

Rényi Entanglement Entropy of Interacting Fermions

A Continuous-time Quantum Monte Carlo Approach

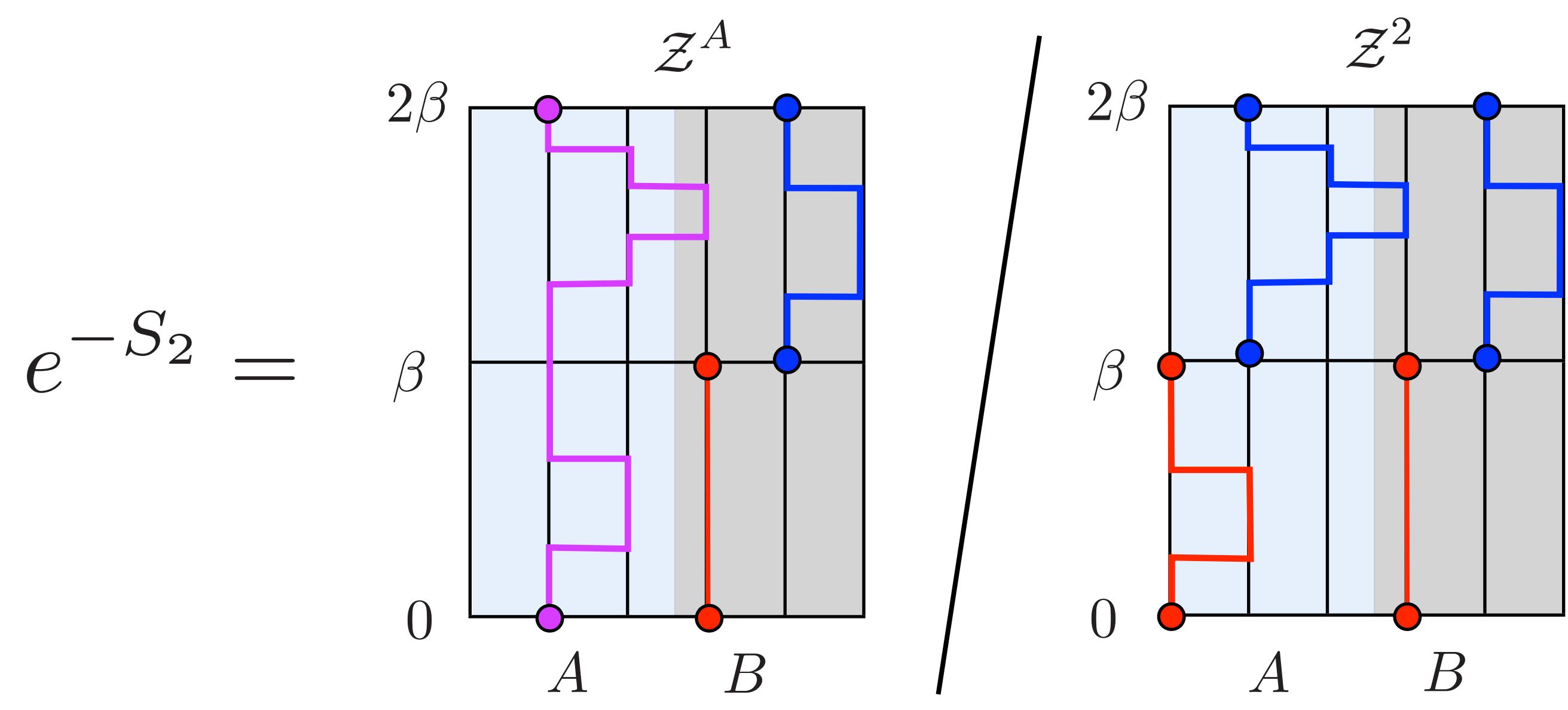
Lei Wang and Matthias Troyer, **ETH** zürich

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], works better than free fermion decomposition approach [2].

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

References

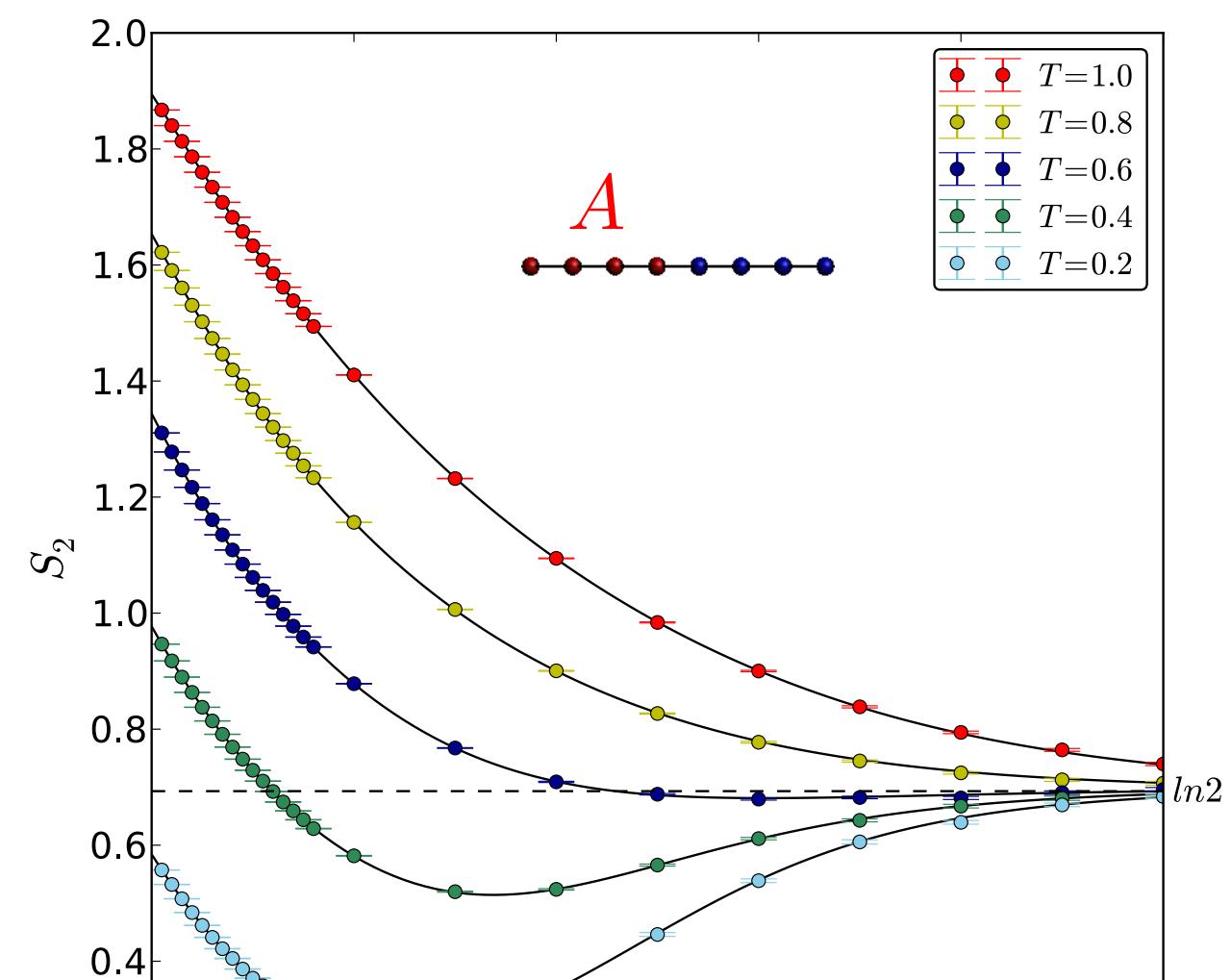
- [1] P. Broecker and S. Trebst, arXiv: 1404.3027
- [2] T. Grover, Phys. Rev. Lett. 111, 130402 (2013)
- [3] I. Peschel, J. Phys. A: Math. Gen. 36, L205 (2003)
- [4] J. E. Gubernatis, D. J. Scalapino, R. L. Sugar, and W. D. Toussaint, Phys. Rev. B 32, 103 (1985)



Benchmarks

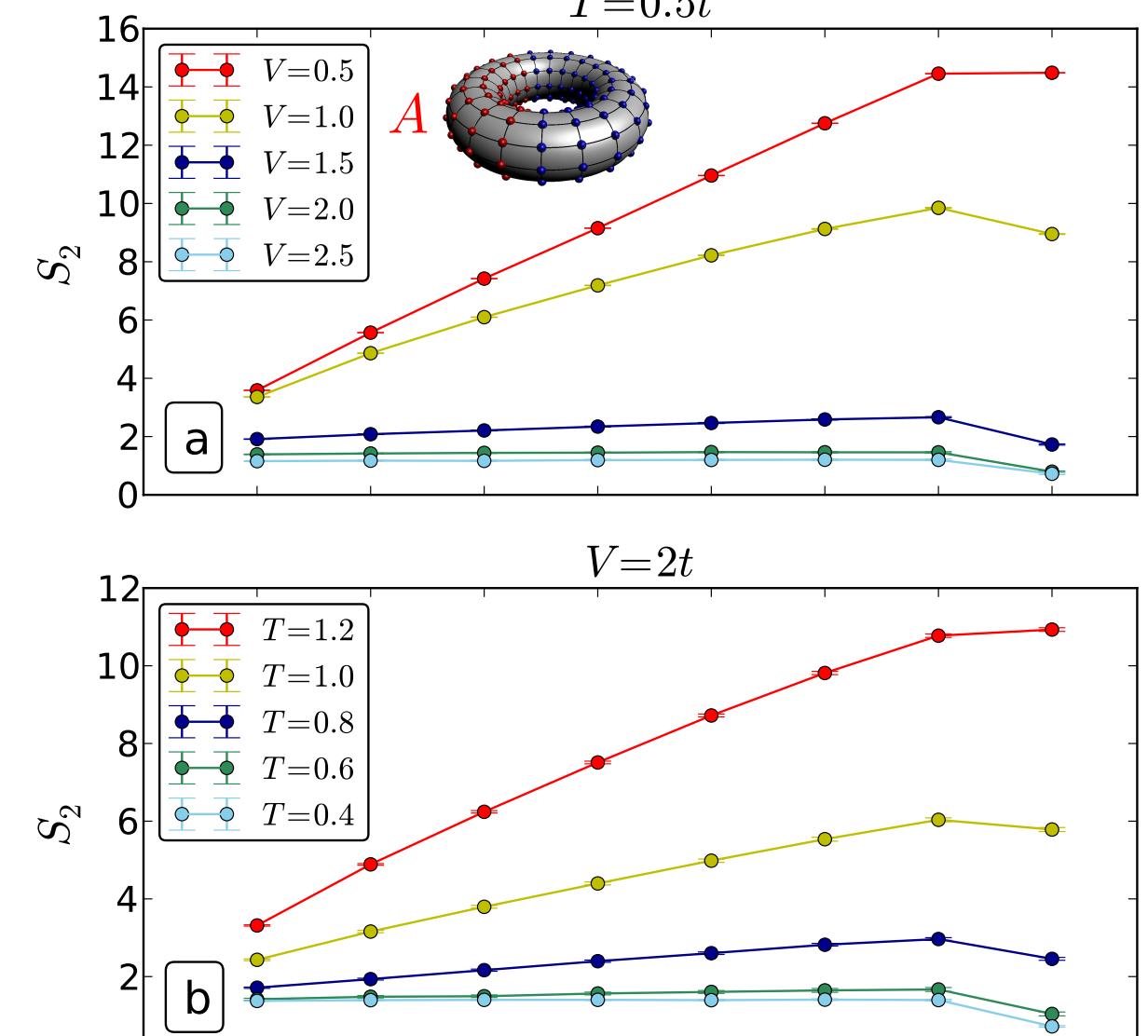
$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i) + V \sum_{\langle i,j \rangle} \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_j - \frac{1}{2} \right)$$

8-site open chain



Agree perfectly with exact diagonalization (solid lines)

8×8 square lattice



Entanglement signature of a CDW transition [4]



CTQMC

$$\begin{aligned} \frac{\mathcal{Z}}{\mathcal{Z}_0} &= \frac{1}{\mathcal{Z}_0} \text{Tr} \left[e^{-\beta \hat{H}_0} \mathcal{T} e^{-\int_0^\beta d\tau \hat{H}_1(\tau)} \right] & \hat{H} = \hat{H}_0 + \hat{H}_1 \\ &= \sum_{k=0}^{\infty} \int_0^\beta d\tau_1 \dots \int_{\tau_{k-1}}^\beta d\tau_k \frac{(-1)^k}{\mathcal{Z}_0} \text{Tr} \left[e^{-\beta \hat{H}_0} \hat{H}_1(\tau_k) \dots \hat{H}_1(\tau_1) \right] \\ &= \sum_c w(c) \end{aligned}$$

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

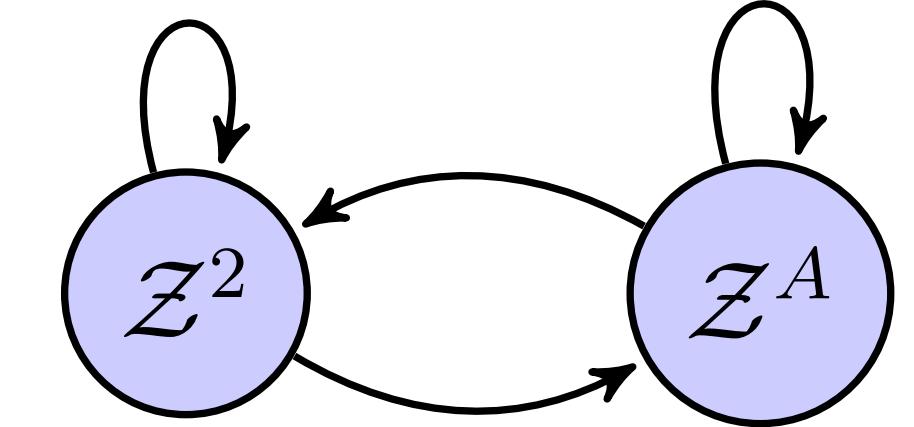
$$S_2^0 = -\ln \left(\frac{\mathcal{Z}_0^A}{\mathcal{Z}_0^2} \right)$$

Easily calculated by correlation matrix method [3]

Sampled use CTQMC

Extended ensemble simulation

$$\begin{aligned} &(\mathcal{Z}/\mathcal{Z}_0)^2 + \eta(\mathcal{Z}^A/\mathcal{Z}_0^A) \\ &= \sum_c [w_{\mathcal{Z}^2}(\mathcal{C}) + \eta w_{\mathcal{Z}^A}(\mathcal{C})] \end{aligned}$$



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

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

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

