Assignment: Phase Diagram and Out-of-Equilibrium Dynamics

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I. INTRODUCTION

We will study the phase diagram and the out-of-equilibrium dynamics of a paradigmatic spin model. The model is defined on an open chain of spin-1/2 constituents of length L. The Hamiltonian is given by [1]:

$$H(p, \lambda) = -\sum_i \left[\sigma_i^z \sigma_{i+1}^z + \lambda \sigma_i^x + p\big(\sigma_i^z \sigma_{i+2}^z + \lambda \sigma_i^x \sigma_{i+1}^x\big)\right] . \tag{1}$$

Key properties of the Hamiltonian:

1. If $p = 0$, the model reduces to the standard transverse-field Ising model.
2. If $\lambda = 1$ and $p \to \infty$, the Ising part becomes negligible, and the model is more complicated.
3. For $p \neq 0$, the Hamiltonian includes next-nearest-neighbor interactions.

The goal of this assignment is to analyze the phase diagram of the model in the (p, λ) plane and to study its out-of-equilibrium dynamics. We will focus on values $p \leq 1$ to stay close to the transverse field Ising model (whose properties you can obtain by setting $p = 0$).

II. PHASE DIAGRAM (5 POINTS)

Using `TeNPy` [2, 3], perform the following tasks:

1. **Define the model in `TeNPy`** (2 points).
2. **Characterize the phase diagram using an infinite MPS ansatz** (2 points).
   (a) For each (p, λ) point, run simulations with bond dimensions $D = 16$ and $D = 32$.
   (b) Compute and plot the correlation length ξ as a function of p and λ for both bond dimensions. Identify regions where D is insufficient to capture the physics.
   (c) Using $\xi \propto 1/\Delta$, discuss implications for the phase diagram.
3. **Extend simulations to larger bond dimensions ($D \leq 64$)** (1 point).
   (a) Identify regions where ξ saturates with D versus where it continues to grow.
   (b) Plot the half-chain entanglement entropy $S(\xi(D))$ versus D and analyze its behavior [4].

III. OUT-OF-EQUILIBRIUM DYNAMICS (5 POINTS)

Using `TeNPy` [2, 3], implement the following quantum quench protocol:

1. **Quench from a product state** using the ITEBD algorithm:
   (a) Initialize all spins in the $|+\rangle$ state (along x-axis).
   (b) Evolve under the Hamiltonian with $p = 0.5$ and $\lambda = 1$ for time $t = 5$, using a maximum bond dimension $D = 100$.
2. Plot the following as functions of time (each worth 0.5 points):
   (a) Magnetization $\langle \sigma^x \rangle(t)$.

(b) Magnetization $\langle\sigma^z\rangle(t)$.

(c) Explain the behavior of $\langle\sigma^z\rangle$ using algebraic reasoning.

(d) Entanglement entropy of half the chain.

(e) Bond dimension D.

(f) Truncation error ϵ.

(g) Discuss the relation between bond dimension growth, truncation error, and entanglement entropy.

3. **Entanglement spectrum analysis** (1 point):

(a) Compute the entanglement spectrum $e_i = -\log(\lambda_i)$, where λ_i are the eigenvalues of the reduced density matrix.

(b) Define gaps $\Delta_i = e_i - e_0$ for the 10 largest eigenvalues and plot both Δ_i and their ratios Δ_i/Δ_1 as functions of time.

4. **Discussion** (0.5 points): Summarize and interpret your results [5].

IV. SUMMARY

This assignment aims to deepen your understanding of quantum phase transitions and non-equilibrium dynamics using tensor network methods. Key takeaways include:

- Identifying quantum phases via correlation length scaling.
- Observing entanglement growth in quench dynamics.
- Understanding computational limitations imposed by bond dimension and truncation errors.

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