Quantum Criticality in Long Range Transverse Field Ising Model

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Abstract

The critical behavior of many quantum systems, like the long-range transverse field Ising model, is not well understood in terms of quantum correlation measures like entanglement entropy because of the lack of efficient computational methods. Projector Quantum Monte Carlo (PQMC), well-established for short-range models, is extended here to the long-range case to comment on the behavior of critical exponents and entanglement entropy at criticality in the thermodynamic limit $L \to \infty$.

Quantum Monte Carlo Methods

Classical Monte Carlo:

- The classical partition function is:

$$Z = \sum_i e^{-\beta E_i}. \tag{1}$$

- One samples each term of this expansion in the simulation, and extracts observables:

$$\langle O \rangle = \sum_i \frac{O_i e^{-\beta E_i}}{Z}. \tag{2}$$

Quantum Monte Carlo (Stochastic Series Expansion) [1]:

- Quantum partition function is the trace over the thermal density matrix.

$$Z = \mathrm{Tr}(\hat\rho) = \mathrm{Tr}(\mathrm{e}^{-\beta \hat H}), \tag{3}$$

$$Z = \sum_{\alpha_0} \langle \alpha_0 \mid \mathrm{e}^{-\beta \hat H} \mid \alpha_0 \rangle = \sum_{\alpha_0} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \langle \alpha_0 \mid \hat H^n \mid \alpha_0 \rangle, \tag{4}$$

$$Z = \sum_{n=0}^{\infty} \sum_{\{\alpha\}} \frac{(-\beta)^n}{n!} \langle \alpha_0 \mid \hat H \mid \alpha_1 \rangle \langle \alpha_1 \mid \hat H \mid \alpha_2 \rangle \cdots \langle \alpha_{n-1} \mid \hat H \mid \alpha_0 \rangle.$$

- If the Hamiltonian is a local operator, then

$$Z = \sum_{n=0}^{M} \sum_{\{\alpha\}} \frac{(-\beta)^n (M-n)!}{M!} \prod_{m=1}^{M} \langle \alpha_{m-1} \mid \hat H_{t_m, a_m} \mid \alpha_m \rangle. \tag{5}$$

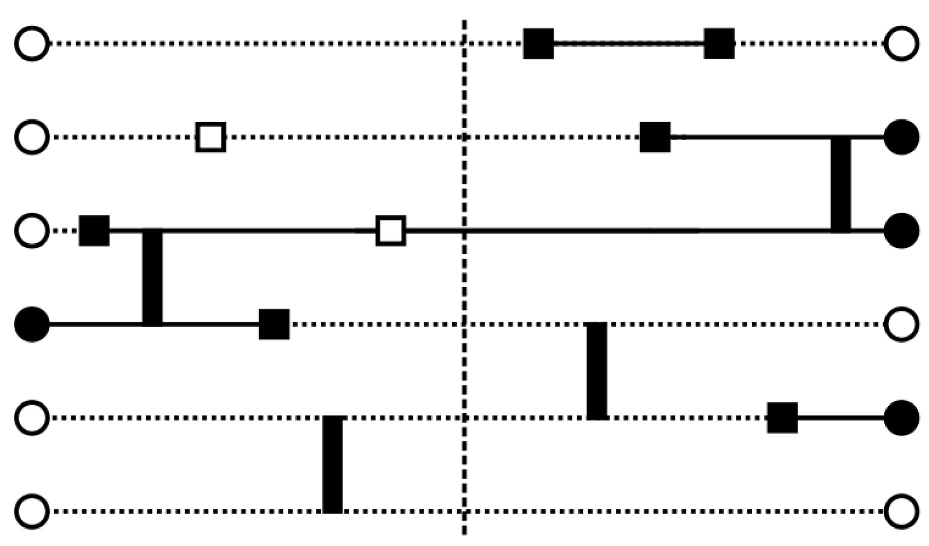

Figure: $(D+1)$-dimensional representation of a configurational cell in SSE

Projector Quantum Monte Carlo:

- To obtain $T = 0$ expectation values, one can increase β but this is computationally costly. Instead, the projector method achieves faster convergence.

$$\left(-\hat H\right)^m \mid \alpha_d \rangle = c_0 |E_0|^m \left(|0\rangle + \frac{c_1}{c_0} \left(\frac{E_1}{E_0} \right)^m |1\rangle + \cdots \right). \tag{6}$$

- Then, the partition function at $T = 0$ is:

$$Z = \sum_{\{\alpha\}} \langle \alpha_k \mid (-\hat H)^p (-\hat H)^r \mid \alpha_d \rangle = \sum_{\{\alpha\}} \sum_{S_{r+p}} \prod_{j=1}^{r+p} \langle \alpha_k \mid (-\hat H_{t_j, a_j}) \mid \alpha_d \rangle. \tag{7}$$

Transverse Field Ising Model

Paradigmatic Model for Quantum Phase Transitions

- This model exhibits an order-disorder transition at $T = 0$ in all dimensions:

$$\hat H = -J \sum_i \sigma_i^z \sigma_{i+1}^z - h^T \sum_i \sigma_i^x, \tag{8}$$

where J is the interaction strength and h^T is the transverse field.

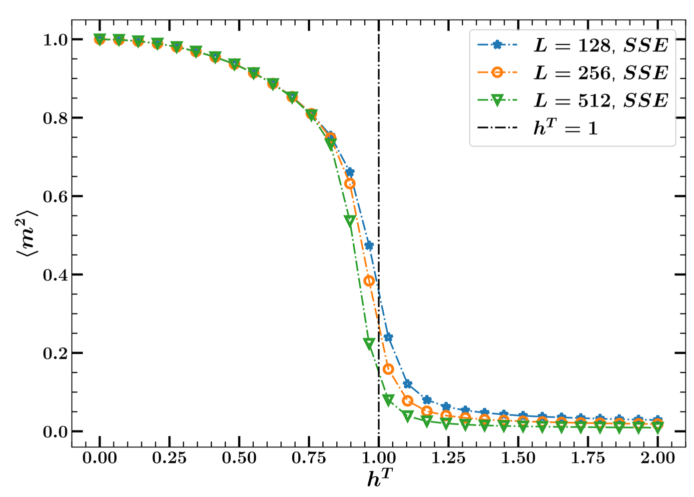

Figure: $\langle m^2 \rangle$ for 1D TFIM at $T = 0$.

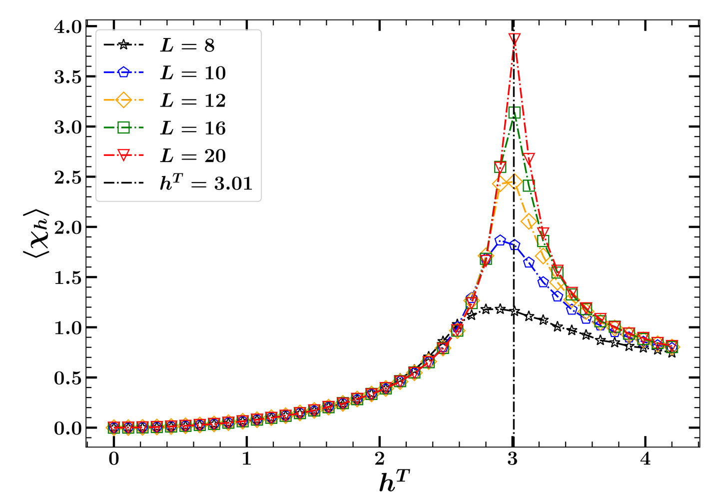

Figure: Susceptibility for 2D TFIM at $T = 0$.

Long Range Interactions

- Model system – 1D Long Range Transverse Field Ising Model (LRTFIM):

$$\hat H = -\sum_{i,j} \frac{J}{r^{d+\sigma}} \sigma_i^z \sigma_j^z - h^T \sum_i \sigma_i^x, \tag{9}$$

where d is the system's dimension and σ is a parameter tuning the interaction range.

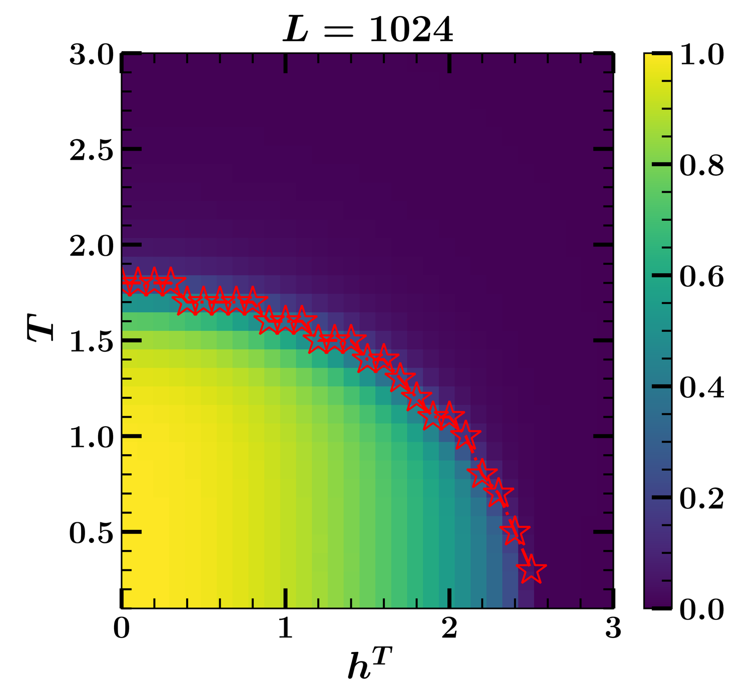

Figure: $\langle m^2 \rangle$ from finite-T SSE (KT transition)

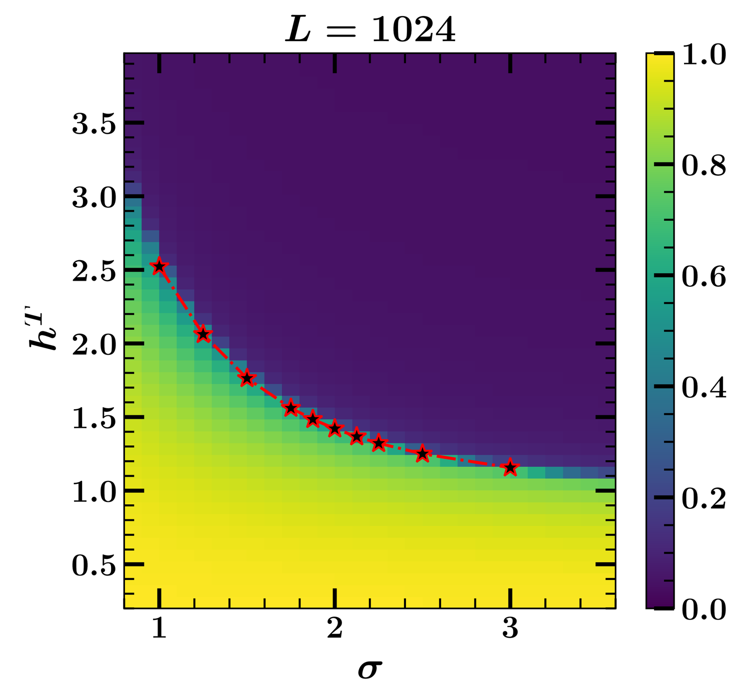

Figure: $\langle m^2 \rangle$ from PSSE

Entanglement Entropy

- Entanglement is a useful quantity to detect quantum phase transitions.
- In SSE, the second-order Rényi entropy is computed via the replica trick:

$$S_A^{(2)} = -\ln \mathrm{Tr}(\rho_A^2) = -\ln \langle SWAP_A \rangle, \tag{10}$$

where $\langle SWAP_A \rangle$ is the expectation value of the SWAP operator for subsystem A between two replicas.

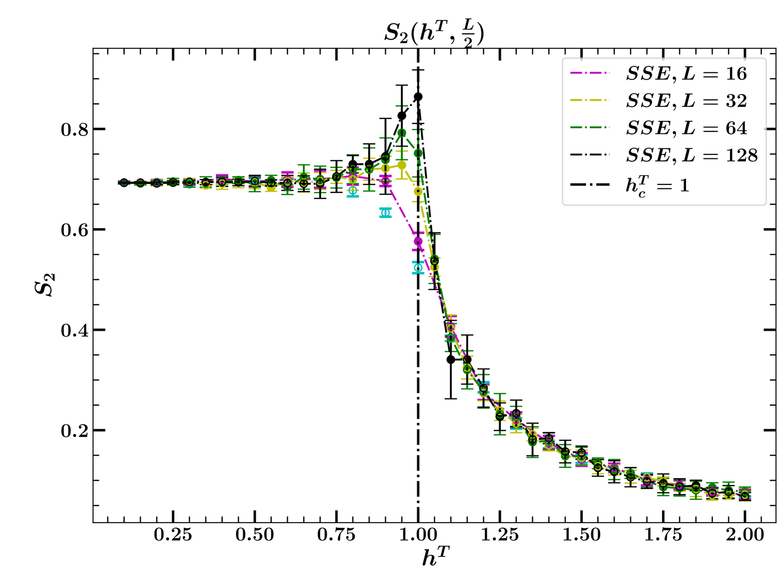

Figure: SRTFIM

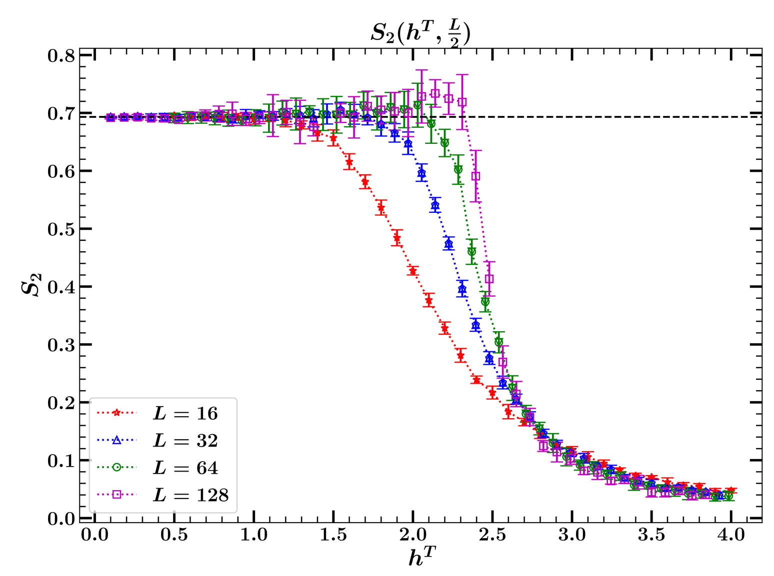

Figure: LRTFIM with $\sigma = 1.0$

- **Area Law:** In SRTFIM, entanglement entropy scales as L^{d-1} outside criticality. These signatures still persists in long range interactions.

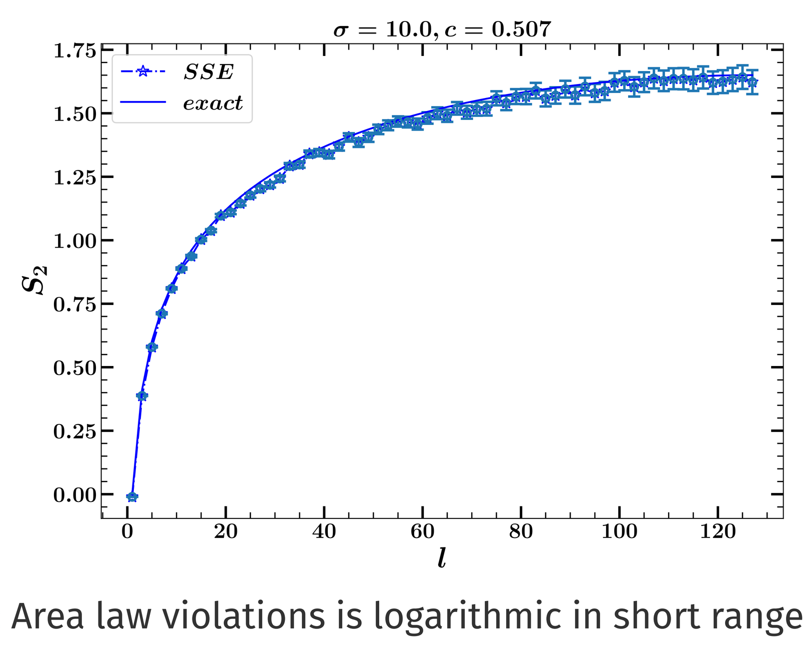

Figure: Area law violations is logarithmic in short range regime[3]

Conclusion and Outlook

- Projector QMC allows us to obtain continuum results for the quantum model at $T = 0$.
- The criticality in LRTFIM exhibits very distinct scaling behavior (in comparison to SRTFIM), significantly affecting the behaviour of entanglement entropy area law.
- Next step: to include the whole regime of long-range interactions, in order to accurately predict the robustness of the area law at the critical point.

References

[1] Anders W. Sandvik, *Ground State Projection of Quantum Spin Systems in the Valence-Bond Basis*, Phys. Rev. Lett. **95**, 207203 (2010).

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[3] Tomotaka Kuwahara et al., *Area Law of Noncritical Ground States in 1D Long-Range Interacting Systems*, Nat. Commun. **11**, 4478 (2020).

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