Revisiting the Hybrid Monte Carlo Method for Hubbard and Electron-Phonon Models

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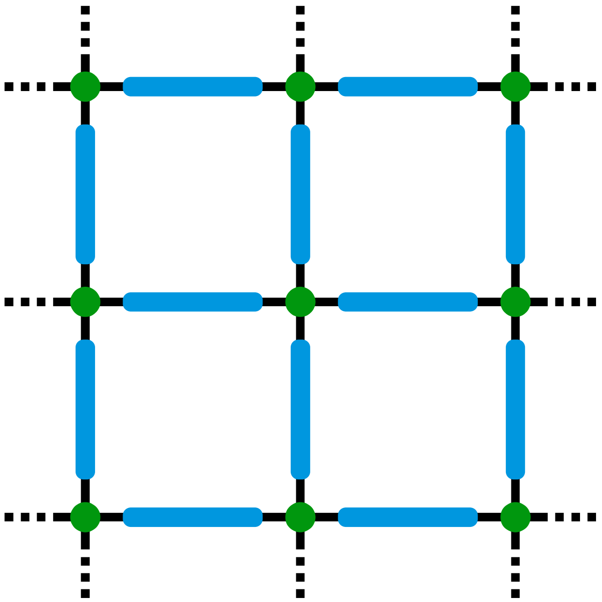

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physics with a twist

Reference Model

Hubbard type model:

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + U \sum_{i} \left(\hat{n}_{i,\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i,\downarrow} - \frac{1}{2} \right)$$

Partition Function with Trotter Decomposition:

$$Z = \mathrm{tr}\, \mathrm{e}^{-\beta H} = \mathrm{tr}\, \left(\mathrm{e}^{-\triangle_\tau H} \right)^{N_\tau} \simeq \mathrm{tr}\, \left(\mathrm{e}^{-\triangle_\tau H_K} \mathrm{e}^{-\triangle_\tau H_V} \right)^{N_\tau}$$

Introduce auxiliary field:

$$\exp\left[-\triangle_\tau U \left(\hat{n}_{i,\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i,\downarrow} - \frac{1}{2} \right) \right] =$$

$$= \left(\triangle_\tau / \pi \right)^{1/2} \mathrm{e}^{-\triangle_\tau U/4} \int_{-\infty}^{\infty} \mathrm{d}x_{i,l} \; \exp\left\{ -\triangle_\tau \left[x_{i,l}^2 + \sqrt{2U} x_{i,l} \left(\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow} \right) \right] \right\}$$

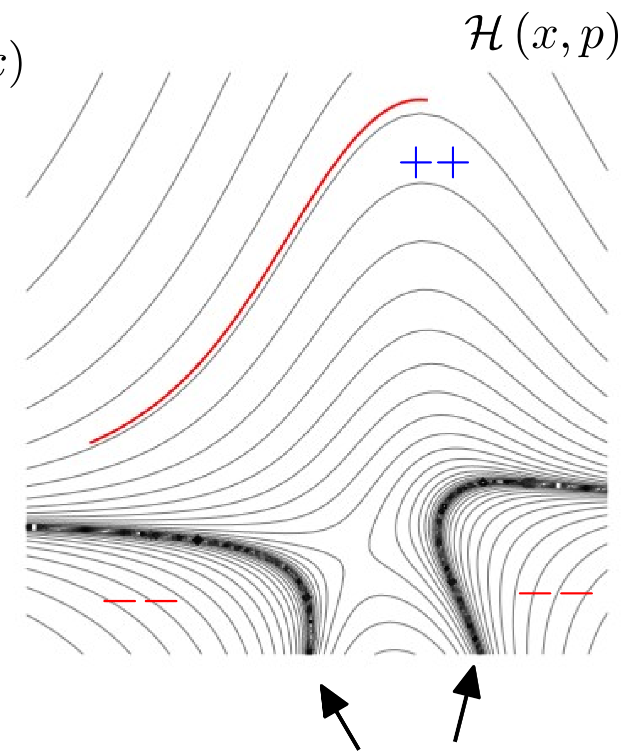
Ergodicity (HQMC)

$$Z = \int [\delta x\, \delta\phi_\uparrow\, \delta\phi_\downarrow\, \delta p] \exp \underbrace{\left\{ -S_B(x) - \sum_\sigma \phi_\sigma \left(M_\sigma^T(x)\, M_\sigma(x) \right)^{-1} \phi_\sigma - \sum_{i,l} p_{i,l}^2 \right\}}_{=:-\mathcal{H}(x,p)}$$

$$= \int [\delta x\, \delta p]\ \mathrm{e}^{-S_B(x) - p^2} \det M_\uparrow(x)\ \det M_\downarrow(x)$$

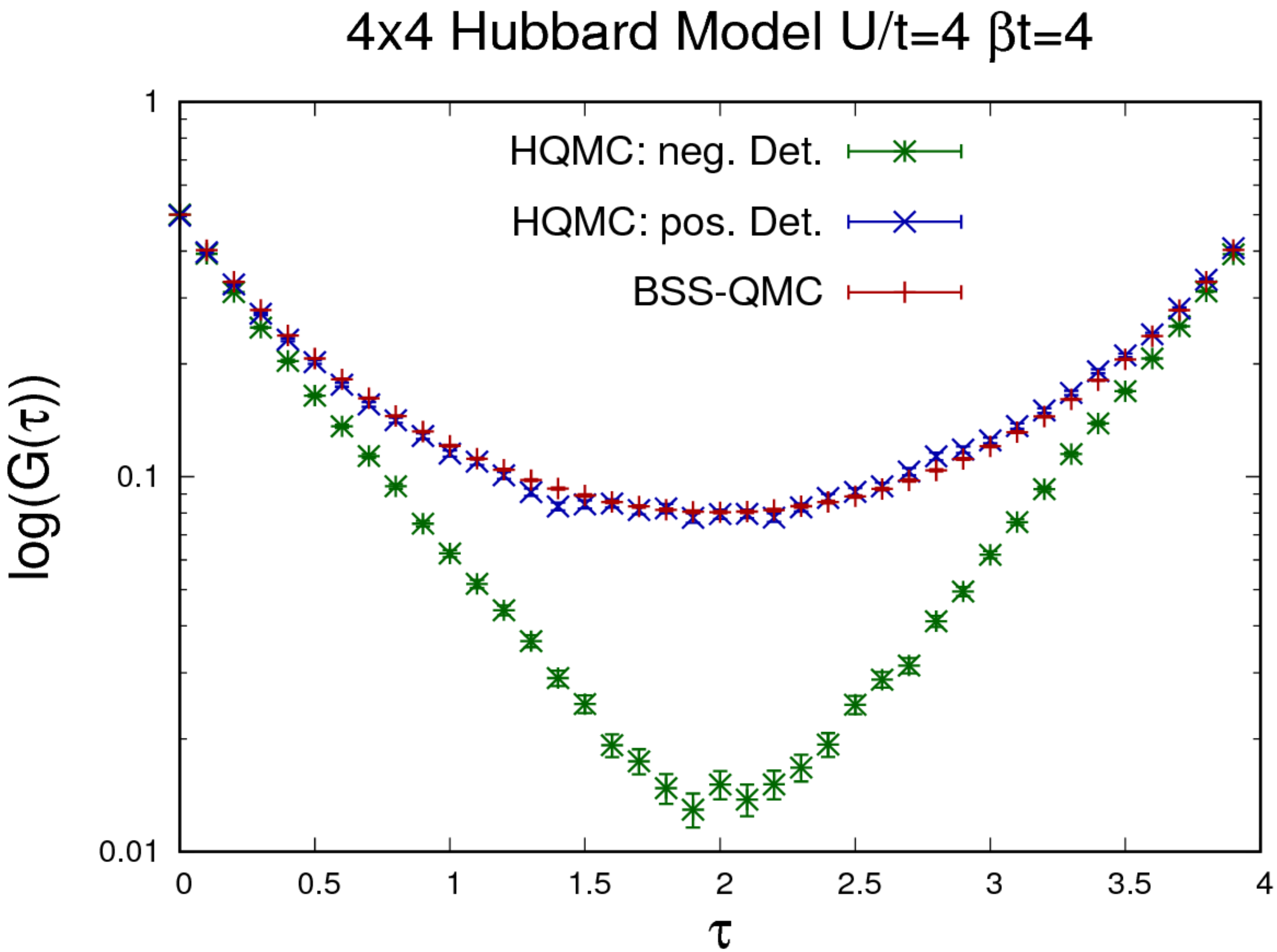
Ergodicity can not be ensured

$\det M_\sigma(x) = 0$ →



Domain walls that cannot be crossed by the leapfrog method

Benchmark Plot



Introduction of Complex Fields (cHQMC)

Rewrite the interaction part of the Hamiltonian:

$$H'_V = \sum_i \alpha \frac{U}{2} \left(\hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow} - 1\right)^2 - \sum_i (1-\alpha) \frac{U}{2} \left(\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow}\right)^2$$

Double Hubbard-Stratonovich-transformation:

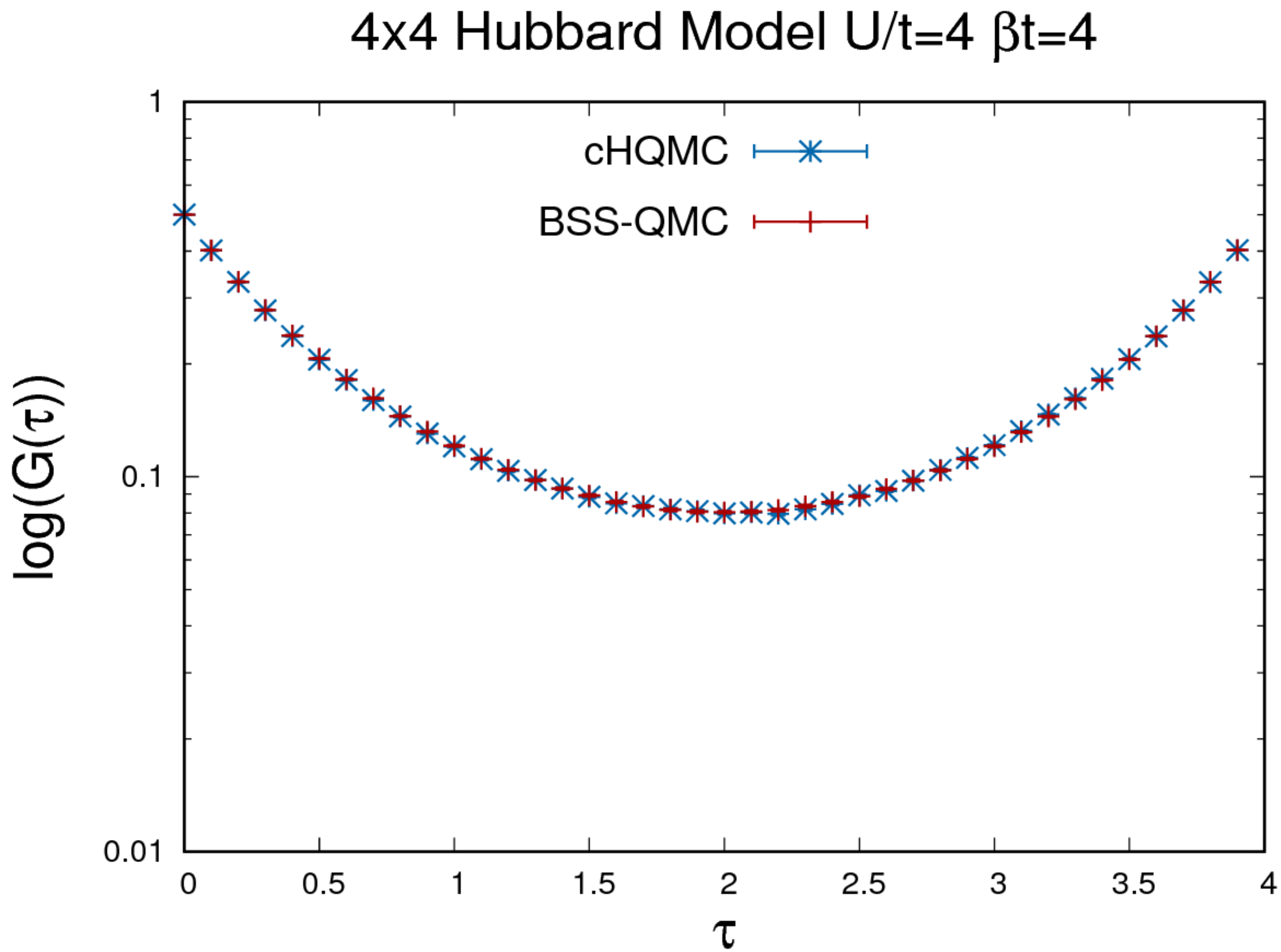
$$\mathrm{e}^{-\triangle_\tau H'_V} \propto \int \mathrm{d}x_{i,l}\, \mathrm{d}y_{i,l} \quad \exp\left\{-\triangle_\tau \sum_i \left[x_{i,l}^2 + y_{i,l}^2 + \left(\sqrt{2U(1-\alpha)}x_{i,l} + \mathrm{i}\sqrt{2U\alpha}y_{i,l}\right)\left(\hat{n}_{i,\uparrow} - \tfrac{1}{2}\right) - \left(\sqrt{2U(1-\alpha)}x_{i,l} - \mathrm{i}\sqrt{2U\alpha}y_{i,l}\right)\left(\hat{n}_{i,\downarrow} - \tfrac{1}{2}\right)\right]\right\}$$

At half filling:

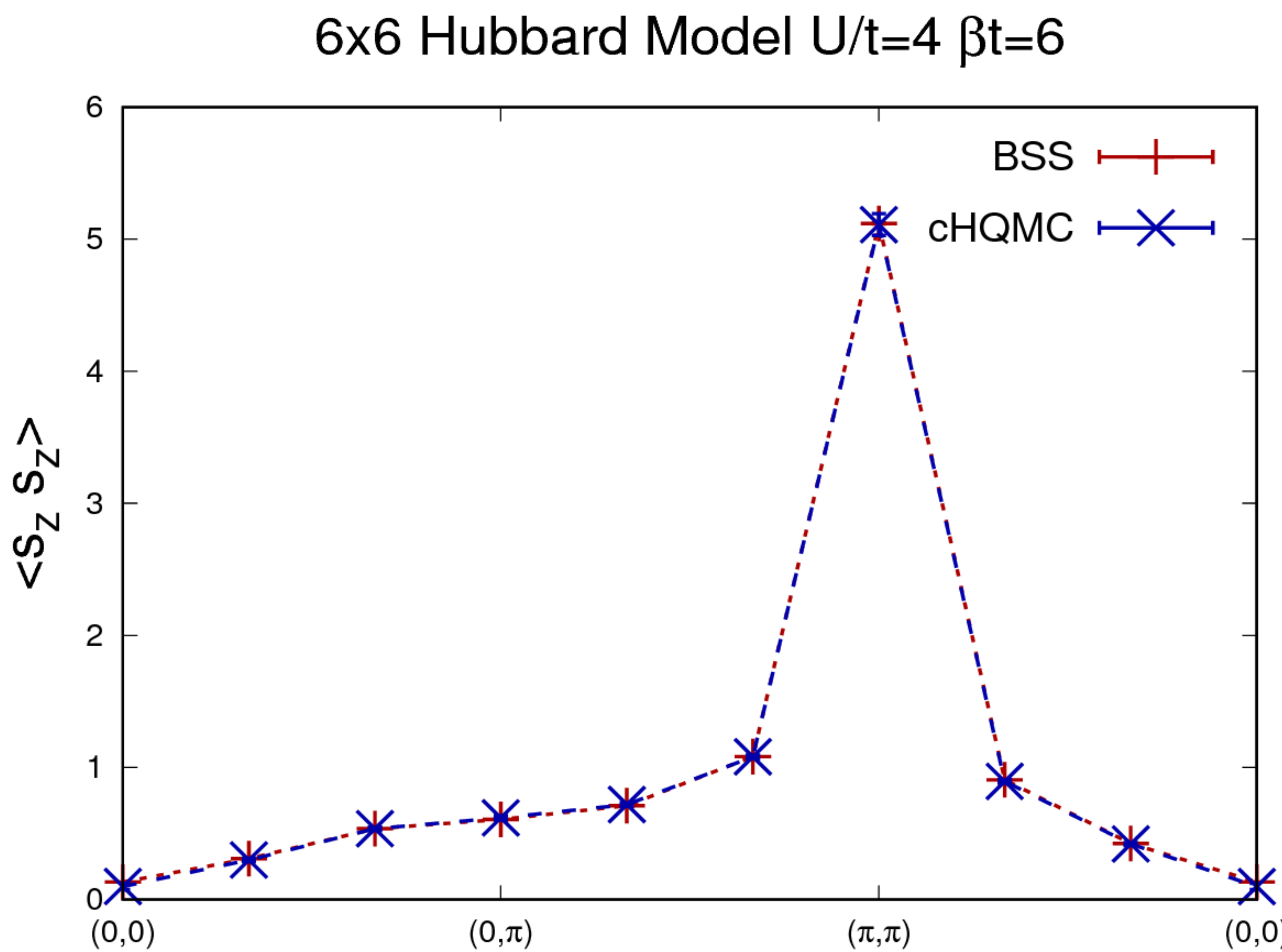
$\det\left[\mathcal{M}_\uparrow(x,y)\right] = \overline{\det\left[\mathcal{M}_\downarrow(x,y)\right]} \Rightarrow$ no sign problem

$\det\left[\mathcal{M}_\sigma(x,y)\right] \in \mathbb{C} \Rightarrow$ no problems with ergodicity

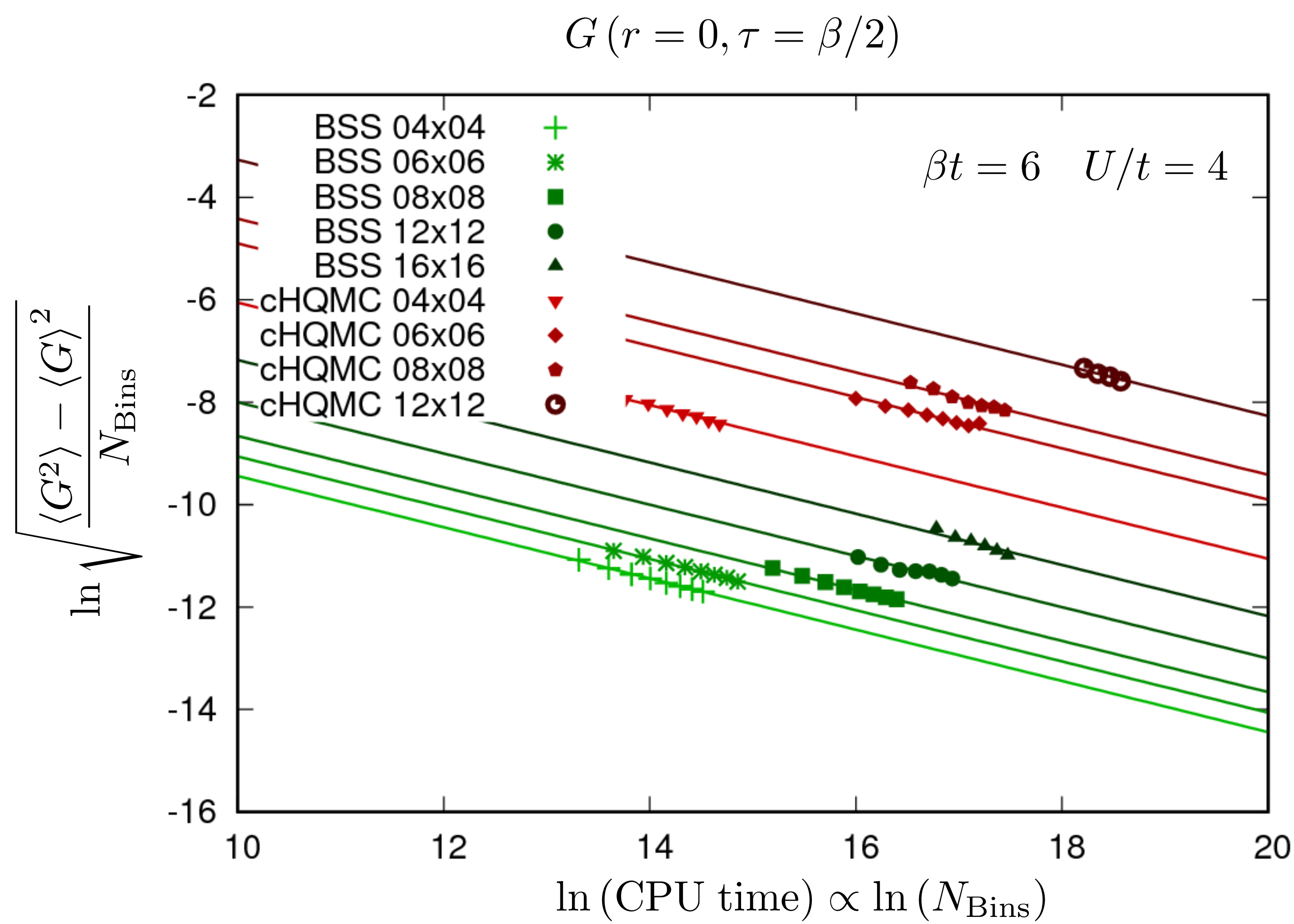
Benchmark Plot



Benchmark Plot



Comparison: cHQMC and BSS-QMC



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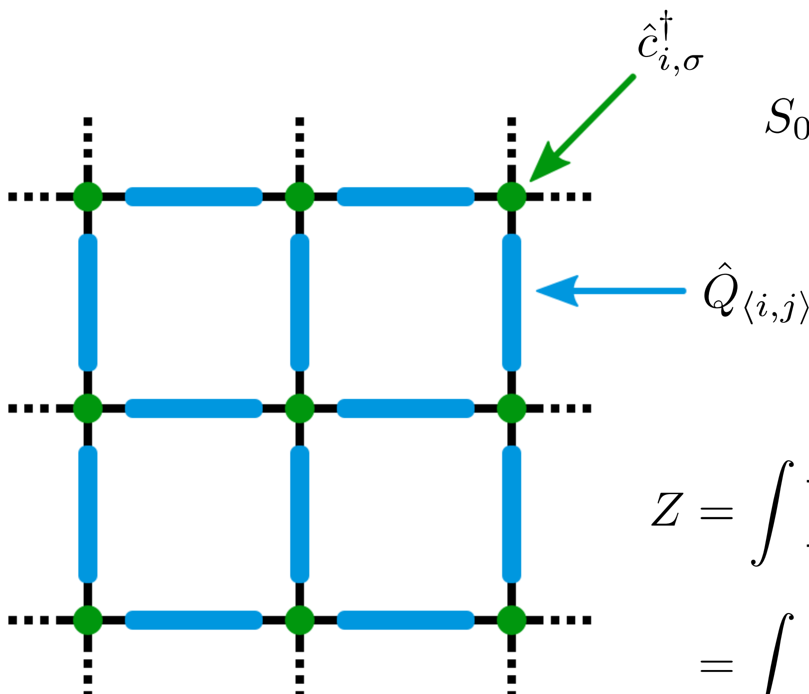
Su-Schrieffer-Heeger model (SSH)

$$H = -t \sum_{\langle i,j\rangle,\sigma} \left(\hat{c}^\dagger_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^\dagger_{j,\sigma}\hat{c}_{i,\sigma}\right) + \sum_{\langle i,j\rangle} \left[\frac{\hat{P}^2_{\langle i,j\rangle}}{2m} + \frac{k}{2}\hat{Q}^2_{\langle i,j\rangle}\right] + g \sum_{\langle i,j\rangle,\sigma} \hat{Q}_{\langle i,j\rangle} \left(\hat{c}^\dagger_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^\dagger_{j,\sigma}\hat{c}_{i,\sigma}\right)$$

$$\hat{Q}_b \left|x_b\right\rangle = x_b \left|x_b\right\rangle \qquad b := \langle i,j\rangle \qquad K_b := \left(\hat{c}^\dagger_i \hat{c}_j + \hat{c}^\dagger_j \hat{c}_i\right)$$

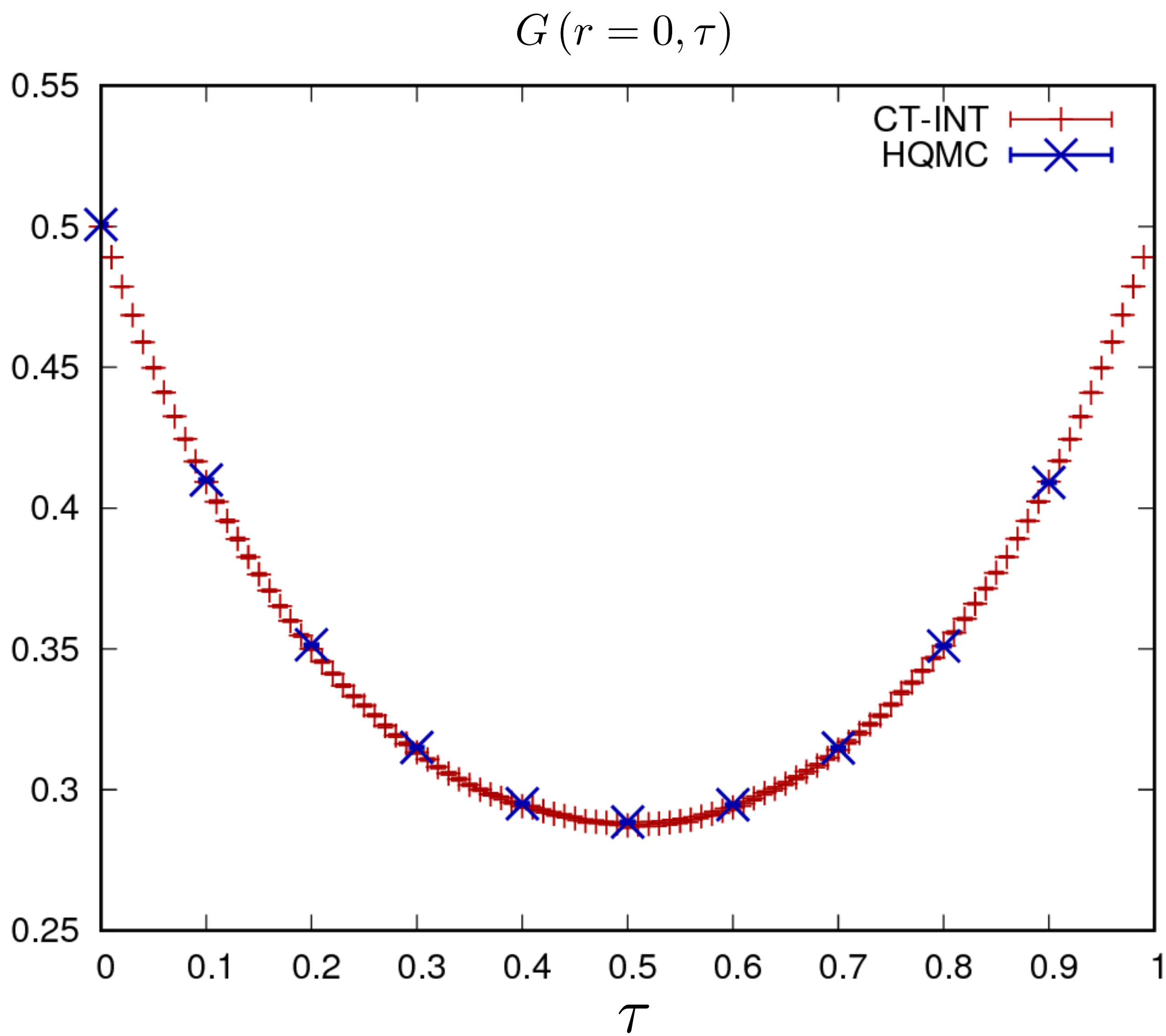


$$S_0\left(x_{b,\tau}\right) := \triangle_\tau \left(\frac{m}{2}\left[\frac{x_{b,\tau+1} - x_{b,\tau}}{\triangle_\tau}\right]^2 + \frac{k}{2} x^2_{b,\tau}\right)$$

$$Z = \int \prod_{b,\tau} \mathrm{d}x_{b,\tau} \mathrm{e}^{-S_0(x_{b,\tau})} \left[\mathrm{tr}\,\mathrm{e}^{-\triangle_\tau \sum_b (g x_{b,\tau} - t) K_b}\right]^{N_{\mathrm{col}}}$$

$$= \int \left[\delta x\right] \mathrm{e}^{-S_0(x)} \left[\det M\left(x\right)\right]^{N_{\mathrm{col}}}$$

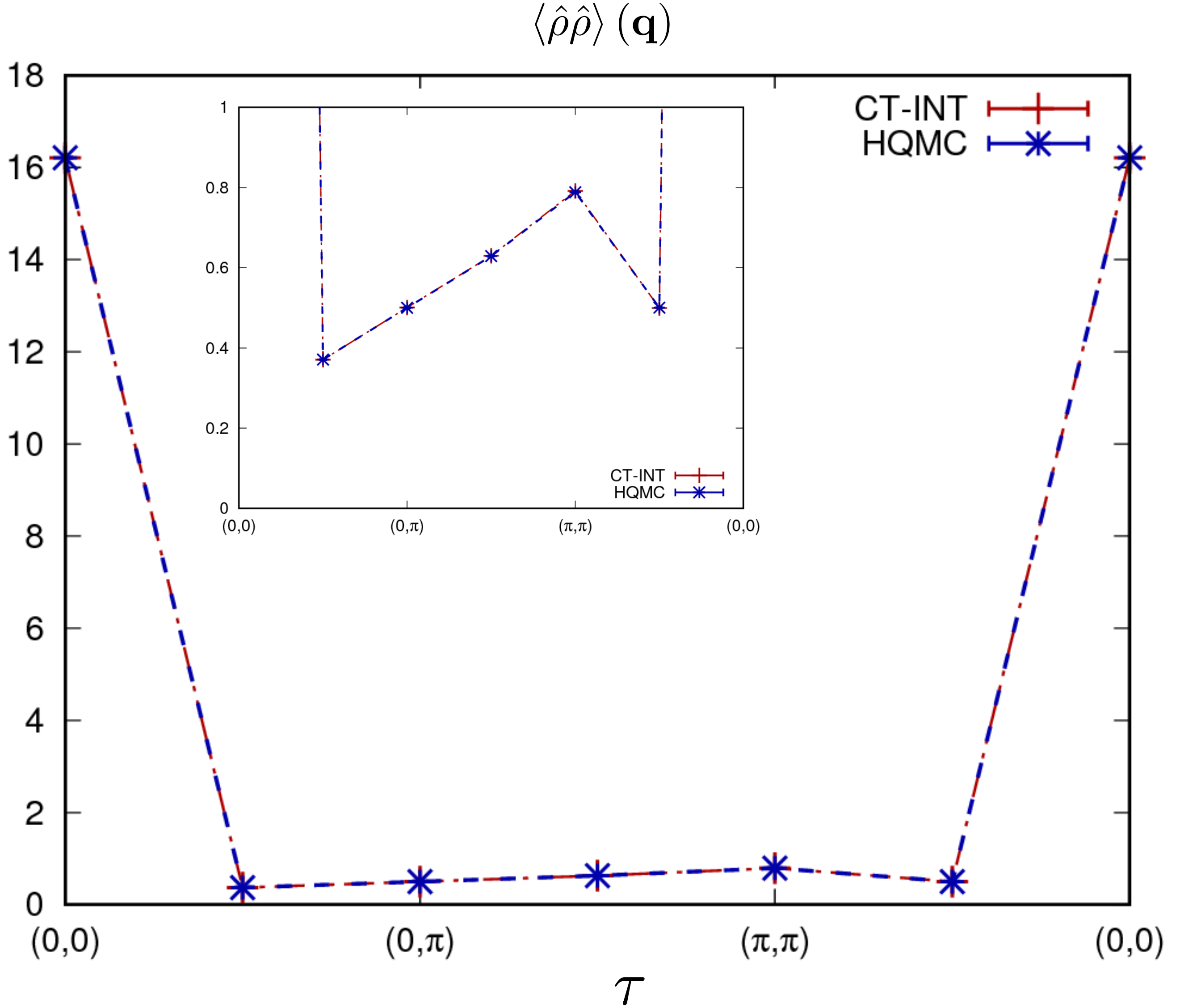
Benchmark Green's Function



Benchmarks provided by Martin Hohenadler.

$$\beta = 1.0 \quad \sqrt{\frac{2}{k}}g = 1.0 \quad \sqrt{\frac{k}{m}} = 1.0 \quad \text{system size: } 4\text{x}4$$

Benchmark Density-Density



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THANKS FOR YOUR ATTENTION