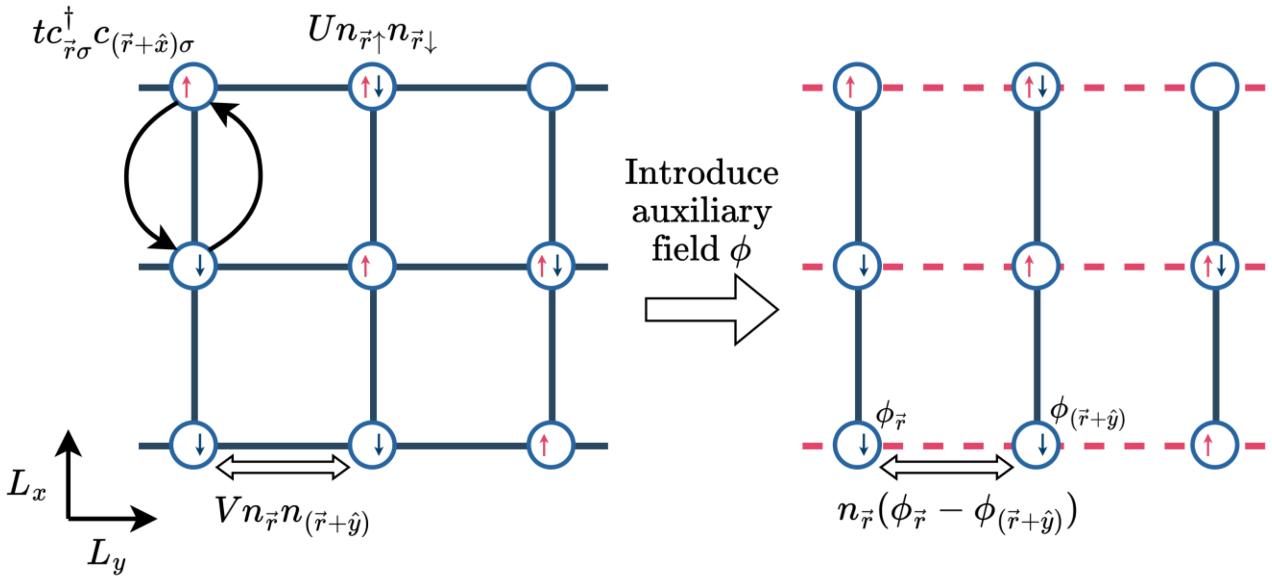

H^2MC: A HYBRID HAMILTONIAN MONTE CARLO FRAMEWORK FOR INTERACTING QUANTUM WIRES

JULY 28TH 2026 I FINN TEMMEN I FORSCHUNGSZENTRUM JÜLICH

Member of the Helmholtz Association

JÜLICH Forschungszentrum

HYBRID HAMILTONIAN MONTE CARLO

A FRAMEWORK FOR INTERACTING QUANTUM WIRES

JULY 28TH 2026 I FINN TEMMEN I FORSCHUNGSZENTRUM JÜLICH

IN COLLABORATION WITH

MARTINA GISTI	(UNIVERSITY OF BONN)
DAVID LUITZ	(UNIVERSITY OF BONN)
JOHANN OSTMEYER	(UNIVERSITY OF BONN)
THOMAS LUU	(FORSCHUNGSZENTRUM JÜLICH)

MOTIVATION

Stochastic vs direct methods

Direct methods

- Exact Diagonalization (ED)
- Thermal trace formalism
- Numerically exact
- Exponential Scaling

Stochastic methods

- Hamiltonian Monte Carlo (HMC)
- Path integral formalism
- Polynomial scaling
- Sign problem
- Autocorrelation times / Ergodicity violations

MOTIVATION

Stochastic vs direct methods

Direct methods
- Exact Diagonalization (ED)
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Stochastic methods
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Hybrid Hamiltonian Monte Carlo ($\mathrm{H^2MC}$)
A Hybrid ED and HMC framework

SETTING THE STAGE

Interacting quantum wires as Hubbard chains

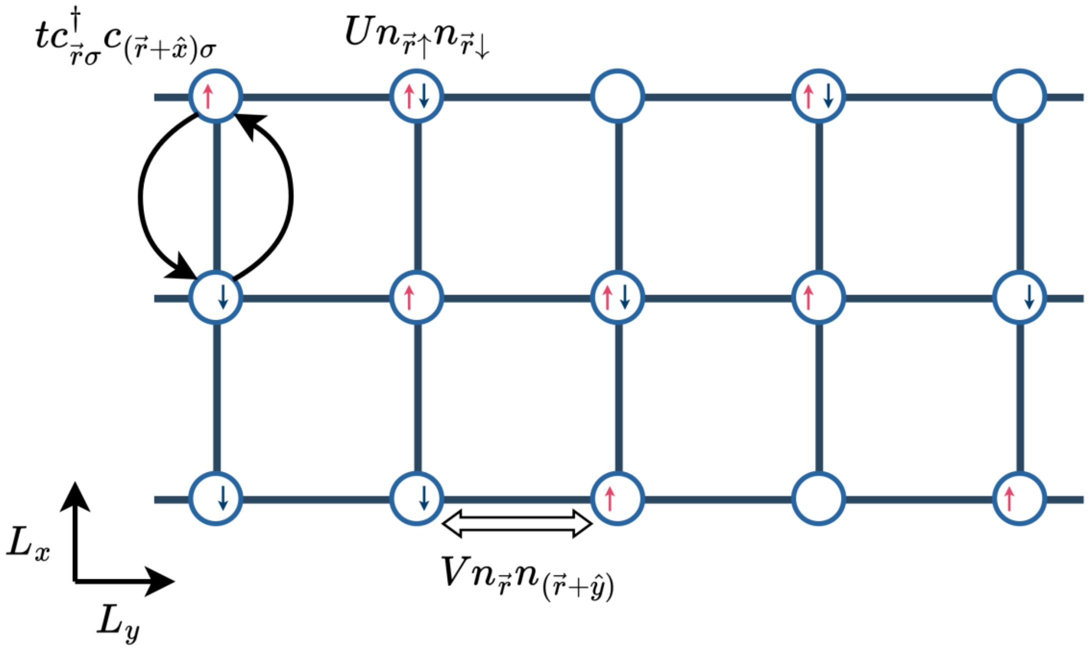
$$n_{xy\sigma} = c^\dagger_{xy\sigma} c_{xy\sigma}$$

$$n_{xy} = \sum_\sigma n_{xy\sigma}$$

Bollmark et al. arXiv:2411.00480 (2024)

$$H^{(y)}_{1\mathrm{D}} = \sum_{x=1}^{L_x} \left[- \sum_{\sigma=\{\uparrow,\downarrow\}} t_\sigma \left(c^\dagger_{xy\sigma} c_{(x+1)y\sigma} + \mathrm{h.c.} \right) + U n_{xy\uparrow} n_{xy\downarrow} + \mu n_{xy} \right]$$

$$H = \sum_{y=1}^{L_y} H^{(y)}_{1\mathrm{D}} - \frac{V}{2} \sum_{y=1}^{L_y} \sum_{x=1}^{L_x} \left(n_{xy} - n_{x(y+1)} \right)^2$$



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SETTING THE STAGE

Decoupling the chains

$$n_{ij\sigma} = c^\dagger_{ij\sigma} c_{ij\sigma}$$

$$n_{ij} = \sum_\sigma n_{ij\sigma}$$

$$H = \sum_{y=1}^{L_y} H_{1\mathrm{D}}^{(y)} - \frac{V}{2} \sum_{y=1}^{L_y} \sum_{x=1}^{L_x} \left(n_{xy} - n_{x(y+1)}\right)^2$$

$$Z = \mathrm{tr}\left[e^{-\beta\left(\sum_{y=1}^{L_y} H_{1\mathrm{D}}^{(y)} + H_V\right)} \right]$$

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SETTING THE STAGE

$$n_{ij\sigma} = c^\dagger_{ij\sigma} c_{ij\sigma}$$

$$n_{ij} = \sum_\sigma n_{ij\sigma}$$

Decoupling the chains

$$H = \sum_{y=1}^{L_y} H^{(y)}_{1\mathrm{D}} - \frac{V}{2} \sum_{y=1}^{L_y} \sum_{x=1}^{L_x} \left(n_{xy} - n_{x(y+1)}\right)^2$$

Suzuki-Trotter decomposition

$$Z = \mathrm{tr}\left[\prod_{t=1}^{N_t} \left(e^{-\Delta_t \sum_y H^{(y)}_{1\mathrm{D}}} \; e^{-\Delta_t H_V}\right)\right] + \mathcal{O}(\Delta_t^2)$$

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SETTING THE STAGE

$$n_{ij\sigma} = c^\dagger_{ij\sigma} c_{ij\sigma}$$
$$n_{ij} = \sum_\sigma n_{ij\sigma}$$

Decoupling the chains

$$H = \sum_{y=1}^{L_y} H^{(y)}_{1\mathrm{D}} - \frac{V}{2} \sum_{y=1}^{L_y} \sum_{x=1}^{L_x} \left(n_{xy} - n_{x(y+1)}\right)^2$$

Suzuki-Trotter decomposition

$$Z = \mathrm{tr}\left[\prod_{t=1}^{N_t} \left(e^{-\Delta_t \sum_y H^{(y)}_{1\mathrm{D}}}\; e^{-\Delta_t H_V}\right)\right] + \mathcal{O}(\Delta_t^2)$$

Hubbard-Stratonovich (HS) transformation

$$e^{\frac{\tilde{V}}{2}\left(n_{xy} - n_{x(y+1)}\right)^2} \propto \int_{-\infty}^{\infty} d\phi_{txy}\; e^{-\frac{\phi^2_{txy}}{2\tilde{V}} - \phi_{txy}\left(n_{xy} - n_{x(y+1)}\right)}$$

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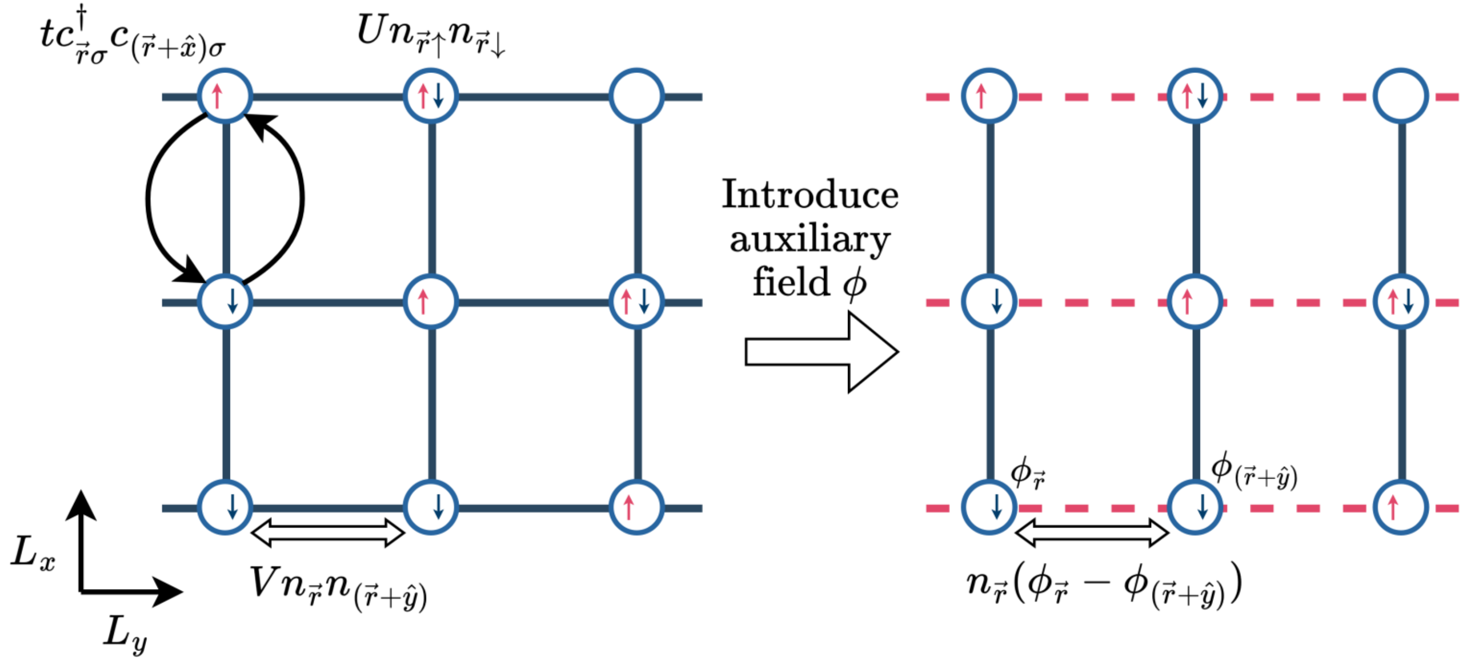
SETTING THE STAGE

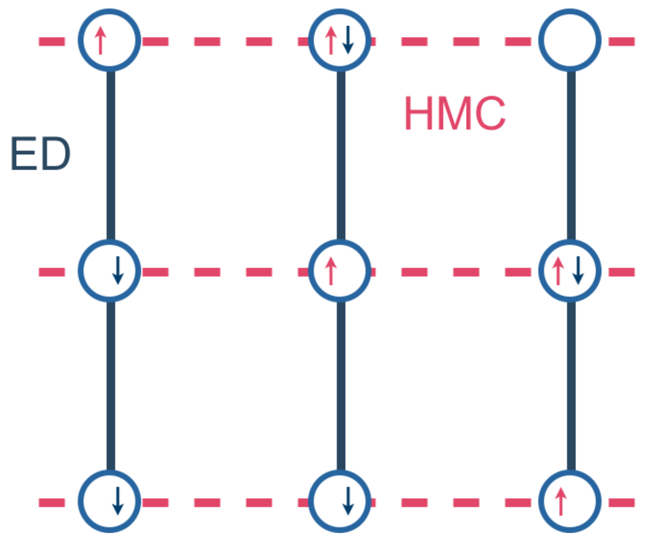
Hybrid formulation

$$\mathrm{tr}\left[\bigotimes_{y=1}^{L_y}\prod_t\left(e^{-\Delta_t H_{1\mathrm{D}}^{(y)}}e^{-\sum_x n_{xy}\Delta\phi_{txy}}\right)\right]=\prod_{y=1}^{L_y}\mathrm{tr}_y\left[\prod_t\left(e^{-\Delta_t H_{1\mathrm{D}}^{(y)}}e^{-\sum_x n_{xy}\Delta\phi_{txy}}\right)\right]$$



SETTING THE STAGE

Hybrid formulation



Action

$$S[\phi] = \sum_{txy} \frac{\phi_{txy}^2}{2\tilde{V}} - \sum_y S_y^{\mathrm{ED}}[\phi]$$

Fermion trace

$$S_y^{\mathrm{ED}}[\phi] = \log \mathrm{tr}_y \left[\prod_t \left(e^{-\Delta_t H_{1\mathrm{D}}^{(y)}} e^{-\sum_x n_{xy} \Delta \phi_{txy}} \right) \right]$$

Force

$$\partial_{\phi_{txy}} S[\phi] = \frac{1}{\tilde{V}} \phi_{txy} + \langle n_{xy}(t) \rangle - \langle n_{x(y+1)}(t) \rangle$$

RESULTS

Benchmarking against pure HMC

- Pure HMC needs **additional HS transformation** in U
- Compare to **two pure HMC formulations** with different sampling properties
    - Real field (χ)
    - Imaginary field ($i\chi$)

RESULTS

Benchmarking against pure HMC

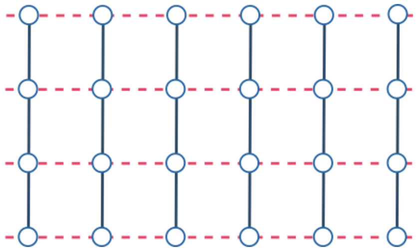
- Pure HMC needs **additional HS transformation** in U
- Compare to **two pure HMC formulations** with different sampling properties
  - Real field (χ)
  - Imaginary field ($i\chi$)

- Quantify sampling efficiency
  - **Average phase** $$\Sigma = \left|\langle e^{-i\mathrm{Im}(S)}\rangle_{\mathrm{Re}(S)}\right|$$
  - **Integrated autocorrelation time** $$\tau_{\mathrm{int},\mathcal{O}} = \frac{1}{2}\sum_{t=-\infty}^{\infty}\frac{\Gamma_{\mathcal{O}}(t)}{\Gamma_{\mathcal{O}}(0)}$$

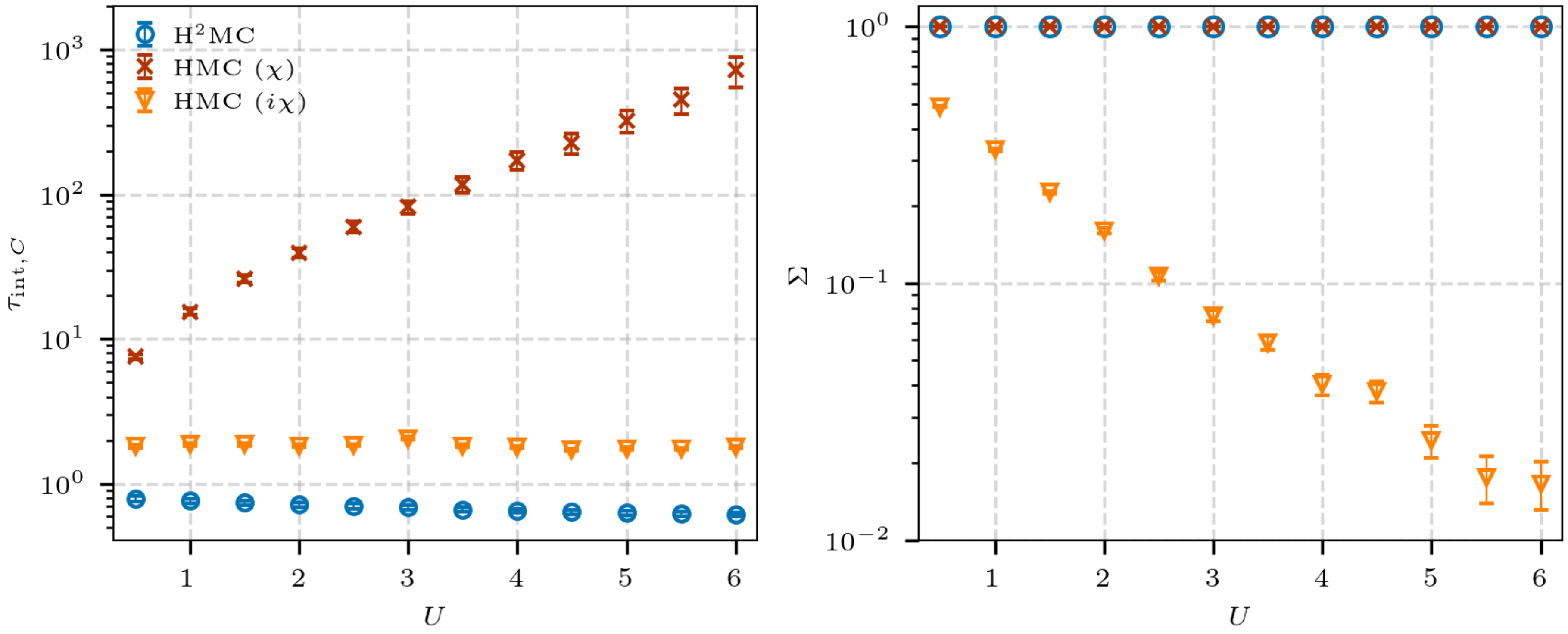
Wolff CPC **156** (2004)

RESULTS

Benchmarking against pure HMC



$\beta = 1$
$V = 0.2$
$\mu = \text{half-filling}$



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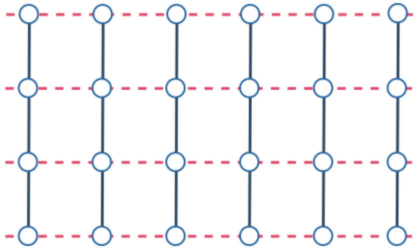
RESULTS

Numerical Stability

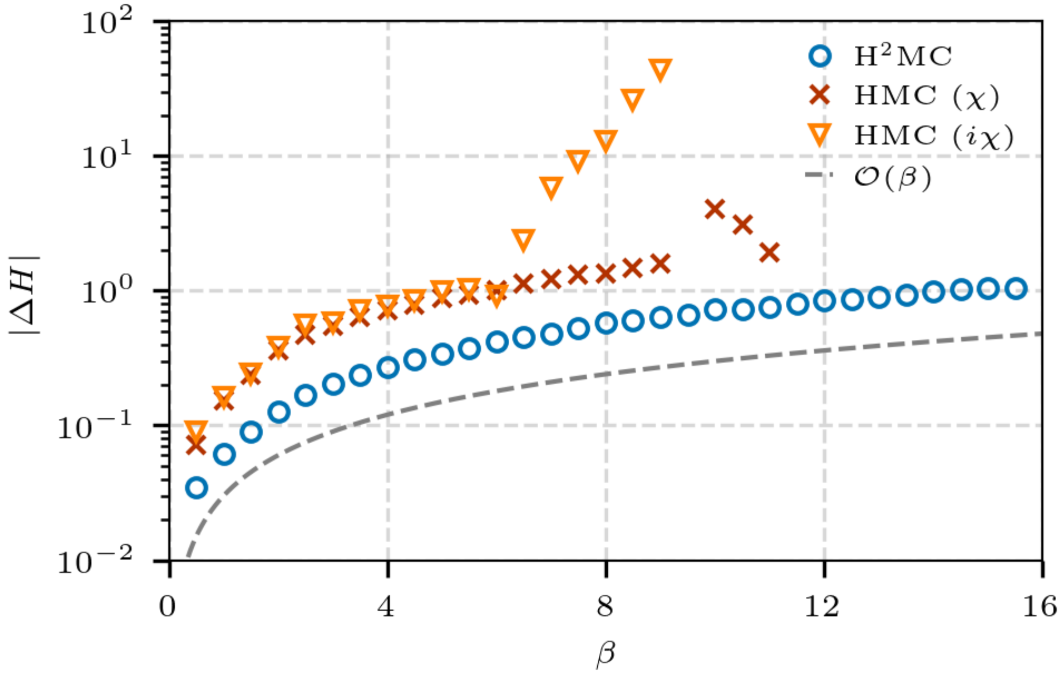


$U = 2$
$V = 0.5$
$\mu = \text{half-filling}$

- **Median of $|\Delta H|$** during molecular dynamics
- **Pure HMC: numerically unstable** with larger β
  - Matrix multiplications with vastly different scales
  - Matrix inversions in gradient
  - Need **stabilization**, separation of scales

Luu, FT et al. arXiv:2604.00815 (2026)

- $\mathrm{H^2MC}$: trace is **numerically benign**



EXTENDING THE MODEL

Interacting quantum chains

- Extend the chains with **s-wave pairing** term

$$H_{1\mathrm{D}}^{(y)} \to H_{1\mathrm{D}}^{(y)} + \Delta_s \sum_x \left(\Delta_{xy}^\dagger + \mathrm{h.c.}\right)$$

$$\Delta_{xy}^\dagger = c_{xy\uparrow}^\dagger c_{xy\downarrow}^\dagger$$

- More involved for pure HMC (**Pfaffian QMC**)

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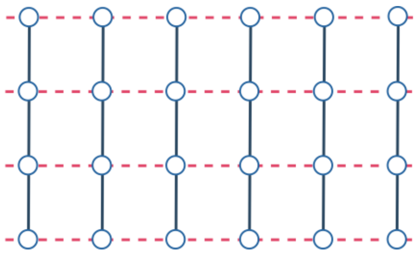
EXTENDING THE MODEL

Interacting quantum chains

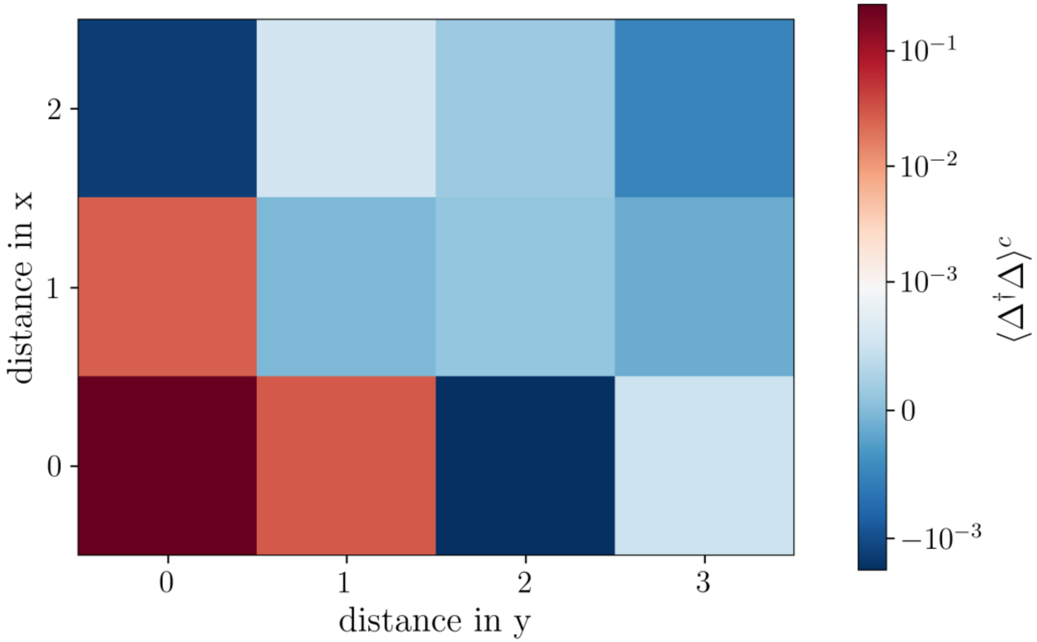


$\beta = 2$
$U = 2$
$V = 0.2$
$\mu = \text{half-filling}$
$\Delta_s = 2$

- Extend the chains with **s-wave pairing** term

$$H_{1\mathrm{D}}^{(y)} \to H_{1\mathrm{D}}^{(y)} + \Delta_s \sum_x \left(\Delta_{xy}^\dagger + \text{h.c.}\right)$$

$$\Delta_{xy}^\dagger = c_{xy\uparrow}^\dagger c_{xy\downarrow}^\dagger$$



- More involved for pure HMC (**Pfaffian QMC**)
- **Connected Cooper pair correlator**

$$\langle \Delta^\dagger \Delta_{(\Delta_x,\Delta_y)} \rangle^c = \frac{1}{L_x L_y} \sum_{x,y} \left(\langle \Delta_{xy}^\dagger \Delta_{(x+\Delta_x)(y+\Delta_y)} \rangle - \langle \Delta_{xy}^\dagger \rangle \langle \Delta_{xy} \rangle \right)$$

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PSEUDO-PSEUDOFERMIONS ($\mathrm{PSEUDO}^2\mathrm{FERMIONS}$)

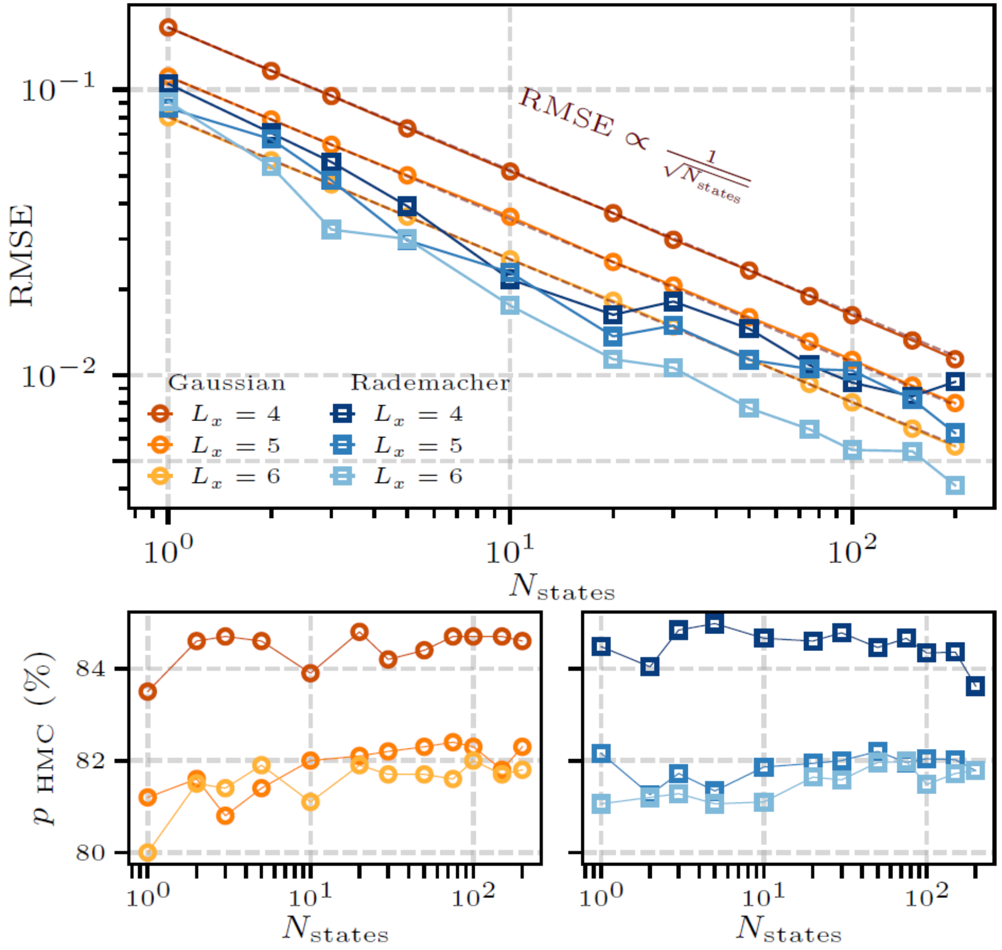
Accelerating the gradient computation

PSEUDO-PSEUDOFERMIONS (PSEUDO²FERMIONS)

Accelerating the gradient computation

- **Stochastic trace estimators**

$$\mathrm{tr}(\mathcal{O}) \approx \frac{1}{N_{\mathrm{states}}} \sum_{k=1}^{N_{\mathrm{states}}} \langle \tilde{\psi}_k | \mathcal{O} | \tilde{\psi}_k \rangle$$



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PSEUDO-PSEUDOFERMIONS (PSEUDO^{2}FERMIONS)

Accelerating the gradient computation

- **Stochastic trace estimators**

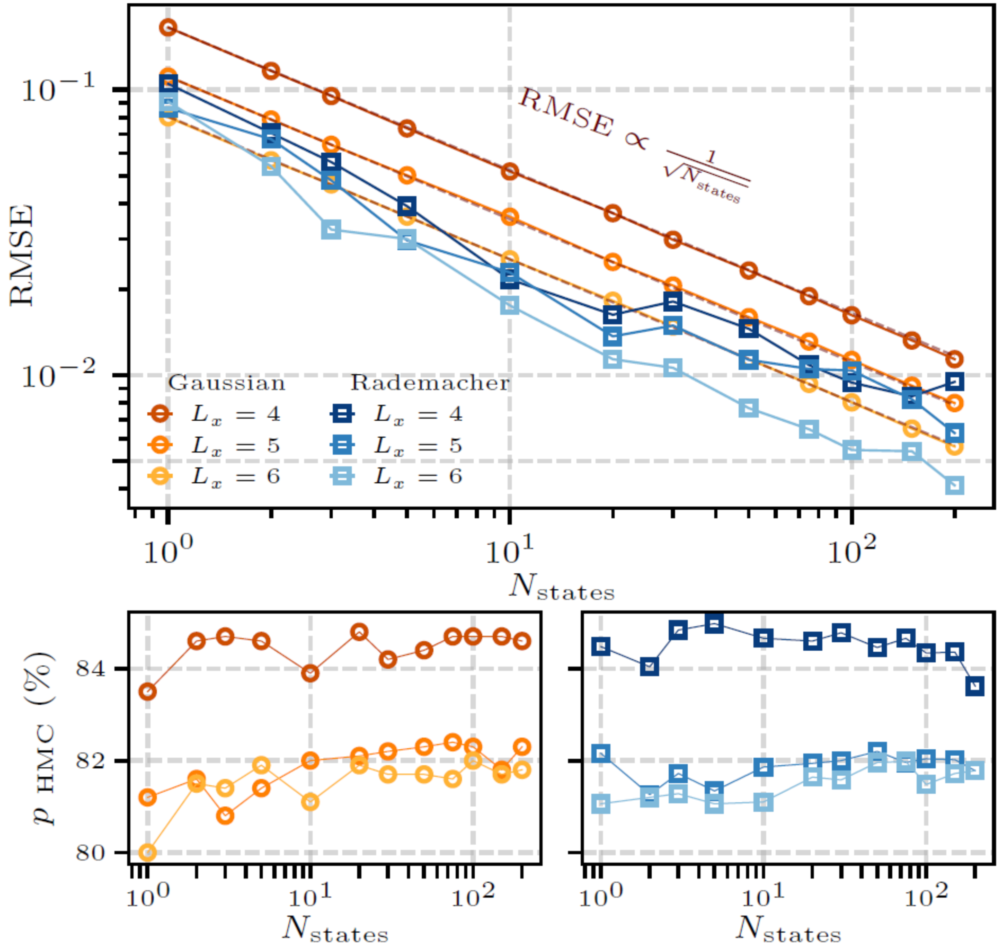
$$\mathrm{tr}(\mathcal{O}) \approx \frac{1}{N_{\mathrm{states}}} \sum_{k=1}^{N_{\mathrm{states}}} \langle \tilde{\psi}_k | \mathcal{O} | \tilde{\psi}_k \rangle$$

- Using sparse matrix vector multiplication

$$\mathcal{O}(L_y N_{\mathrm{states}} N_t 4^{L_x})$$

- Leading order scaling from action

$$\mathcal{O}(L_y N_t 4^{2L_x})$$



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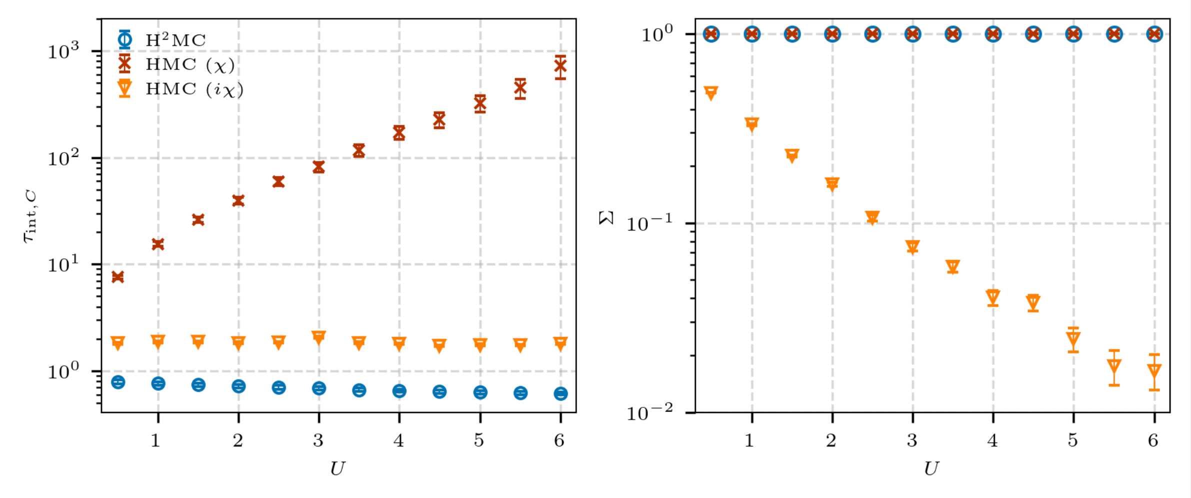
SUMMARY AND OUTLOOK

Take home message and future avenues

FT, Martina Gisti et al.
arXiv:2603.17788 (2026)

$\mathrm{H^2MC}$: Hybridizing direct (ED) and stochastic (HMC) methods

- Interactions between chains treated with HMC
- Fermion determinant replaced by trace and solved via ED
- Outperforms ED in scaling
- Can outperform pure HMC



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SUMMARY AND OUTLOOK

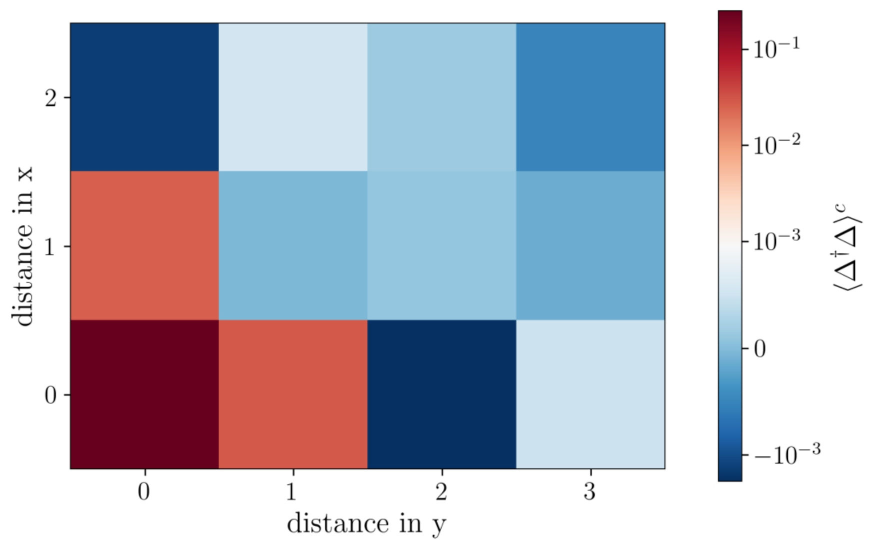
Take home message and future avenues

FT, Martina Gisti et al.
arXiv:2603.17788 (2026)

$\mathrm{H^2MC}$: Hybridizing direct (ED) and stochastic (HMC) methods

Extension of the model

- Extension on chains
  - Quantum/Kitaev chains
  - Extended interactions
- Equivalent formulation for other quartic operators



SUMMARY AND OUTLOOK

Take home message and future avenues

FT, Martina Gisti et al.
arXiv:2603.17788 (2026)

- $\mathrm{H^2MC}$: **Hybridizing direct (ED) and stochastic (HMC) methods**
- **Extension of the model**
- **Extension of the algorithm**
  - Pseudo-Pseudofermions for action
  - Radial updates
  - Replacing ED with Tensor Networks
    - Matrix Product Operators (MPOs) and Time-evolving block decimation (TEBD)

Kennedy, Yu PoS Lattice (2024)
Ostmeyer JPhysA **58** (2025)
FT et al. PhysRevB **112** (2025)

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BACKUP SLIDES

APPENDIX

Ambiguity in Hubbard-Stratonovich transformation

- Ambiguity in Hubbard-Stratonovich transformations

$$e^{+\frac{\tilde{V}}{2}\left(n_{xy}-n_{x(y+1)}\right)^2} \propto \int_{-\infty}^{\infty} d\phi_{txy}\ e^{-\frac{\phi_{txy}^2}{2\tilde{V}}-\phi_{txy}\left(n_{xy}-n_{x(y+1)}\right)}$$

$$e^{-\frac{\tilde{V}}{2}\left(n_{xy}+n_{x(y+1)}\right)^2} \propto \int_{-\infty}^{\infty} d\phi_{txy}\ e^{-\frac{\phi_{txy}^2}{2\tilde{V}}-i\phi_{txy}\left(n_{xy}+n_{x(y+1)}\right)}$$

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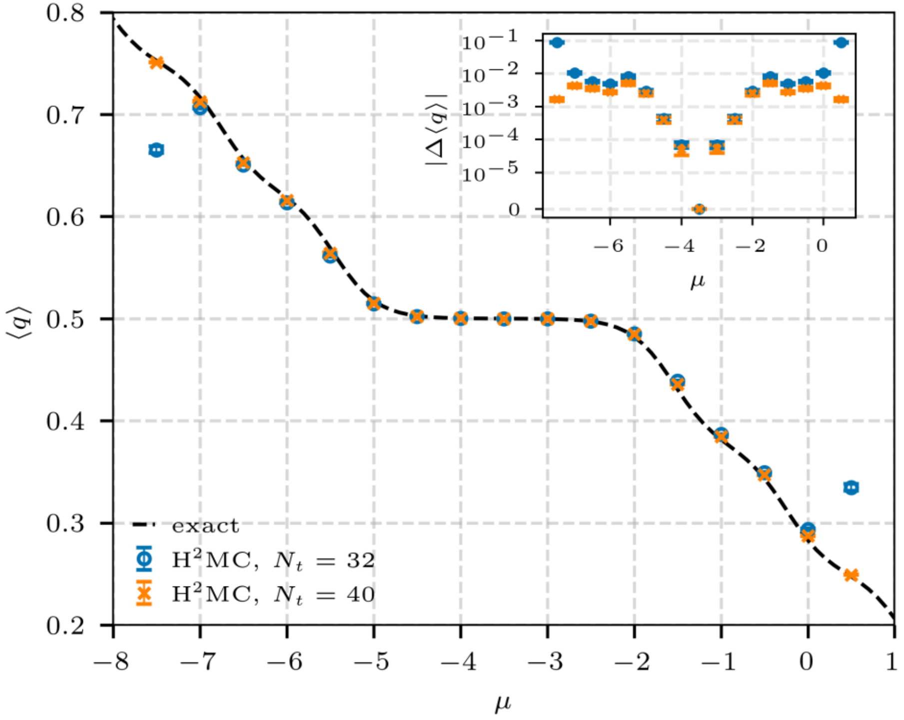
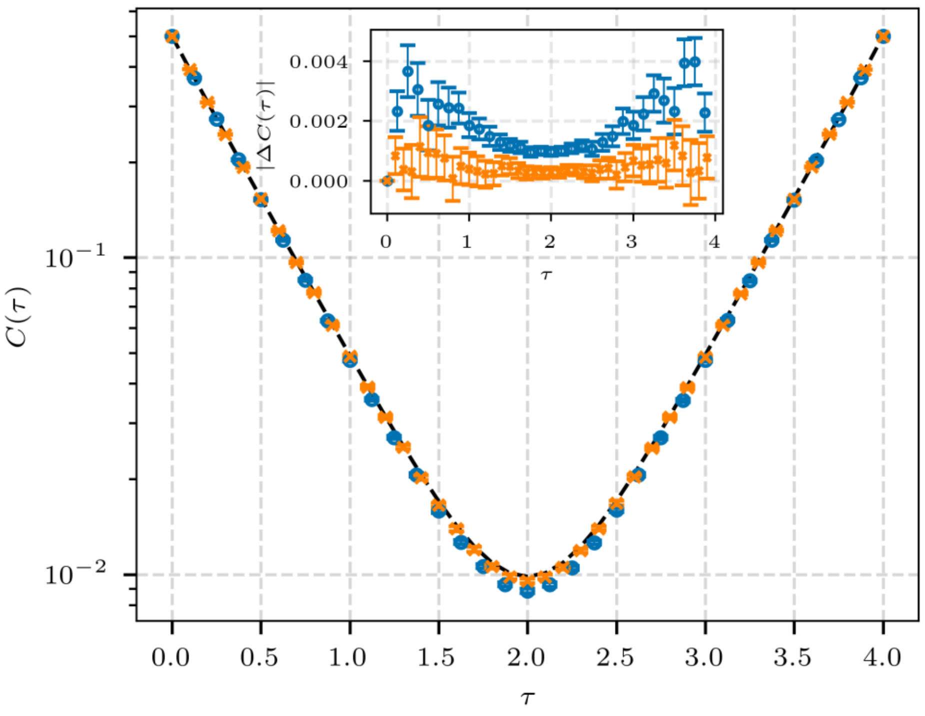
APPENDIX

Benchmarking with full ED

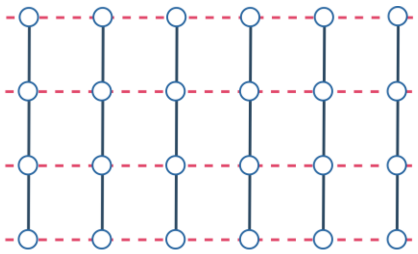
$L_x = 2$
$L_y = 2$
$\beta = 4$
$U = 3$
$V = 1$

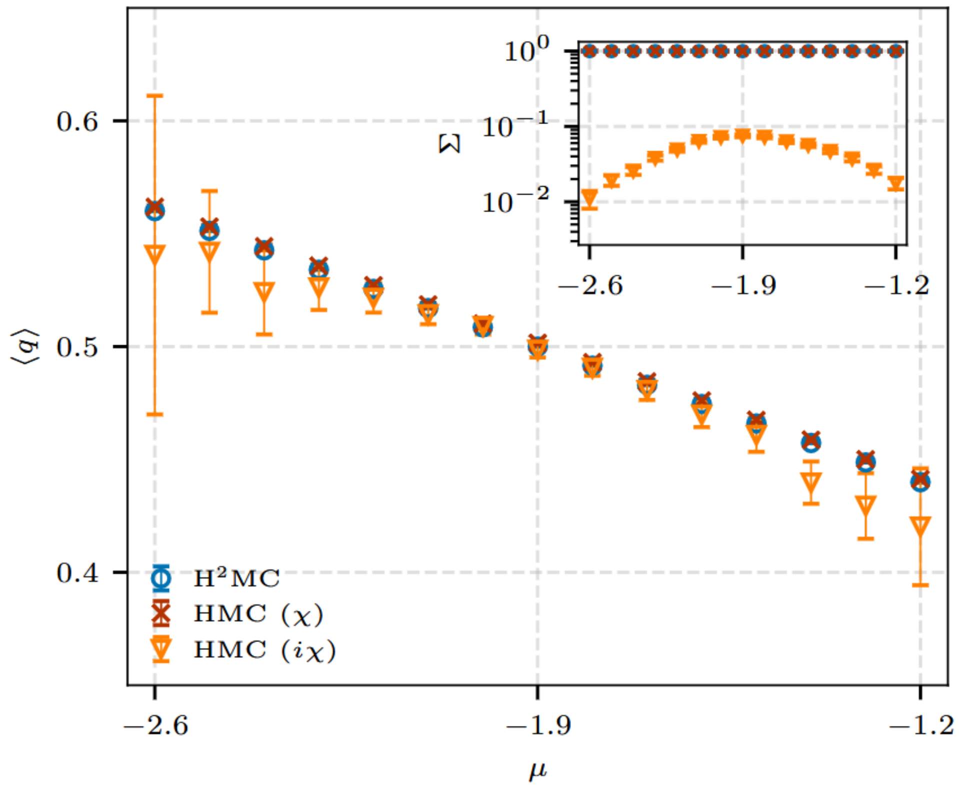


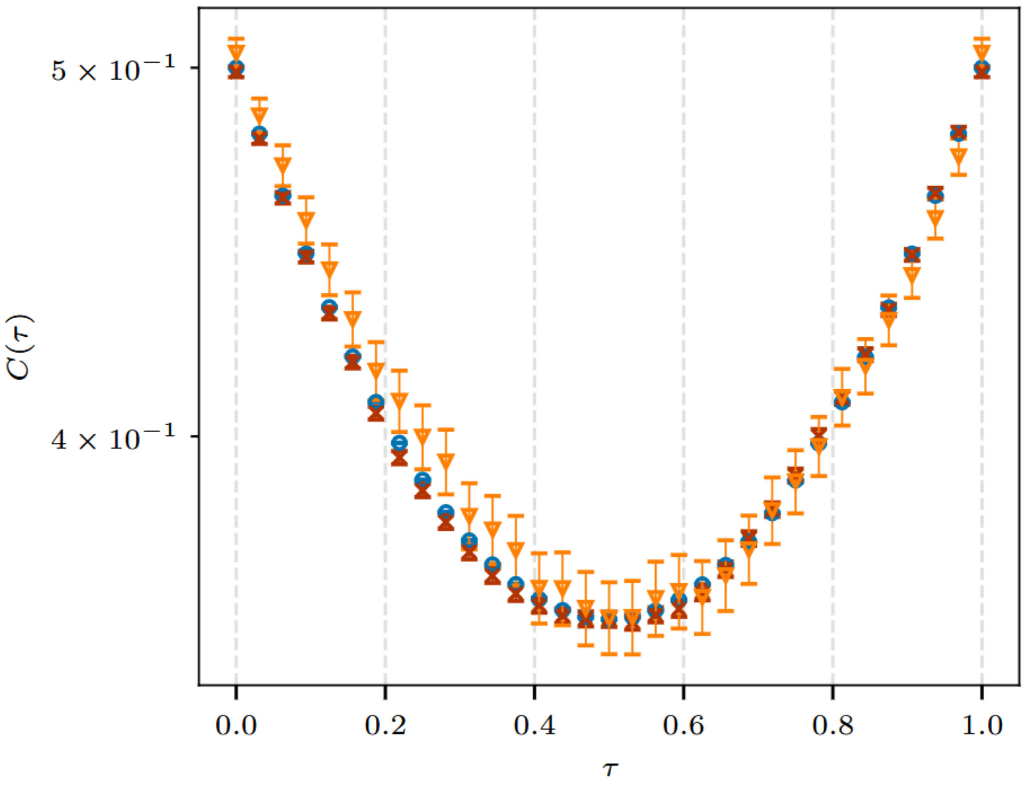


APPENDIX

Benchmarking against pure HMC







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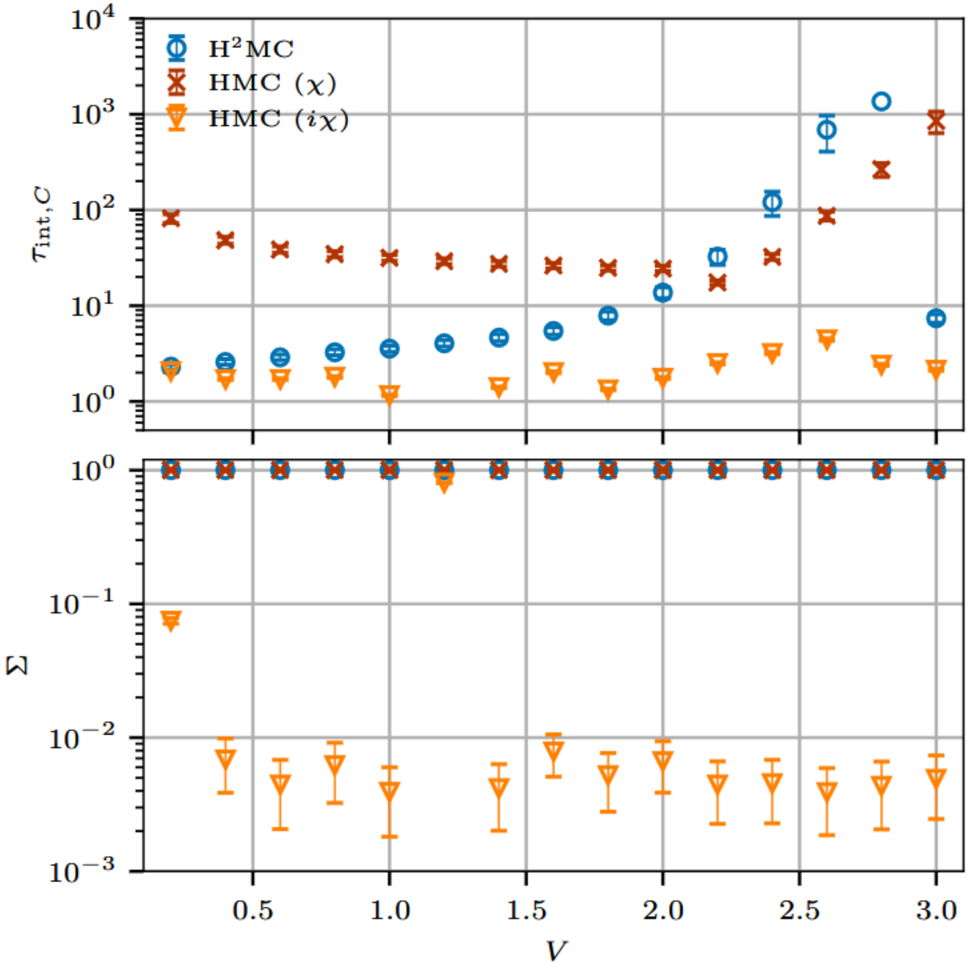
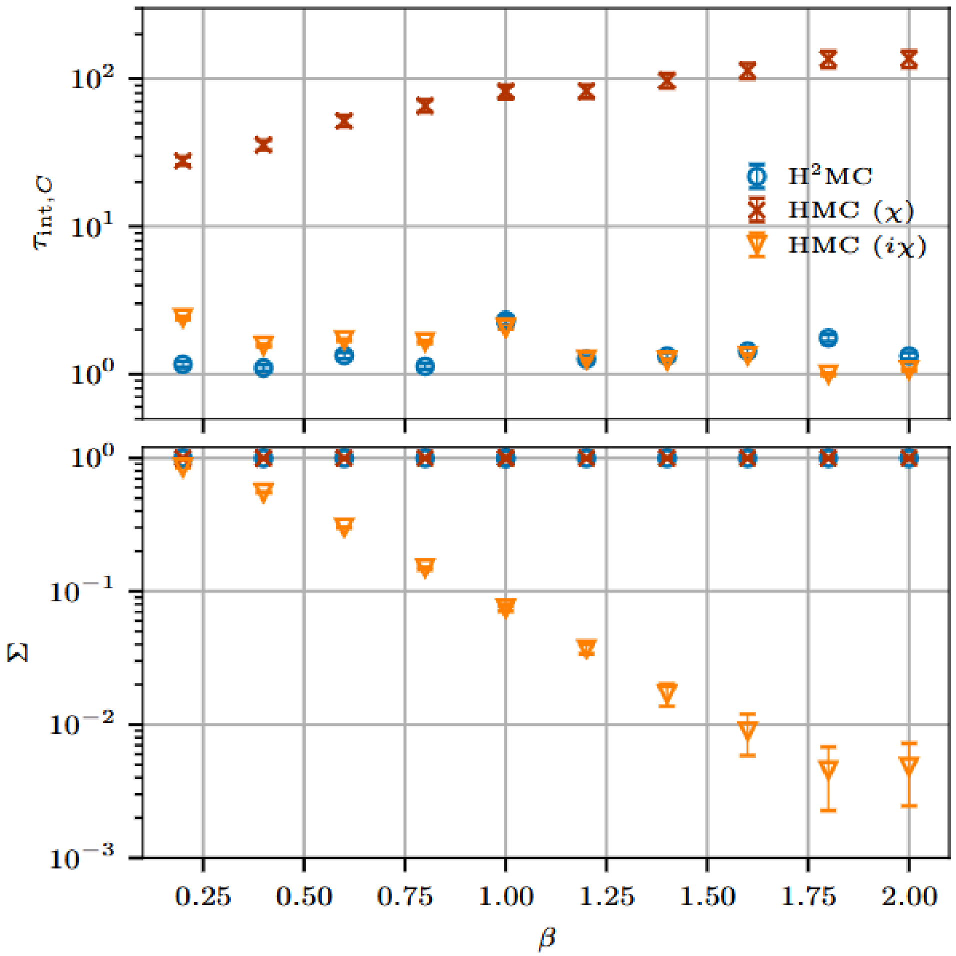
APPENDIX

Benchmarking against pure HMC





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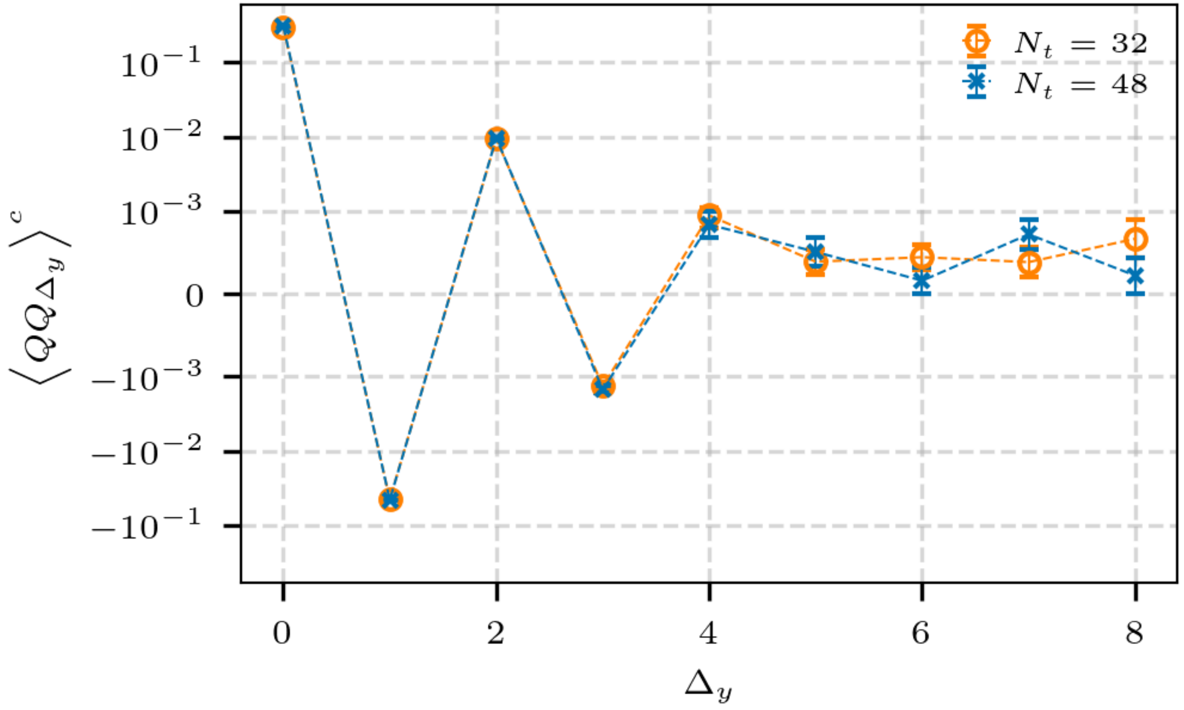
APPENDIX

Interchain correlations

$$\langle QQ_{\Delta_y}\rangle^c = \frac{1}{L_x L_y}\sum_{x=1}^{L_x}\sum_{y=1}^{L_y}\langle Q_{xy}Q_{x(y+\Delta_y)}\rangle^c$$



$$Q_{xy} = n_{xy\uparrow} - (1 - n_{xy\downarrow})$$

$$\Delta_y \in \{0, \ldots, \lfloor L_y/2 \rfloor\}$$