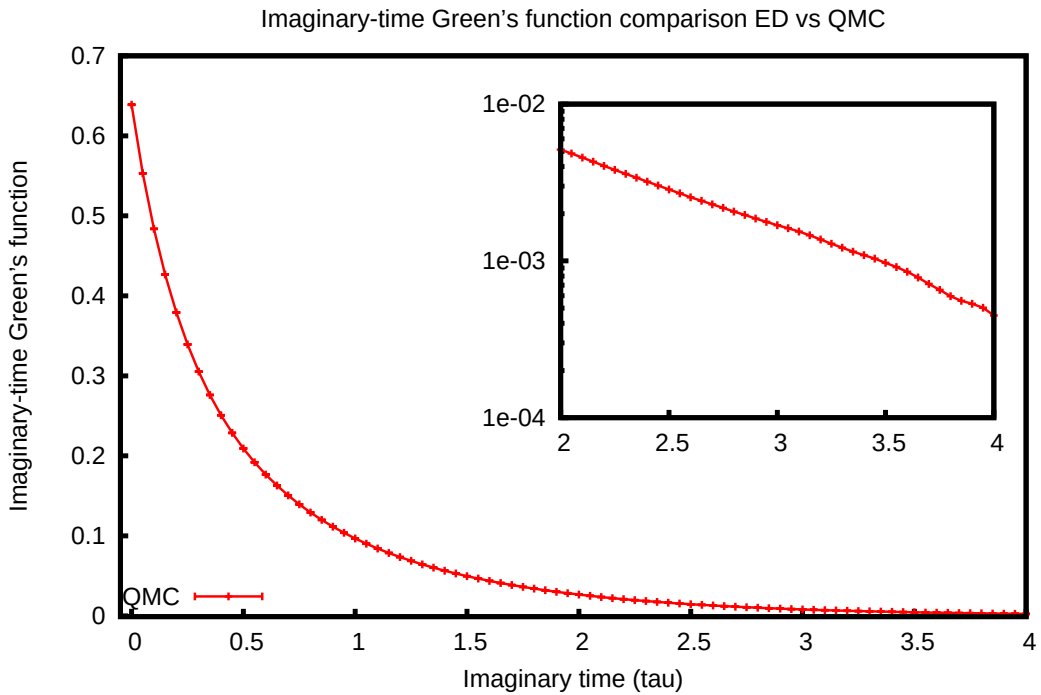
Benchmark: 4×4 lattice, $5 \uparrow 5 \downarrow$, $U = 4$

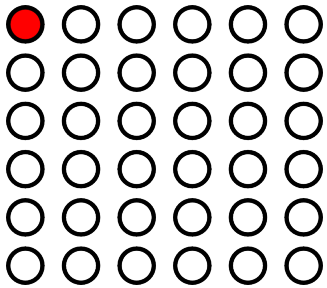
Application



- 6×6 lattice, $13 \uparrow 13 \downarrow$ electrons.
- Hilbert space dimension: 5.4×10^{18}
  - 156m times larger than largest ED system.

Application

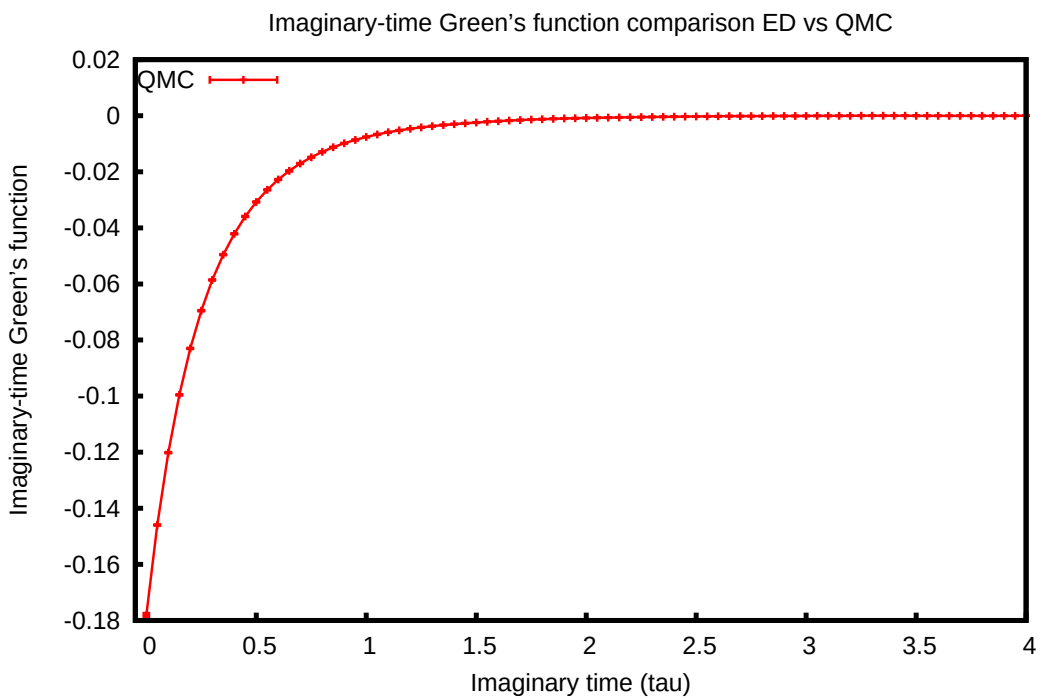


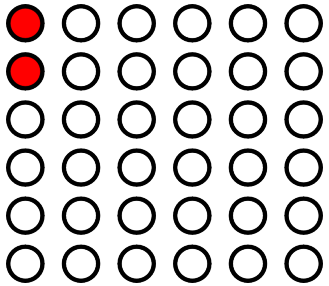


Benchmark: 6×6 lattice, $13 \uparrow 13 \downarrow$, $U = 4$

Chemical potential: $-1.179(5)$ ($\tau = 3$ to 4).

Application





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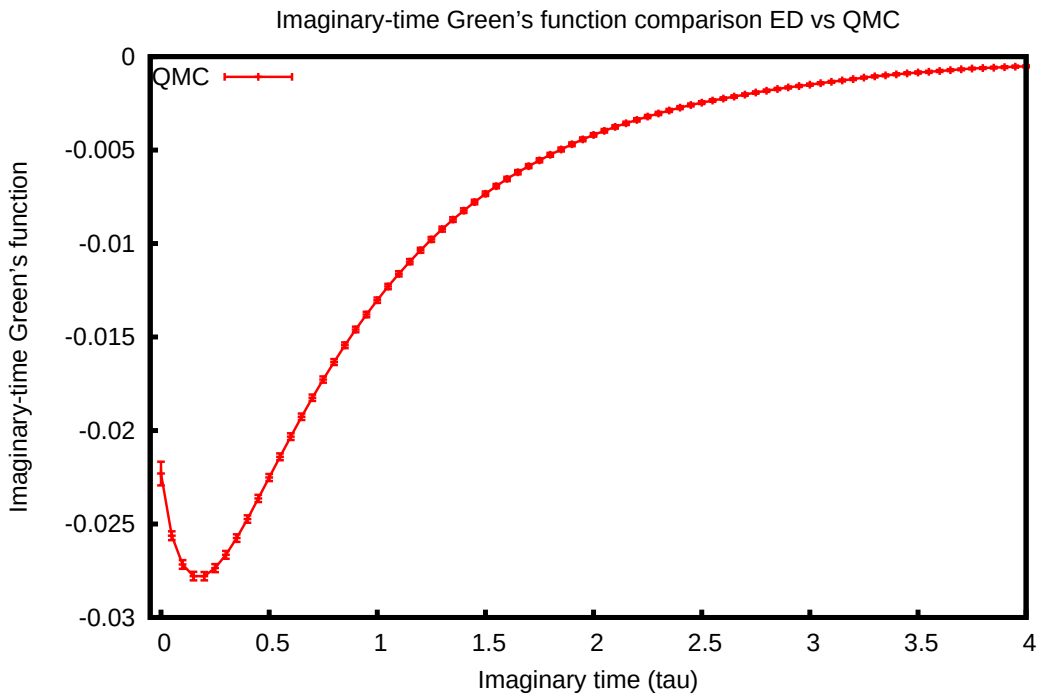

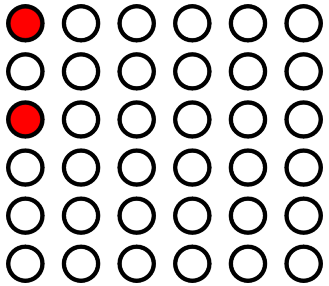

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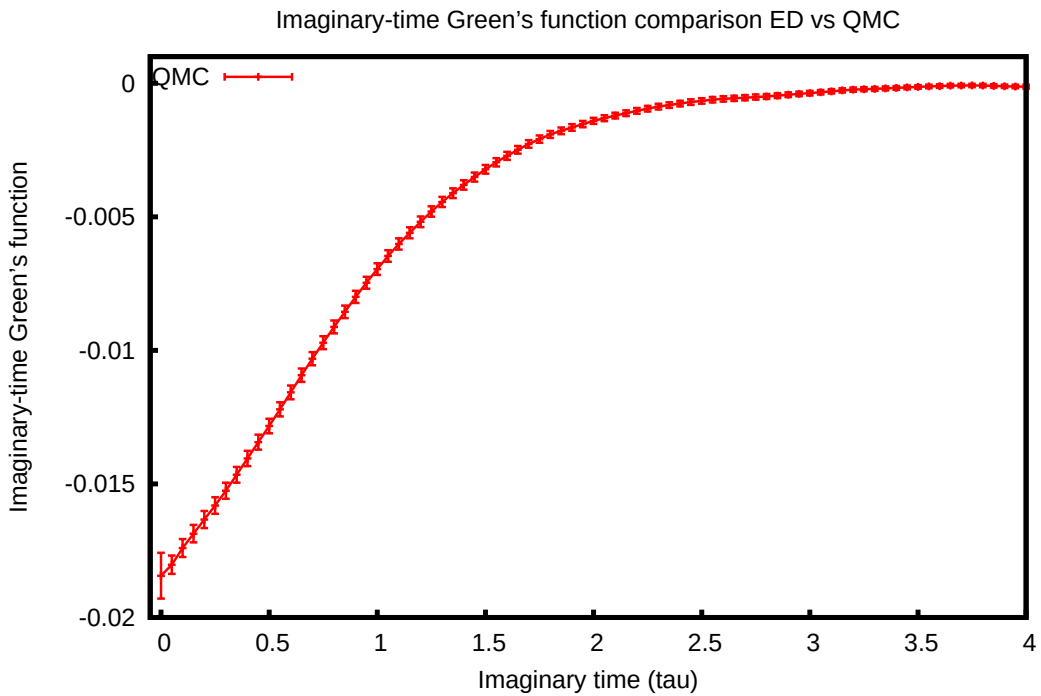

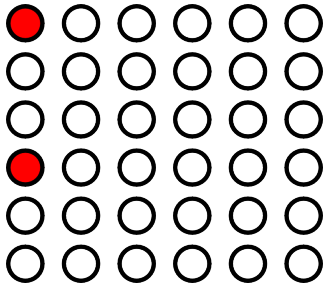

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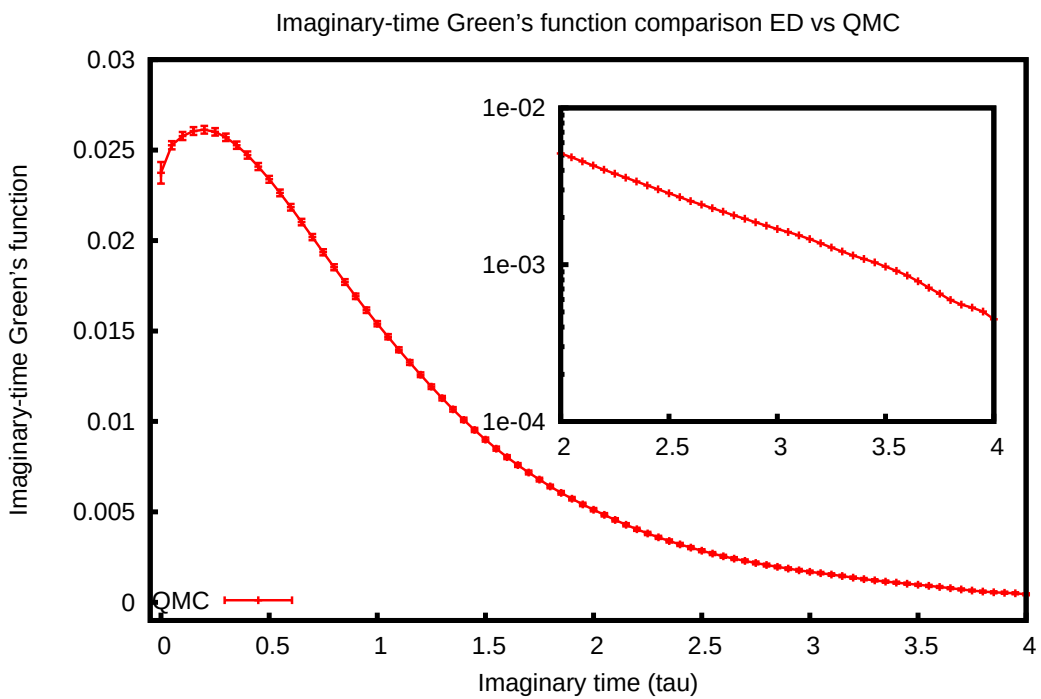

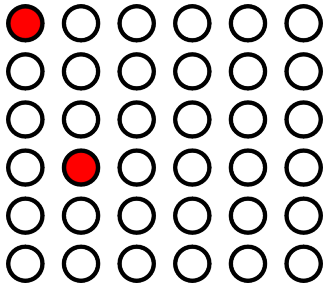

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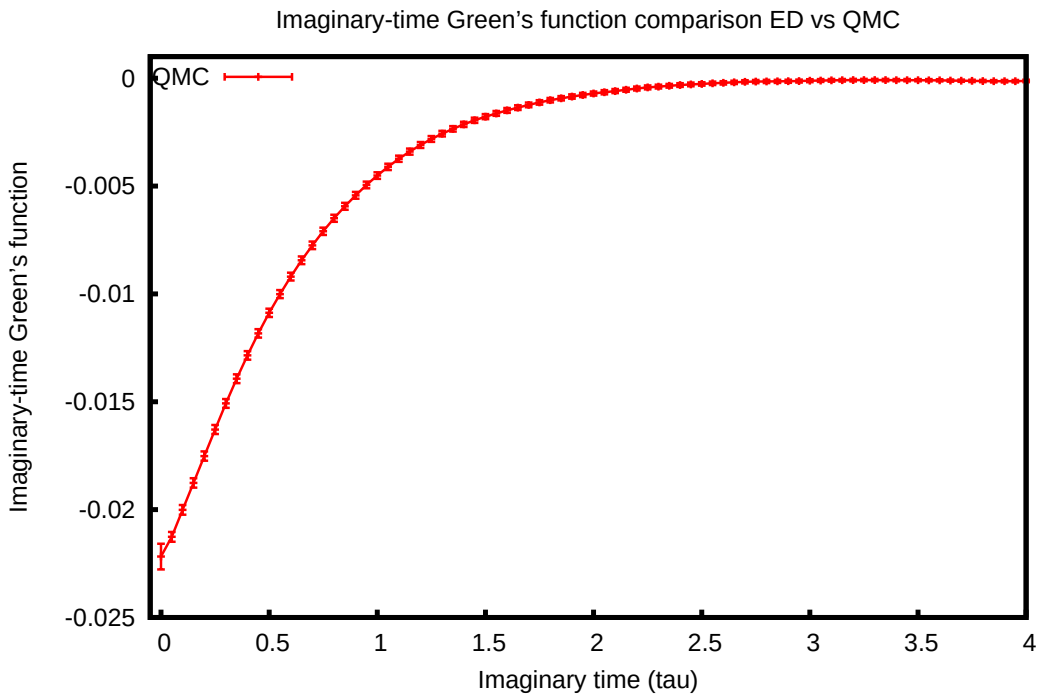

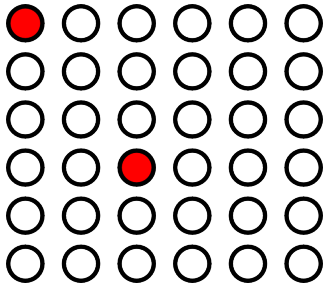

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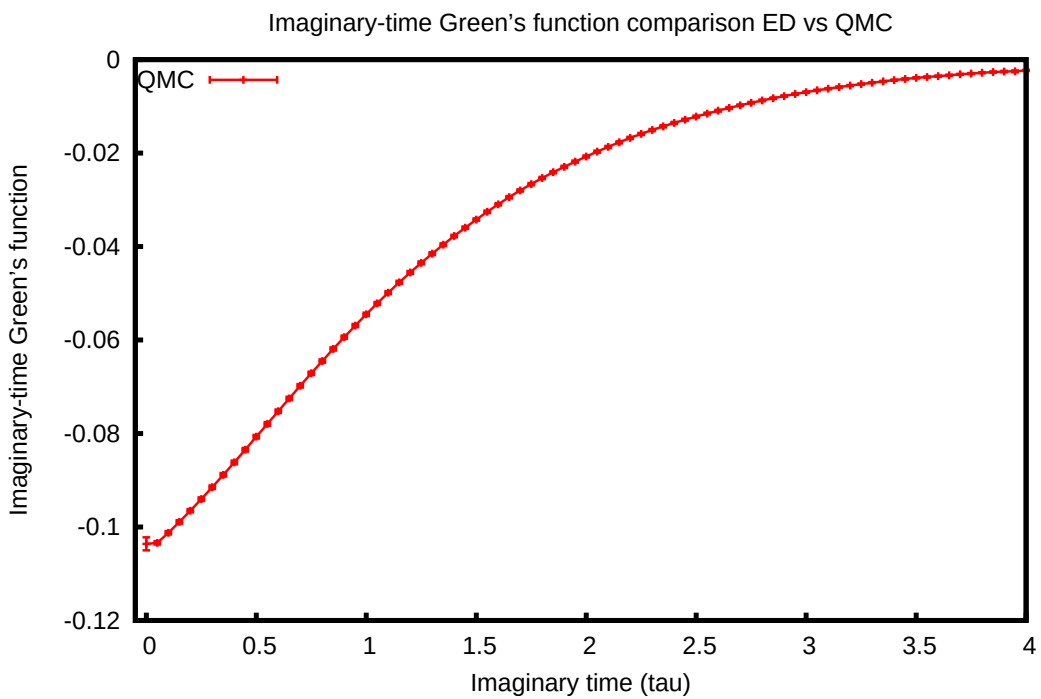
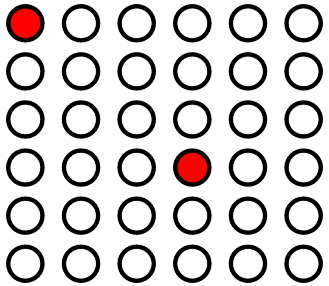
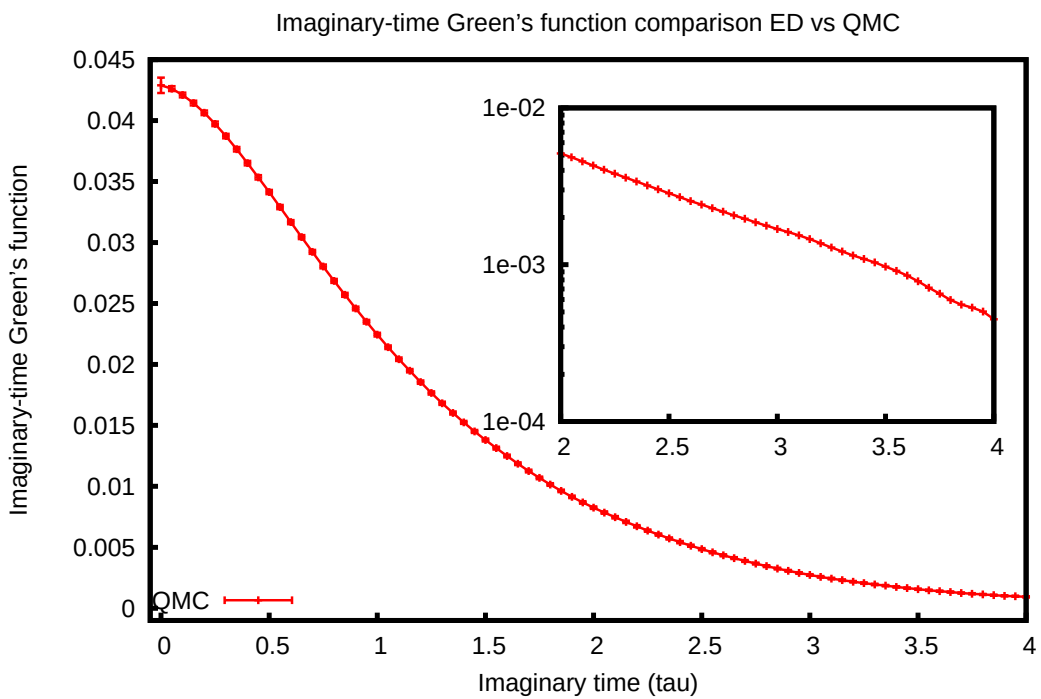
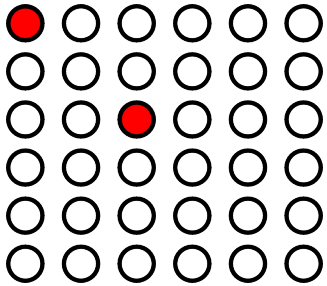




Benchmark: 6×6 lattice, $13 \uparrow 13 \downarrow$, $U = 4$

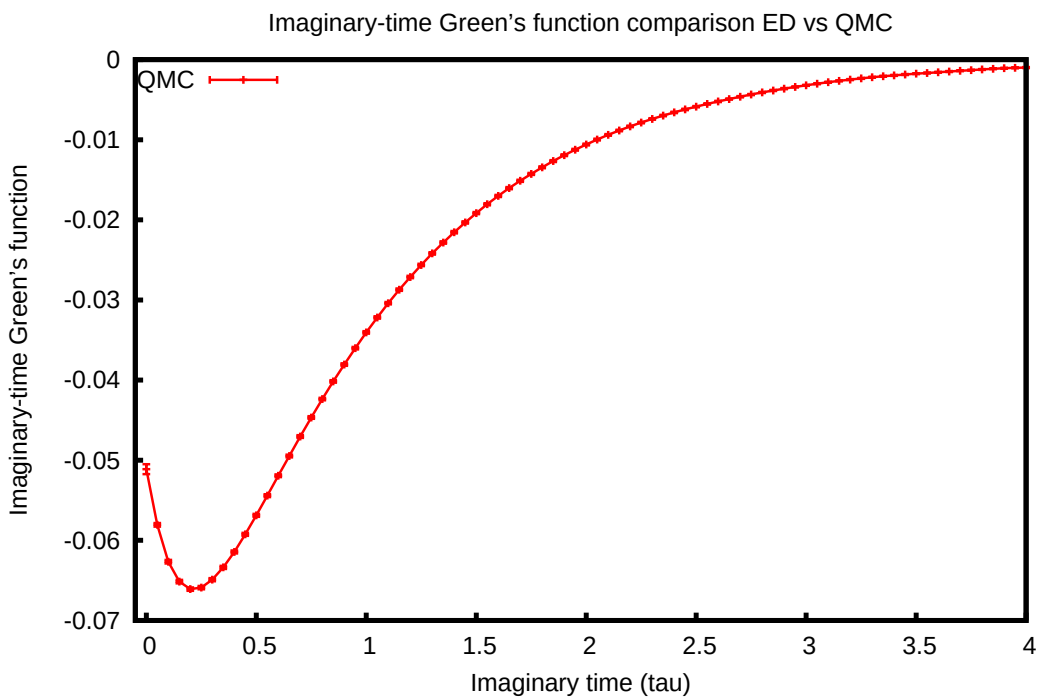
Application

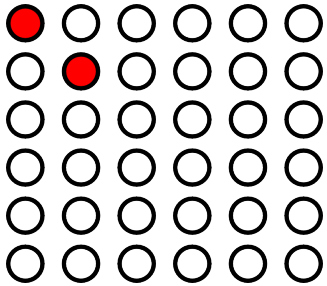




Benchmark: 6×6 lattice, $13 \uparrow 13 \downarrow$, $U = 4$

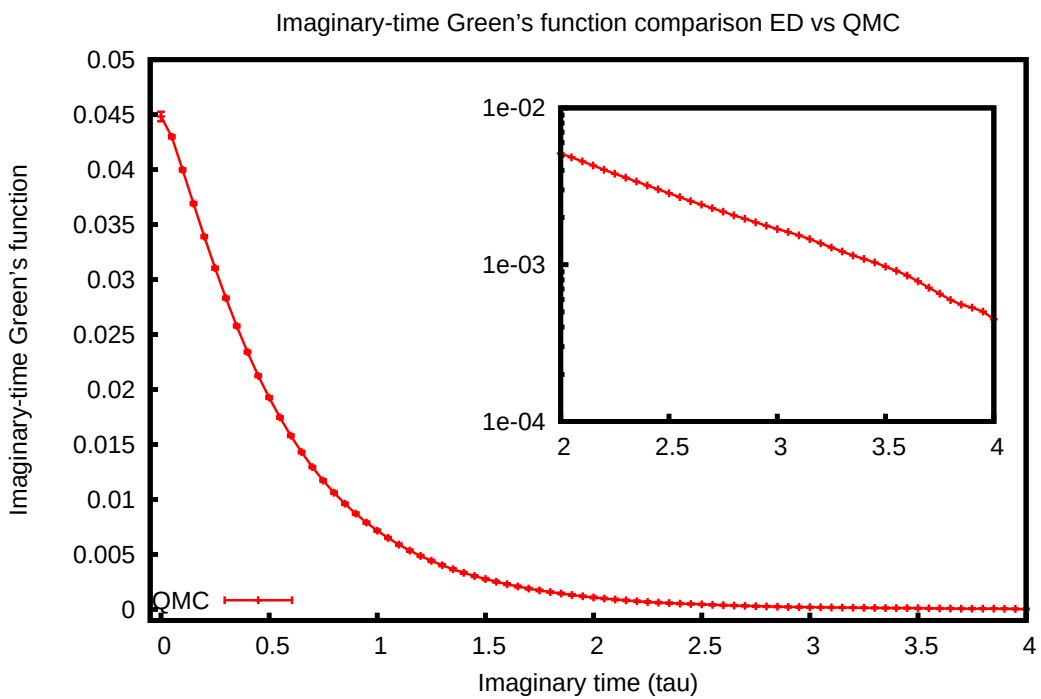
Application

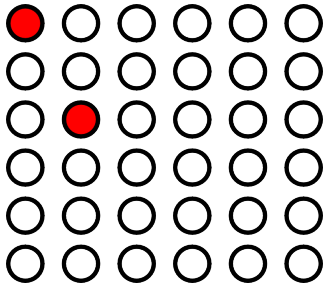




Benchmark: 6×6 lattice, $13 \uparrow 13 \downarrow$, $U = 4$

Application





Benchmark: 6×6 lattice, $13 \uparrow 13 \downarrow$, $U = 4$

Future work

- Better ED benchmarks.
- Multi-determinant trial wave function.
- Calculate physical quantities:
  - Charge and magnetic structure factors and susceptibility.
  - Current-current correlator, Drude weight.
- Convert imaginary-time Green's function calculation to FORTRAN.

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- For more details, visit `www.huy-nguyen.com/Reed-thesis` .

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