Learning ground states of quantum Hamiltonians with graph networks

Daniele Montagnani

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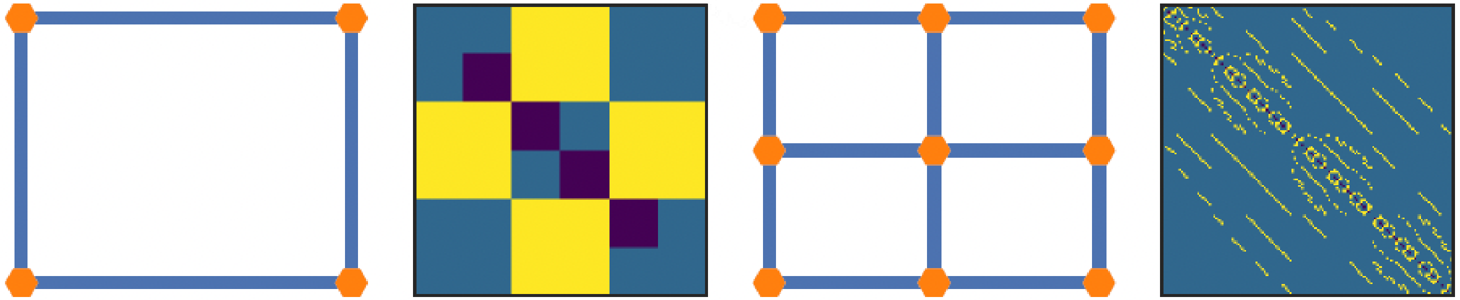
Project @ https://github.com/danmonuni/quant_sim_fp

Introduction

The Problem: Finding the Ground states of an Heisenber Hamiltonian

- Why is it difficult? Exponential Growth in Complexity



SOTA

- Variational Monte Carlo with Ansatz f

Paper Contribution

- Use a GNN as Ansatz f
- Highly Expressive and amenable to optimisation
- Distributer representation
- Better one shot transfer capabilities

Variational Monte Carlo

Address the complexity of the Hilbert Space by:

- Working in a low dimensional variational manifold $V \subseteq H$
- Use stochastic sample-based approximations for evaluation and optimisation

The manifold: $|\psi_{f,w}> = \sum f(w, c_i)|c_i>$

Stochastic method:

- Sample computational basis states from f, with Metropolis Hastings
- Obtain stochastic estimates of physical observables (Overlap, Energy)

Optimisation:

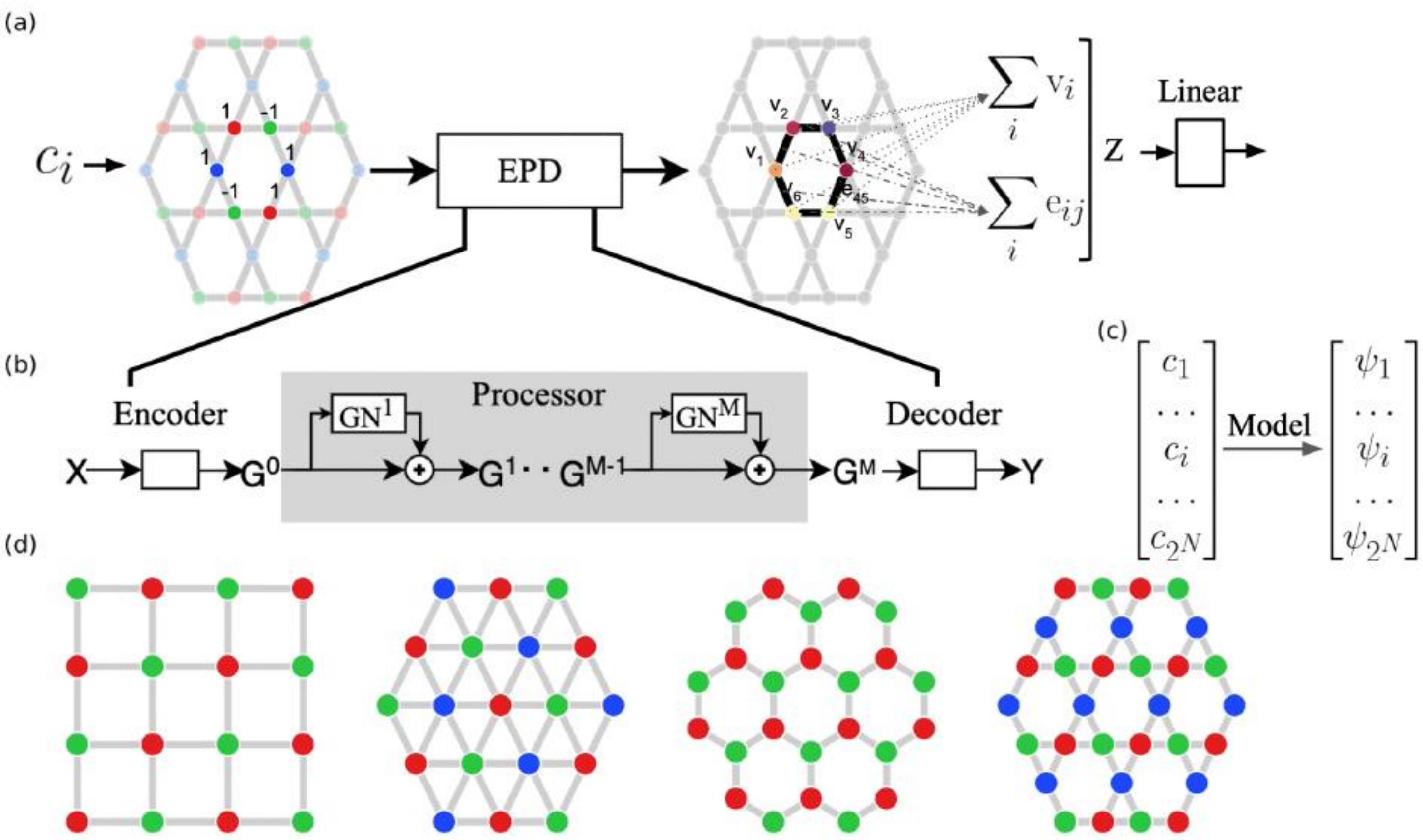
- Energy gradient descent
- Imaginary Time Evolution

GNN as a Variational Model

GNN to predict log(amp) and pha

Architecture:

1. Input basis element and sublattice encoding
2. Compute a distributed latent representation with an encode process decod GNN
3. Sum pool node and edge features, obtain a final latent vector (size invariance)
4. Process it with a linear layer to predict scalar outputs



Optimisation

Imaginary Time Supervised Wave Optimisation:

- Compute the current state
- Obtain an imaginary time evolved state: $|\phi> = (1 - \beta H)|\psi>$
- Maximize the **overlap** between the current state and the time evolved one

- A beautiful view of the Schrödinger equation

Energy Gradient Descent:

- Compute the current state
- Compute its energy
- Use it as the loss fro gradient descent

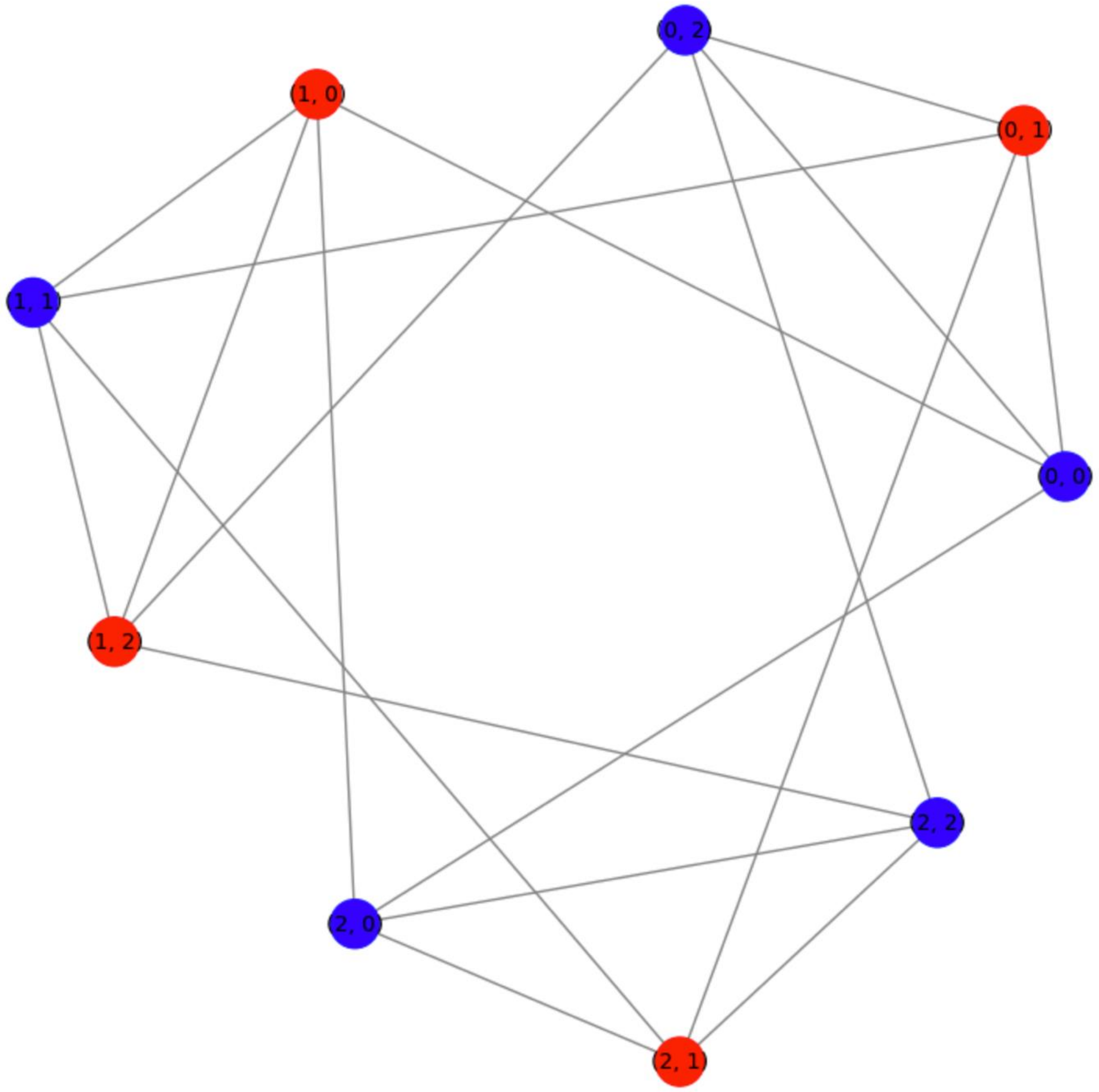
Test Problem

9x9 Square Lattice with Continuity Condition

512 x 512 Quantum Hamiltonian:

$$\hat{H} = \sum_{<i,j>} \hat{S}_i \hat{S}_i$$

Diagonalizable with traditional methods so that I could check my results



Approach Followed

Incremental Approach

Follow a Diamond Progression:

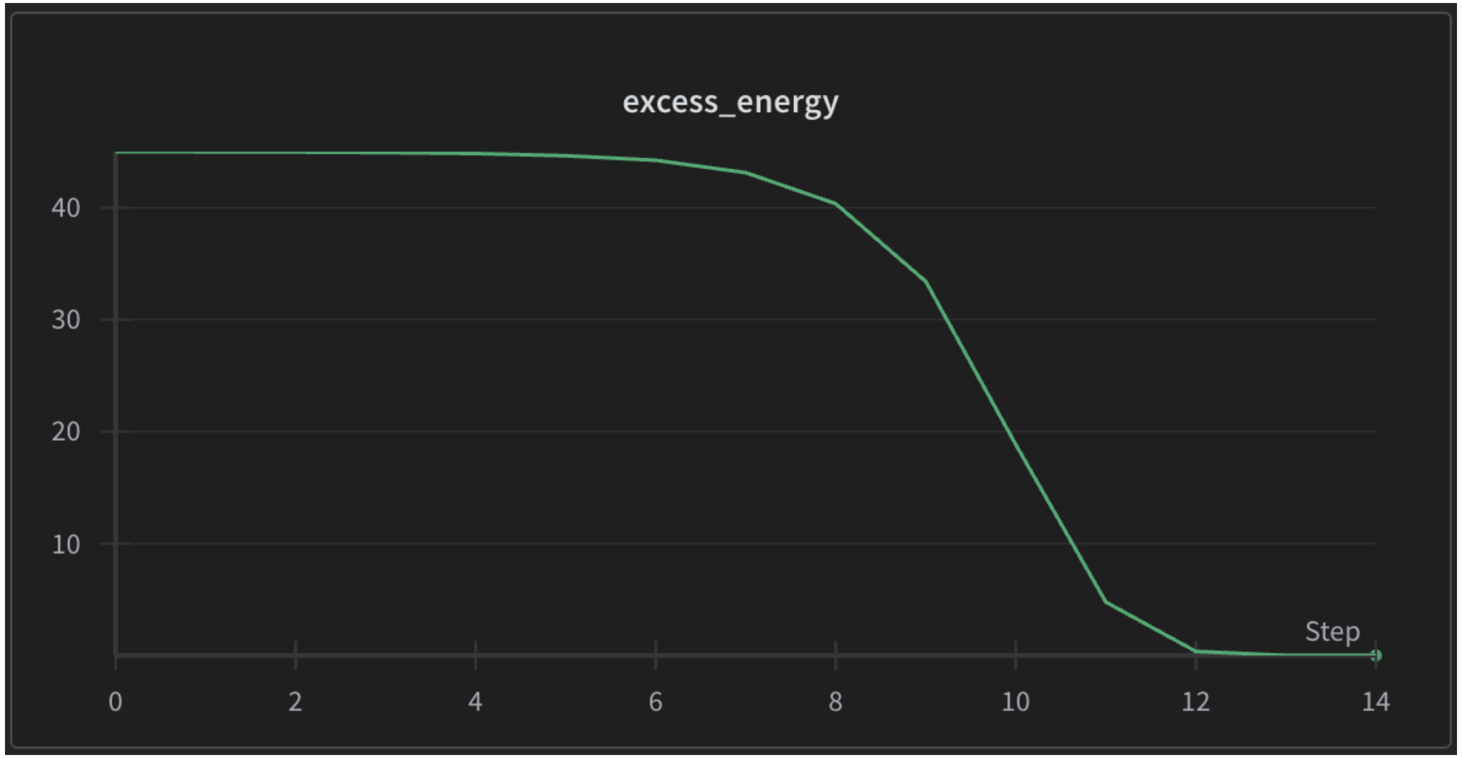
- Root: exhaustive evaluation, classical mixture
- Branch 1: stochastic evaluation, classical mixture
- Branch 2: exhaustive evaluation, quantum superposition
- Merge: stochastic evaluation, quantum superposition

Why the classical mixture? Isn’t it pointless?

root - exhaustive evaluation, classical mixture

Optimization Method: Energy gradient descent

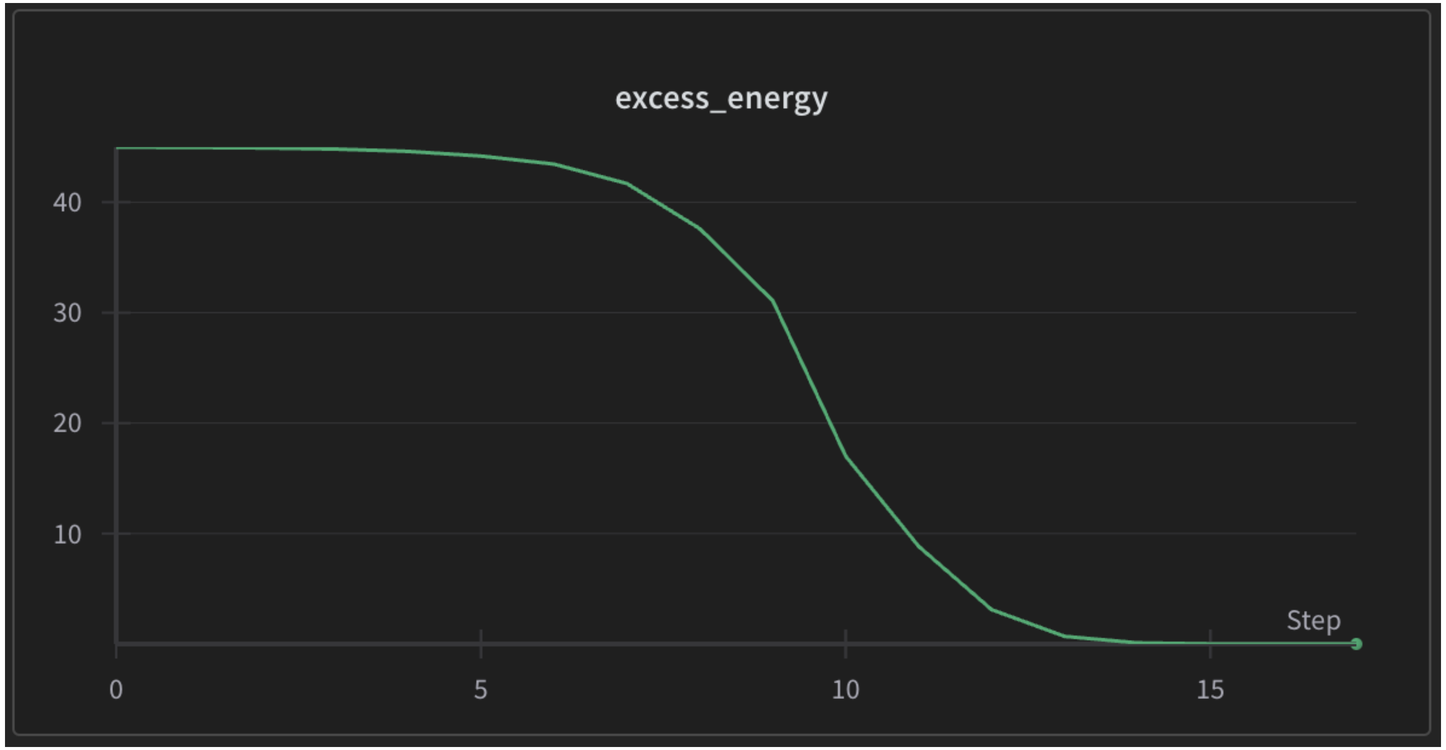
Result: obtain an indicator on the state fully magnetized in the external field direction



root - stochastic evaluation, classical mixture

Optimization Method: Energy gradient descent with a stochastically estimated energy

Result: obtain an indicator on the state fully magnetized in the external field direction



root - stochastic evaluation, classical mixture

Optimization Method: ITSWO
Results:
best overlap with ground states ~25%
Difficulty in overcoming numerical issues
Tried different solutions (clipping, regularization terms)