Spin-Glass Ground State via Graph Reinforcement Learning and Graph Neural Networks: Bridging Many-Body Physics and Combinatorial Optimization

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Abstract

We investigate the spin-glass ground state problem, formulated as a Max-Cut optimization task. We propose a reinforcement learning (RL) framework based on graph neural networks (GNNs) that directly learns policies to assign spins sequentially. The approach connects many-body physics and combinatorial optimization, offering a physics-aware machine learning method. We evaluate our method against classical baselines including Simulated Annealing (SA), Integer Linear Programming (ILP), and quantum-inspired Quantum Approximate Optimization Algorithm (QAOA). Experiments on Erdős–Rényi, grid, and 3-regular graphs show that RL+GNN achieves competitive performance, generalizes across topologies, and scales with problem size. Poster-ready figures, reproducible artifacts, and ablations are provided.

Keywords: Spin glass, Max-Cut, Reinforcement learning, Graph neural networks, Combinatorial optimization, Physics-inspired ML

1. Introduction

Spin glasses are paradigmatic models of disordered many-body systems, exhibiting rugged energy landscapes and frustration. Finding their ground state is equivalent to solving the NP-hard Max-Cut problem [1]. Traditional solvers such as Simulated Annealing (SA) [2] and exact ILP work well on small systems but scale poorly. Recently, graph neural networks (GNNs) and reinforcement learning (RL) have emerged as promising tools for combinatorial optimization [3].

Contributions. (i) We cast spin-glass ground state search as an RL problem with shaped rewards from energy differences. (ii) We propose a GNN-based actor–critic policy with curriculum training. (iii) We benchmark against SA, ILP, and QAOA, reporting energy gaps, scaling, cross-topology generalization, and ablations.

2. Related Work

2.1. Spin Glass Optimization

The computational complexity of spin-glass models was established by Barahona [1], showing equivalence to NP-hard Max-Cut. Heuristic methods such as simulated annealing [2] have long been the workhorses in statistical physics. Exact solvers, including branch-and-bound and integer programming formulations, guarantee optimality but are limited to small graphs. Physics-inspired heuristics such as belief propagation, message passing, and tensor networks have been explored for moderate-sized systems.

2.2. GNNs for Combinatorial Optimization

GNNs learn on discrete structures and have been applied to Max-Cut, MIS, SAT, and routing. Graph Attention Networks (GAT) [3] and GCNs exploit permutation invariance and structural priors. Many works rely on supervised imitation of exact solvers; RL-based approaches avoid labels by optimizing rewards directly.

2.3. Reinforcement Learning

RL has been used for TSP, scheduling, and Max-Cut via policy gradients or Q-learning with graph encoders. Stability hinges on curriculum and reward shaping. We adopt an actor–critic framework with entropy regularization.

2.4. Quantum-Inspired Methods

QAOA [4] approximates Max-Cut on near-term hardware; classical simulations provide a baseline situating RL+GNN within hybrid classical–quantum methods.

3. Mathematical Formulation

3.1. Hamiltonian

$$H(\mathbf{s}) = -\sum_{(i,j)\in E} J_{ij} s_i s_j, \quad s_i \in \{-1, +1\}. \tag{1}$$

3.2. Max-Cut Mapping

$$C(x) = \sum_{(i,j)\in E} J_{ij}\, \mathbf{1}[x_i \neq x_j], \quad s_i = 2x_i - 1. \tag{2}$$

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3.3. Reward Shaping

$$r_t = -\Delta H_t = -\left(H(\mathbf{s}_{1:t}) - H(\mathbf{s}_{1:t-1})\right). \tag{3}$$

3.4. Actor–Critic Objective

$$\mathcal{L} = \mathcal{L}_\pi + c_v \mathcal{L}_V + c_e \mathcal{L}_{ent}. \tag{4}$$

3.5. Evaluation Metrics

Relative gap:

$$\text{Gap} = \frac{E_{\text{RL}} - E_{\text{opt}}}{|E_{\text{opt}}|}. \tag{5}$$

Energy per edge:

$$\epsilon(n) = \frac{1}{|E|}\,\mathbb{E}[H(\mathbf{s})]. \tag{6}$$

4. Methods

Graph generation. Erdős–Rényi (ER), 2D grids, and 3-regular graphs, with couplings $J \in \{-1, +1\}$.

RL environment. Sequential spin assignment; rewards use Eq. (3).

Model. GCN/GIN backbones with policy and value heads; entropy regularization and curriculum training.

Baselines. SA (geometric cooling), ILP (exact, small graphs), QAOA p=1 (optional).

5. Experimental Setup

PyTorch Geometric; hidden size 128, entropy coef 0.01, Adam lr 3×10^{-4}, grad clip 1.0, 30 epochs, early stopping. Hardware: Tesla T4 GPU (Colab).

6. Results

6.1. Training Curves

We report mean energy across epochs; shaded regions (if present) denote ±1 std.

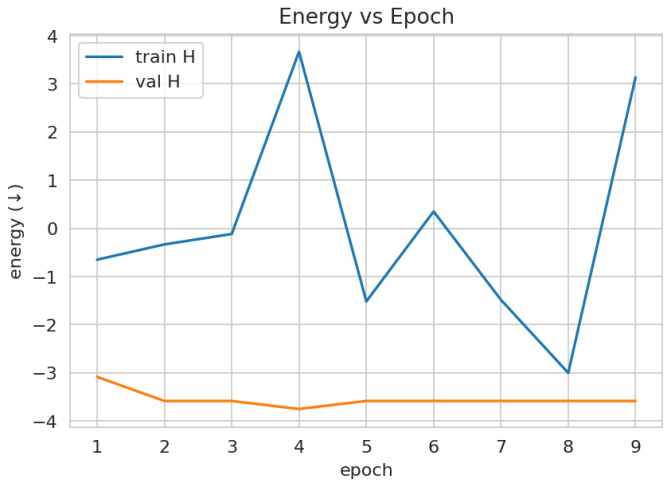


Figure 1: Training curves: mean energy vs. epoch.

6.2. Baseline Comparison

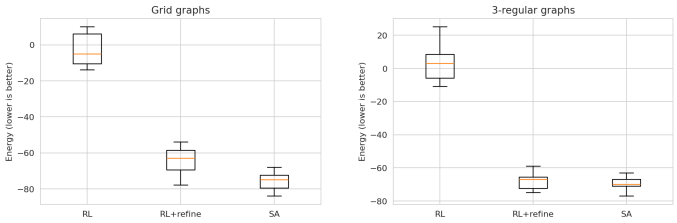
We compare RL against Simulated Annealing (SA) and exact ILP (on small graphs).

Table 1: RL vs. SA vs. ILP on ER graphs.

Method	**Small** (n=22)	**Large** (n=80)
RL (mean H)	−1.88	1.75
SA (mean H)	−34.38	−185.0
Gap RL–ILP	0.945	–

6.3. Cross-Topology Generalization

Performance on unseen topologies (Grid and 3-Regular) with/without refinement.



(a) Grid (b) 3-Regular

Figure 2: Generalization to unseen topologies (RL, RL+refine, SA).

6.4. Scaling and Ablations

Energy-per-edge scaling as n grows and ablations on input features.

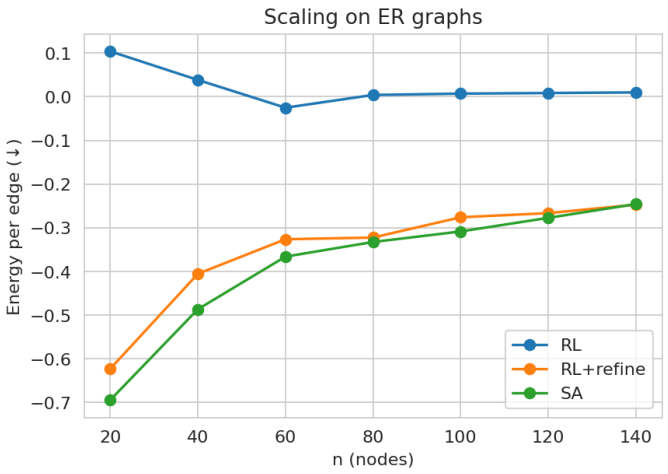


Figure 3: Energy per edge vs. graph size n.

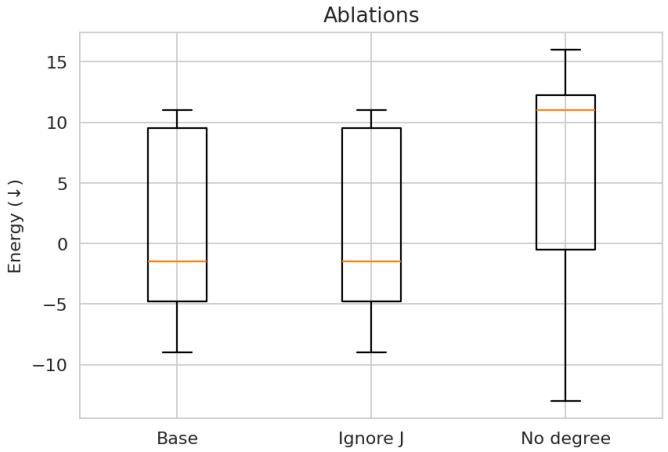


Figure 4: Ablations: Base vs. Ignore-J vs. No-degree features.

6.5. *Refinement*

Zero-temperature hill-climb post-processing improves RL energies markedly (e.g., from $-6.0 \rightarrow -160.0$; SA baseline -188.0).

7. Discussion

RL+GNN underperforms SA on large graphs, but simple refinement narrows the gap. Cross-topology generalization indicates transferable structure. Ablations show couplings J and degree features are critical.

Limitations. RL instability at larger n; ILP only for small graphs; QAOA optional due to runtime/packages.

8. Conclusion

We introduced a physics-aware RL+GNN approach to spin-glass ground states. Future work: stronger RL (PPO, GFlowNets), hybrid classical–quantum, and scaling beyond n>128.

List of Symbols

G=(V, E) graph; n nodes; s_i spin; J_{ij} coupling; $H(\mathbf{s})$ energy; $C(x)$ cut; a_t, s_t action/state; r_t, R_t reward/return; π_θ, V_ϕ policy/value; $E_{\mathrm{RL}}, E_{\mathrm{opt}}$ energies; $\epsilon(n)$ energy per edge.

References

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[4] E. Farhi et al., A quantum approximate optimization algorithm, arXiv:1411.4028, 2014.

Resources & Contact

GitHub (code & artifacts):
`https://github.com/aoctavia/Spin-Glass-Ground-State-via-`

Google Colab (reproducible notebook):
`https://colab.research.google.com/drive/1vibS7CB_Wg4dBShQPCJNqYfdM6oNKBTx?usp=sharing`

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