Hamilton-Zero - A Neural Tensor Network Foundation Model

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A central problem in quantum many-body systems is computing the ground state of a given spin-1/2 Hamiltonian. Efficient ground state computation is relevant from materials design through to drug discovery [1, 2, 3], with the former especially relevant when mapping out the phase diagram of a many-body system.

For a large many-body system, however, computing such ground states has proven famously difficult due to the curse of dimensionality. This curse refers to the fact that a spin-$\frac{1}{2}$ Hamiltonian on N sites has a ground state in 2^N complex dimensions. Decades of research have uncovered many complementary methods to solve this problem as generally as possible, from variational quantum algorithms, to tensor networks and neural quantum states (NQS). NQS, has taken off in popularity over the last years, solving for variational upper-bounds to ground states on large systems, with the largest systems approaching $1500 - 2000$ qubits [4]. Conventionally, the training cost for NQS requires optimizing an architecture from scratch for each given instance of a many-body system, including in electronic NQS such as FermiNet, PauliNet, and DeepErwin [5, 6, 7]. Foundation neural quantum states (FNQS) [8, 9, 10, 11] changed this paradigm, amortizing that cost with one model trained across a Hamiltonian family such as a family of Ising models with differing interaction and transverse field strengths [12]. Thus far however, the community has gone in a direction where they fix the Hamiltonian's interaction graph, varying only in the parameter space of that Hamiltonian and train a pure-state foundation model. This means every time the particle number, interaction topology (e.g. from 1D chain to a 2D lattice to an amorphous material), or interaction type (e.g. from XX to XZ couplings), a new model must still be trained anew.

In this contribution, we introduce Hamilton-Zero [13], a foundation model that generalises across both multiple system sizes, different interaction topologies, and different interaction types, trained on hundreds of thousands of distinct training Hamiltonian topologies, system sizes and interaction types spanning a century of quantum many-body literature. In order to scale to thousands of qubits, we derive a novel phase-space variational principle for centrally odd scalar functions $\psi_\theta : SU(2)^N \to \mathbb{C}$, with each $SU(2) \hookrightarrow \mathbb{R}^4$ a continuous Lie-group-valued input. This enables us to act arbitrary quadratic qubit Hamiltonians via custom auto-diff primitives for pretraining, fine-tuning and evaluation. The architecture itself uses an LLM-style embedding of interaction graphs via a featuriser and L-blocks of alternating attention and FFN layers. To contract to a scalar-value, we build a tree tensor-network, with attention layers between each layer of the tree to allow entangling information to flow between sites of a contraction. The ordering of the sites in the tree also sets the entanglement structure of the model, which, since it acts on varying system sizes and interaction topologies, is a learned map trained by deep reinforcement learning.

At $\sim$ 0.5B parameters, this proof of principle shows one model can serve hundreds of thousands of different Hamiltonian systems, generalising to scales $\sim 100\times$ the number of qubits seen in training, and to unseen interaction types and topologies. Applications to materials science are unprecedented. When a single model can serve differing topologies and interaction types, a paradigm emerges where researchers in materials science no longer need specialist deep-learning knowledge to solve for phase-diagrams with neural methods. Furthermore, since such models can serve a range of qubits spanning orders of magnitude, we can for the first time use a single model to investigate numerical signatures of phase transitions in a universal manner. This means that future research could sweep a large candidate set of Hamiltonians as models scale and their quality improves, where currently mapping a novel phase diagram is often a publication-worthy feat. This shift happened in drug discovery with hit generation in protein interactions, and biochemistry with the protein folding problem.

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