

Rényi Entanglement Entropy of Interacting Fermions

A Continuous-time Quantum Monte Carlo Approach

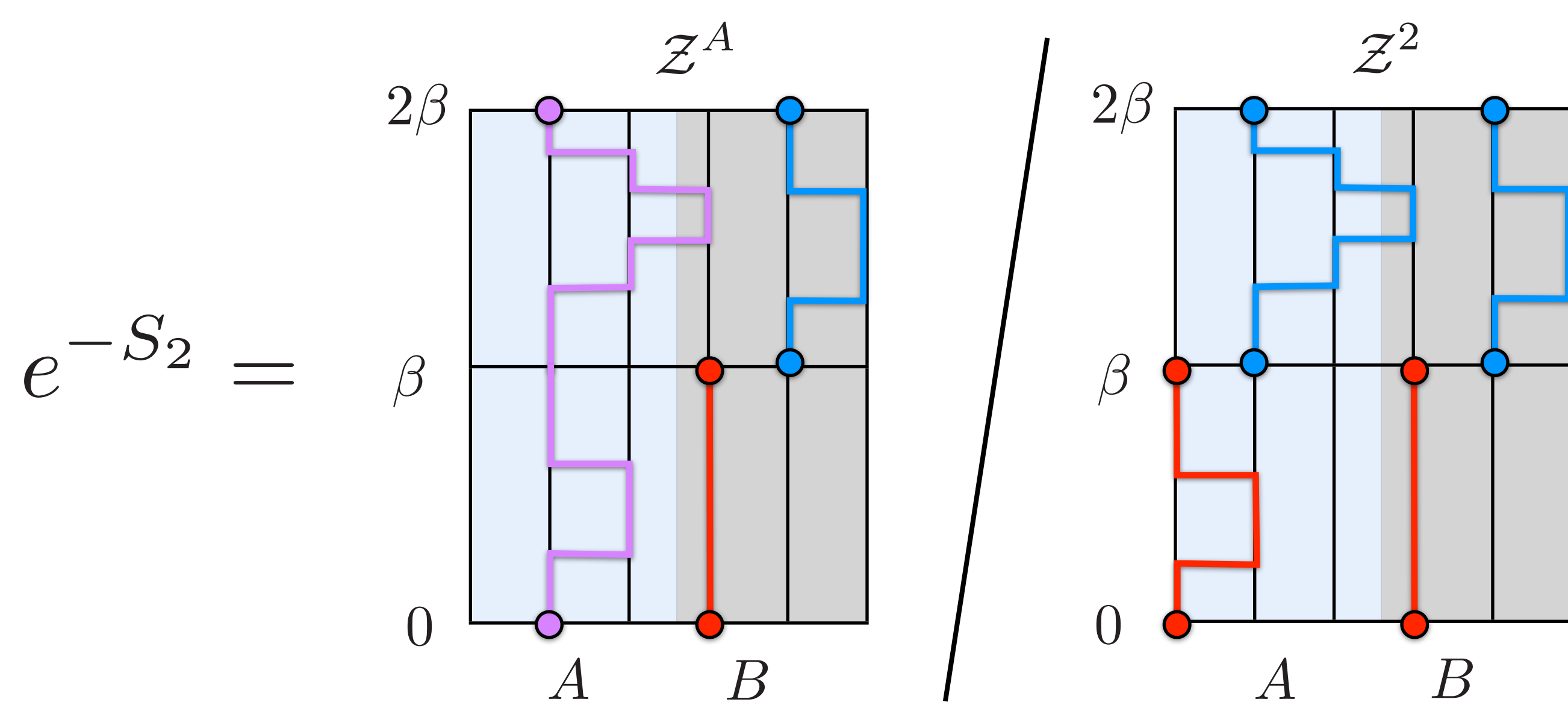
Lei Wang and Matthias Troyer, **ETH** zürich

Rényi Entanglement Entropy

Rényi entanglement entropy is calculated using replica method in quantum Monte Carlo simulation

$$S_2 = -\ln [\text{Tr}_A(\hat{\rho}_A^2)] = -\ln \left(\frac{\mathcal{Z}^A}{\mathcal{Z}^2} \right)$$

$$\hat{\rho}_A = \frac{1}{\mathcal{Z}} \text{Tr}_B(e^{-\beta \hat{H}}) \quad \mathcal{Z} = \text{Tr}(e^{-\beta \hat{H}})$$



Implemented for interacting fermions [1], performs better than free fermion decomposition approach [2].



Area law scaling of entanglement entropy implies *exponentially* vanishing Monte Carlo signal.

References

- [1] P. Broecker and S. Trebst, J. Stat. Mech., P08015 (2014)
- [2] T. Grover, Phys. Rev. Lett. **111**, 130402 (2013)
- [3] I. Peschel, J. Phys. A: Math. Gen. **36**, L205 (2003)
- [4] J. E. Gubernatis, D. J. Scalapino, R. L. Sugar, and W. D. Toussaint, Phys. Rev. B **32**, 103 (1985)

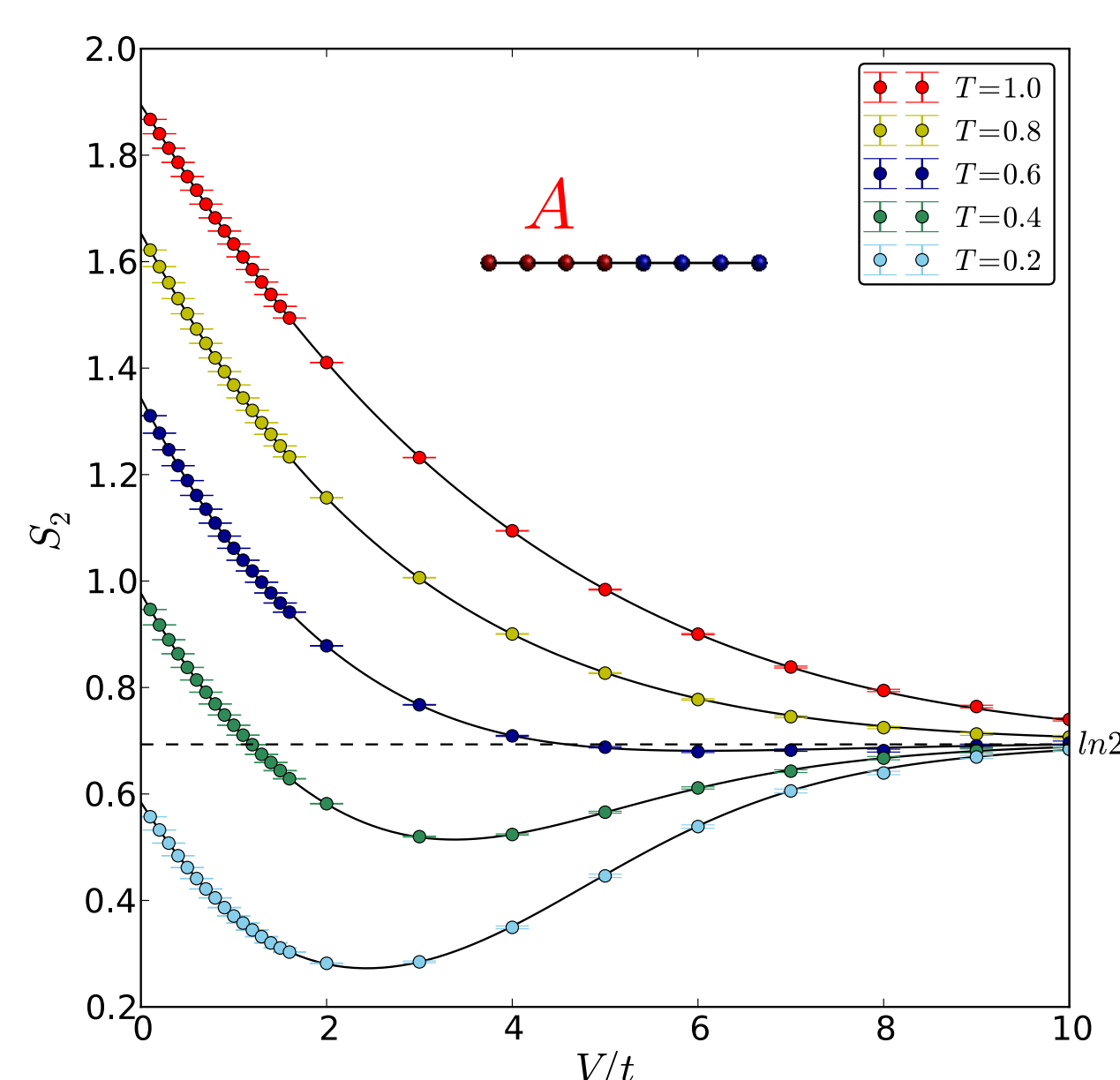


arXiv:1407.0707
PRL in press

Benchmarks

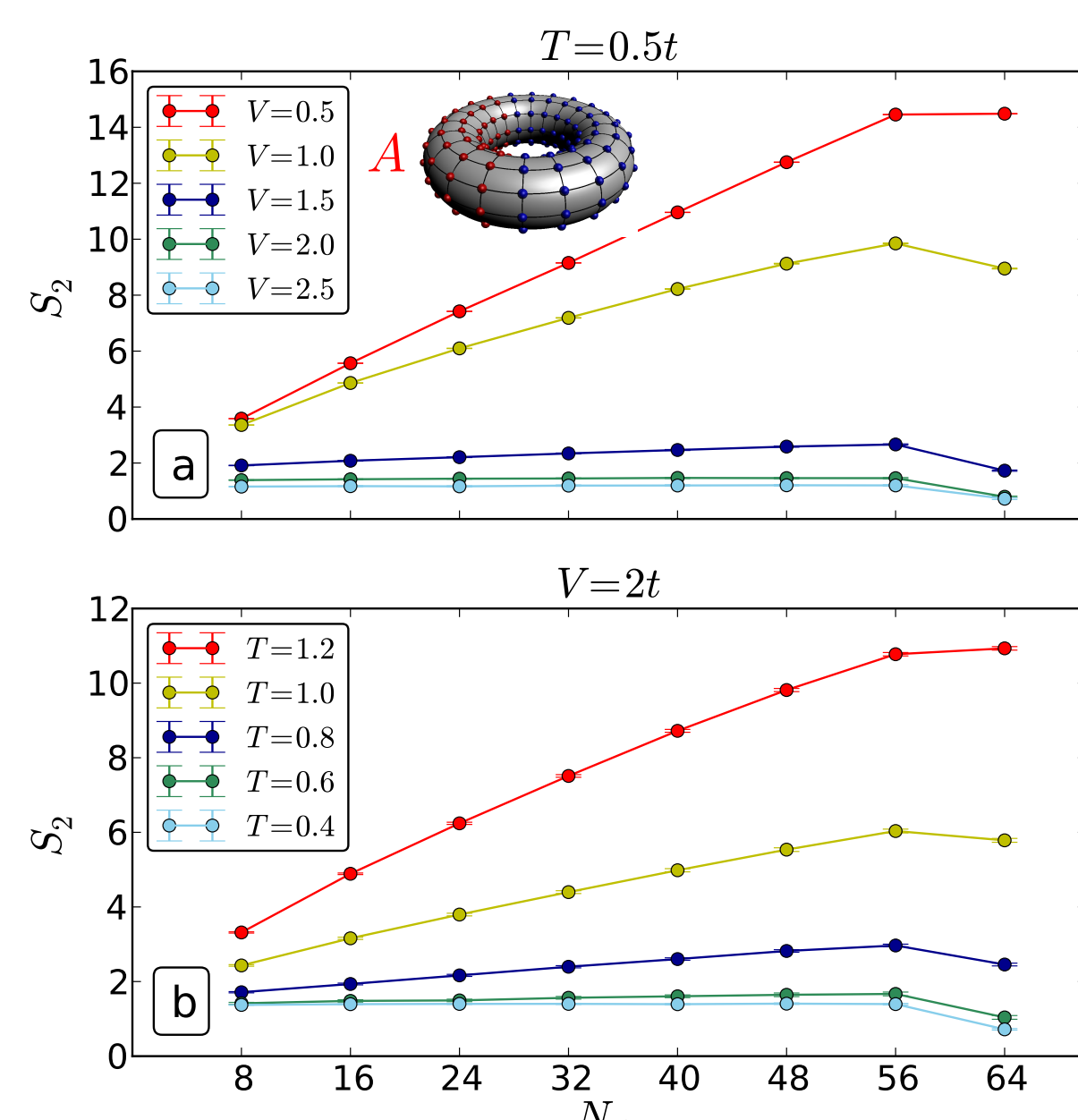
$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i) + V \sum_{\langle i,j \rangle} \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_j - \frac{1}{2} \right)$$

8-site open chain

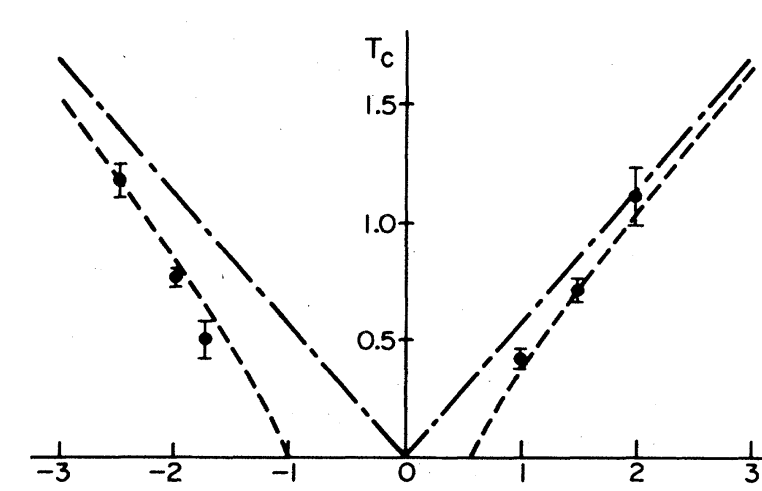


Agree perfectly with exact diagonalization (solid lines)

8x8 square lattice



Entanglement signature of a CDW transition [4]



CTQMC

$$\frac{\mathcal{Z}}{\mathcal{Z}_0} = \frac{1}{\mathcal{Z}_0} \text{Tr} \left[e^{-\beta \hat{H}_0} \mathcal{T} e^{-\int_0^\beta d\tau \hat{H}_1(\tau)} \right] \quad \hat{H} = \hat{H}_0 + \hat{H}_1$$

$$= \sum_{k=0}^{\infty} \int_0^\beta d\tau_1 \dots \int_{\tau_{k-1}}^\beta d\tau_k \frac{(-1)^k}{\mathcal{Z}_0} \text{Tr} \left[e^{-\beta \hat{H}_0} \hat{H}_1(\tau_k) \dots \hat{H}_1(\tau_1) \right]$$

$$= \sum_{\mathcal{C}} w(\mathcal{C})$$

CTQMC offers an unbiased way to sample the ratio between *interacting* and *noninteracting* partition functions

Algorithm

$$S_2 = S_2^0 + \Delta S_2$$

Noninteracting entanglement entropy

$$S_2^0 = -\ln \left(\frac{\mathcal{Z}_0^A}{\mathcal{Z}_0^2} \right)$$

Easily calculated by correlation matrix method [3]

Interaction Corrections

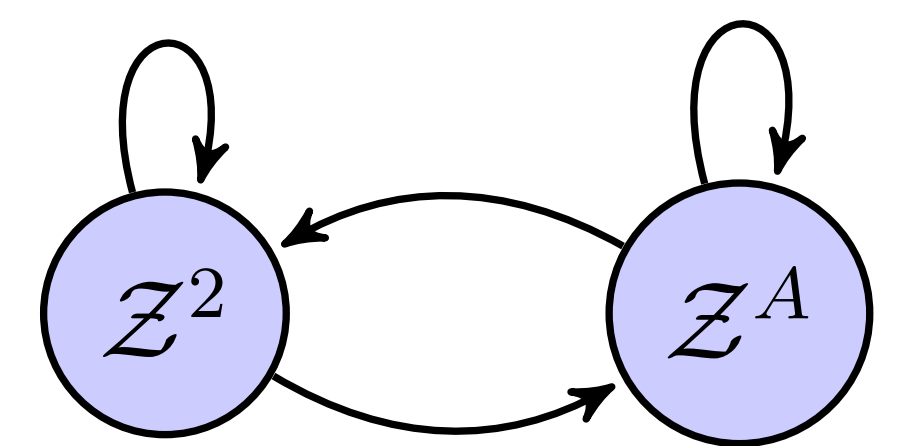
$$\Delta S_2 = -\ln \left[\eta \frac{\mathcal{Z}^A / \mathcal{Z}_0^A}{(\mathcal{Z} / \mathcal{Z}_0)^2} \right] + \ln(\eta)$$

Sampled use CTQMC

Extended ensemble simulation

$$\left(\mathcal{Z} / \mathcal{Z}_0 \right)^2 + \eta \left(\mathcal{Z}^A / \mathcal{Z}_0^A \right)$$

$$= \sum_{\mathcal{C}} [w_{\mathcal{Z}^2}(\mathcal{C}) + \eta w_{\mathcal{Z}^A}(\mathcal{C})]$$



$$\Delta S_2 = -\ln \left[\frac{\langle \delta_{\mathcal{Z}^A} \rangle_{\text{MC}}}{\langle \delta_{\mathcal{Z}^2} \rangle_{\text{MC}}} \right] + \ln(\eta)$$

Critical Point

Square lattice t-V model undergoes an Ising phase transition to a CDW phase at large interaction or low temperature.

Mutual information crossing locates the critical point

$$I_2(A : B) = S_2(\hat{\rho}_A) + S_2(\hat{\rho}_B) - S_2(\hat{\rho}_{A \cup B})$$

