Unsupervised learning of thermal phase diagram of the long-range XXZ model

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Objective

The objective of the project is to study in an unsupervised manner the thermal phase diagram of the finite-size L spin-1/2 chain described by the long-range XXZ Hamiltonian

$$\hat{H} = -\sum_{i,j} J_{ij}(\hat{\sigma}_i^x \hat{\sigma}_j^x + \hat{\sigma}_i^y \hat{\sigma}_j^y + \Delta \hat{\sigma}_i^z \hat{\sigma}_j^z) - h \sum_i \hat{\sigma}_i^z, \tag{1}$$

where J_{ij} couplings are $J_{ij} = \frac{1}{|i-j|^\alpha}$. Note that for $\alpha = 3$ system has dipolar-type of interaction, for $\alpha = 0$ system has all-to-all couplings, while for $\alpha > 6$ system is effectively nearest-neighbour interacting.

Start with zero temperature $T = 0$ analysis.

- Perform an analysis of the system's ground state properties for $\alpha = 6, 3, 0$ and find a range of parameters δ, h_z indicating distinct phases. Perform PCA, and t-SNE analysis. Comment on how clusterization depends on α, what observables allow separate cluster coloring.
- Perform unsupervised phase detection with the autoencoder. Propose your own architecture. Apply normalization techniques and find the optimal hyperparameters. Analyze the clustering of laten space with PCA.
- Analyze reconstruction phase diagram with the reconstruction loss, and with quantum distances: trace distance and Hilbert-Schmidt distance.
- Analyze the situation when training data are only from a finite part of the phase diagram (for example, with a given value of $\langle \hat{S}_z \rangle$).
- Analyze the problem for different numbers M of samples used to train the autoencoder. How does reconstruction quality change with $M = 1, 2, 10, 20, 100, 200$?
- Perform similar analysis for thermal Gibbs states for few temperatures $T = 0.01, 0.05, 0.1, 1$.

Follow the methodology described in this tutorial.