FUJITSU

Meta-learning of Gibbs states for many-body Hamiltonians with applications to Quantum Boltzmann Machines

Background

Preparing Gibbs states of many-body Hamiltonian at low and intermediate temperatures are as hard as preparing the ground states.
For a parametrized many-body Hamiltonian $H(\vec{h})$, Gibbs state at temperature T takes the form :

$$\rho(\vec{h}) = \frac{e^{-\beta H(\vec{h})}}{\sum e^{(-\beta H(\vec{h}))}}, \text{ where } \beta = 1/k_B T$$

Why Gibbs State preparation ?

Gibbs state finds application in:
- Modelling open quantum systems
- Combinatorial optimization
- Training of Quantum Boltzmann Machines

Challenges & Our Proposal

- High cost: Each parameterized Hamiltonian requires separate execution.
- Need for expressive ansatz: Must handle varying parameters and temperatures, especially near finite-temperature crossovers/phase transitions.

Proposed NISQ algorithms to address these challenges

Collective optimization based :
- Meta-Variational Quantum Thermalizer (Meta-VQT)
- Neural Network Meta-Variational Quantum Thermalizer (NN Meta-VQT)

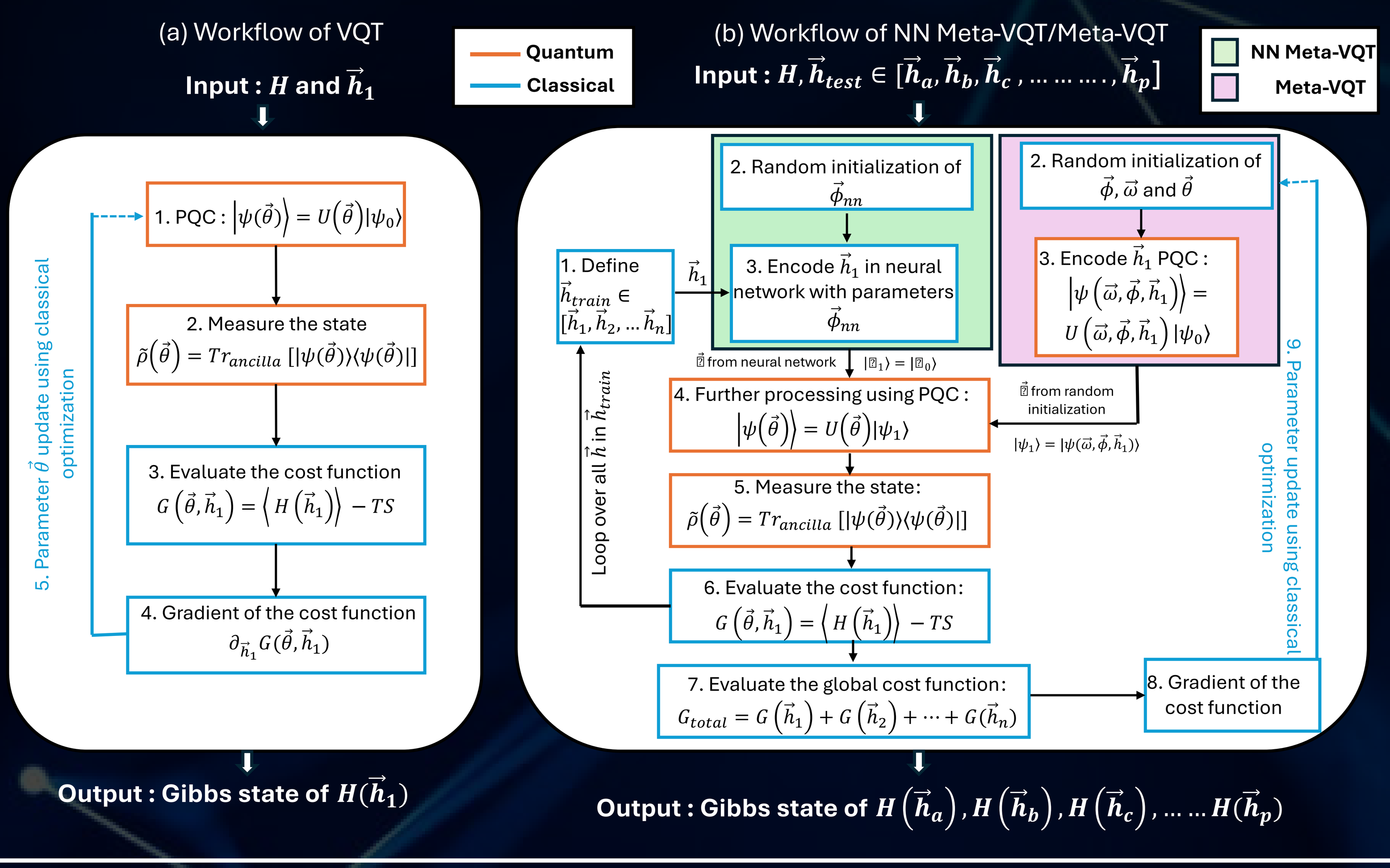
Novel ansatz for capturing correlations in Gibbs state

Results

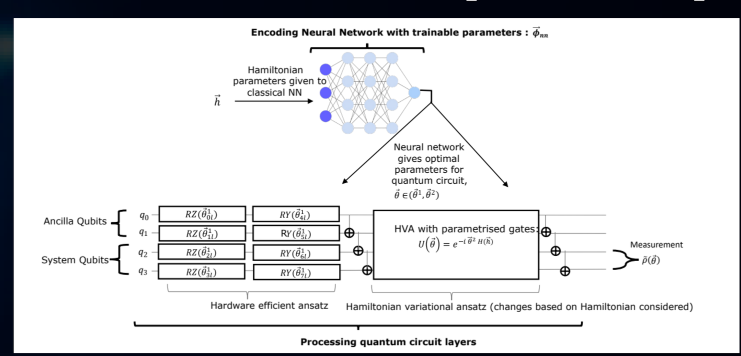
- After training, our ansatz prepares Gibbs states for unseen Hamiltonian parameters with high accuracy.
- If precision is insufficient, the meta-trained circuit serves as an efficient starting point for traditional VQT, avoiding random initializations.
- When used in QBM training :
  - Enhances training speed
  - Requires fewer QPU calls
  - More accurate Gibbs state preparation

Workflow of traditional VQT, Meta-VQT, NN Meta-VQT and novel ansatz design

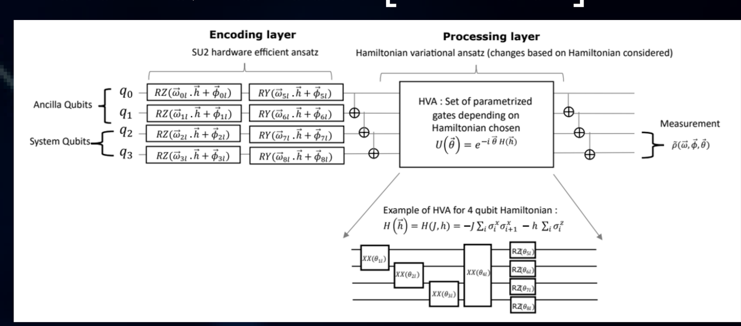
- **Traditional VQT : Separate training required for each Hamiltonian parameter.**
- **Meta-VQT/NN Meta-VQT : Encodes multiple Hamiltonian parameters during training, can generate Gibbs state of unseen parameters without retraining.**
- **Novel design of ansatz enables efficient representation of Gibbs state across parameter space.**



NN Meta-VQT ansatz [Green box]

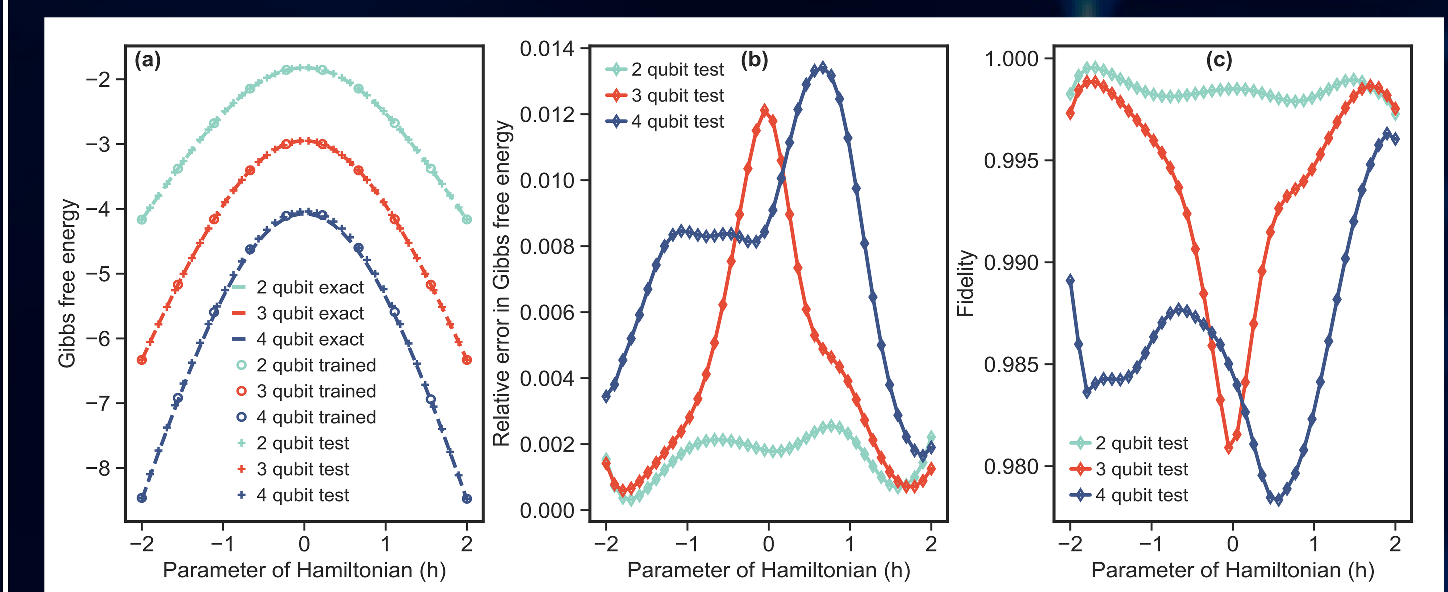


Meta-VQT ansatz [Pink box]



Demonstrative numerical examples

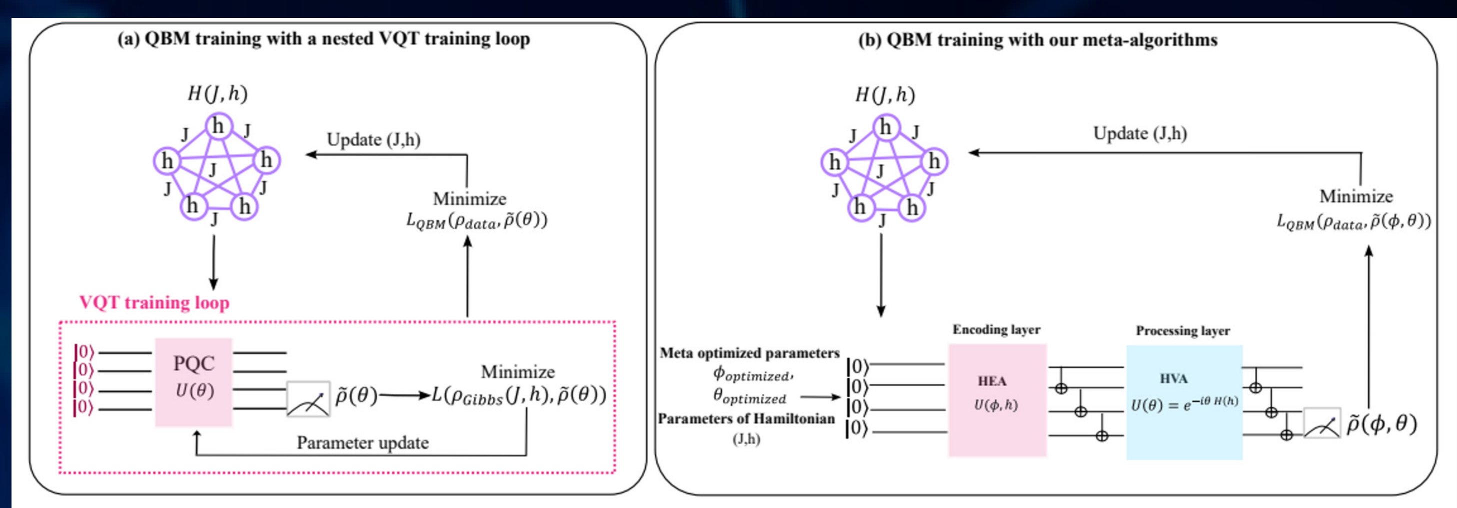
Accurate preparation of Gibbs state of Transverse Field Ising Model



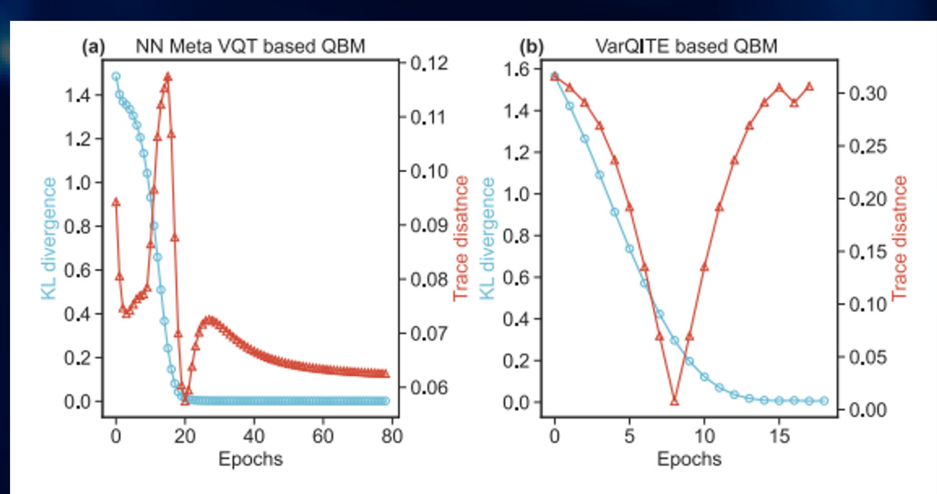
Conclusions

- Our algorithms learn Gibbs states across multiple Hamiltonian parameters, generalizing to unseen cases without retraining.
- Our meta-trained ansatz serves as better initializations for traditional VQT for Gibbs state preparation compared to existing techniques.
- In variational QBM, Meta-VQT and NN Meta-VQT remove the nested optimization loop, support complex many-body models, cut runtime by up to 30×, and improve Gibbs state precision and final loss.

Avoiding nested loop in traditional QBM training using our Meta-trained ansatz for Gibbs state preparation



Comparison of NN Meta-VQT based QBM (our proposal) and VarQITE based QBM (existing) for learning a random 2-qubit state using a Heisenberg model with all field terms



VarQITE-based QBM shows large trace distance from target Gibbs state at convergence, while NN Meta VQT based QBM shows much lower trace distance.

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Check out our full paper here!