Exploring Dynamic Circuits through Gibbs Free Energy Calculations and Error Mitigation

IBM Quantum QRISE Challenge, Maximizing Performance and Tayloring Noise

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Problem Statement

Dynamic circuits are an exciting feature of IBM Quantum hardware that incorporates quantum circuits with real-time classical communication. Different from the static counterpart, dynamic circuits can not only implement a set of basic quantum operations like the Hardmard gate, CNOT gate, or qubit reset but also can implement measurement in the middle of a circuit, store the measurement results to classical bits, evaluate classical expressions on the fly, and determine what quantum operation to do next. This capability has a variety of applications, for example, quantum error correction, quantum simulation, and so on. We encourage you to explore what you can do with dynamic circuits in this challenge.

Introduction to Dynamic circuits I

Dynamic circuits are a groundbreaking advancement in quantum computing that enable the integration of real-time classical communication within quantum circuits. Unlike static circuits, where quantum operations are predetermined and independent of runtime data, dynamic circuits incorporate classical processing during the coherence time of qubits. This allows for mid-circuit measurements and feed-forward operations, where the outcomes of measurements dictate subsequent gate applications. dynamic circuits offer a bridge between classical and quantum computation by leveraging classical information to dynamically adjust the quantum operations performed within a circuit. This capability significantly expands the range of quantum algorithms and applications that can be implemented on near-term quantum hardware. By optimizing the trade-off between circuit depth and width, dynamic circuits pave the way for more efficient and effective quantum computations, potentially unlocking quantum advantage in various domains..

Gibbs State Free energy I

In statistical mechanics and thermodynamics, the Gibbs state free energy, denoted as
F, is a fundamental quantity that characterizes the equilibrium state of a thermodynamic system at constant temperature
T, pressure
P, and particle number
N. It is defined as the difference between the internal energy
U and the product of temperature
T and entropy
S, i.e., $F = U - TS$

Gibbs State Free energy I

Gibbs State Free energy II

The Gibbs free energy plays a crucial role in various areas of physics, chemistry, and engineering. Some key aspects of its importance include:

- **Thermodynamic Stability**: In a closed system at constant temperature and pressure, a process will occur spontaneously if and only if the change in Gibbs free energy is negative
- **Chemical Reactions**: The Gibbs free energy change (ΔG) for a chemical reaction determines whether the reaction is thermodynamically favorable ($\Delta G < 0$) or unfavorable ($\Delta G > 0$). It helps predict the feasibility and direction of chemical reactions under given conditions.
- **Phase Transitions**: At phase equilibrium, the Gibbs free energies of coexisting phases are equal. The Gibbs free energy change between different phases (ΔG_{phase}) governs phase transitions such as melting, vaporization, and sublimation.
- **Equilibrium Conditions**: The Gibbs free energy is minimized at equilibrium, providing a criterion for determining the equilibrium state of a system. At equilibrium, the chemical potential (μ) of each component is equal across phases ($\mu_i^\alpha = \mu_i^\beta$), ensuring a balance of chemical potentials.

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Calculating Gibbs Free energy using Variational Quantum eigensolver

- We have used The Transverse Field Ising Model (TFIM) Hamiltonian describes a system of quantum spins interacting with each other under the influence of an external magnetic field. The Hamiltonian for the TFIM is given by.
- This Hamiltonian describes the interplay between the interaction energy (first term) that tends to align neighboring spins either parallel or antiparallel, and the external magnetic field energy (second term) that tends to align spins along the x-axis.Adjusting the values of N, J, and h allows for the exploration of different system sizes, interaction strengths, and external field strengths.

$$H = -\sum_{ij} J_{ij}\sigma_i^z\sigma_j^z - \sum_i h_i\sigma_i^x.$$

Figure: Transverse Field Ising Model Hamiltonian

Hamiltonian

Construction of Hamiltonian

We then Construct the initial and final Hamiltonians for the TFIM with adjustable parameters.Here are the steps

- Initialize Parameters
- num-sites $= 3$: Number of sites or spins in the system.
- J $= 1$: Coupling constant for spin-spin interaction.
- h $= 1$: Strength of external magnetic field along the x-direction
- Create an operator list oplist
- Use SparsePauliOp.from-sparse-list() to create the initial Hamiltonian hamiltonian-i

1. Update the external magnetic field strength h to a new value (e.g., h $=$ 1.5)
2. Repeat the construction process to create the final Hamiltonian hamiltonian-f
3. Add interaction terms $\sigma_i^z \sigma_{i+1}^z$ and external field term σ_i^x to `oplist`.

EfficientSU2 ansatz

we utilized the EfficientSU2 ansatz to initialize the circuit structure, where the number of parameters was determined by the attribute num-params..

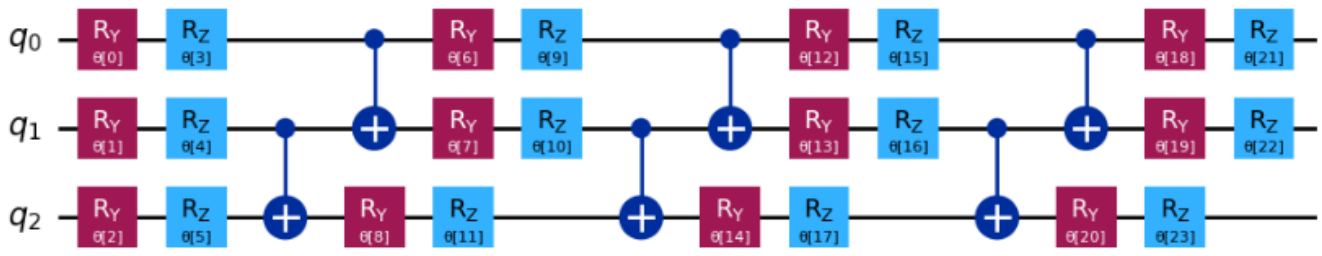

Figure: EfficientSU2 ansatz

Calculating the Final Energy

Calculating the Final Energy

We then Minimized the energy of a Transverse Field Ising Model Hamiltonian using the EfficientSU2 ansatz..Here are the steps

- Initialization: Initialize parameters randomly.
- Define a cost function that estimates the energy from the ansatz using an Estimator instance.
- Implement a callback function to track intermediate results during optimization.
- Utilize the minimize function to minimize the cost function using the COBYLA method.
- Compute the expectation value of the initial and the final Hamiltonian using optimized parameters.
- Calculate the difference in energy between initial and final states, and compute the Gibbs free energy using the Boltzmann factor.
- We get the Free energy value- -0.4211741499226242 5 which is quite a good value

Calculating Gibbs Free energy using Dynamic Circuits

- We started by defining the Hamiltonian, Spin-1/2 Hamiltonian is defined using the Transverse Field Ising Model (TFIM) Hamiltonian. This model describes a system of spin-1/2 particles with interactions between neighboring spins and an external magnetic field. The Hamiltonian is constructed using the qiskit.quantum-info.SparsePauliOp class, which allows us to represent Hamiltonians in terms of Pauli operators efficiently.
- we defined an ansatz circuit using the EfficientSU2 class provided by Qiskit. An ansatz circuit is a parameterized quantum circuit used to prepare trial states for variational quantum algorithms. The EfficientSU2 ansatz is a common choice for variational quantum algorithms as it provides a flexible and efficient way to explore the Hilbert space of the quantum system. The number of parameters in the ansatz circuit determines the expressiveness of the trial states and influences the accuracy of the results obtained from the variational algorithm.

Calculating Gibbs Free energy using Dynamic Circuits

we formulated a cost function equation for the minimization method. This equation, derived from the Gibbs Free Energy expression, involves the Hamiltonian H and the density matrix ρ of the system. By minimizing this equation with respect to the parameters θ of the ansatz circuit, we aim to determine the Gibbs Free Energy associated with the measured Hamiltonian.

$$\mathcal{F}_2(\boldsymbol{\theta}) = \mathrm{tr}(H\rho(\boldsymbol{\theta}))+\beta^{-1}\left(2\,\mathrm{tr}(\rho(\boldsymbol{\theta})^2) - \frac{1}{2}\,\mathrm{tr}(\rho(\boldsymbol{\theta})^3) - \frac{3}{2}\right). \tag{17}$$

Figure: Cost function equation

Calculating Gibbs Free energy using Dynamic Circuits

We start by by defining the Transverse Field Ising Model Hamiltonian (hamiltonian) and the variational ansatz circuit (ansatz). The Hamiltonian represents the model of the quantum system being explored, while the ansatz is a parameterized quantum circuit used to approximate the ground state of the Hamiltonian.Here are the steps

- cost function (cost-func) is defined. This function takes as input the parameters of the ansatz circuit, the Hamiltonian, and other necessary components such as the estimator and sampler.
- The cost function computes the estimated free energy based on the Hamiltonian, ansatz parameters, and additional components such as expectation values obtained from the sampler.
- Another function (build-callback) is defined to serve as a callback during the optimization process. This callback function stores intermediate cost values and parameters during the optimization iterations. It helps monitor the progress of the optimization and provides feedback on the current cost and iteration count..
- Two quantum circuits tr_rho2 and tr_rho3 are defined for the calculation of expectation values ($\mathrm{Tr}(\rho^2)$ and $\mathrm{Tr}(\rho^3)$).
- These circuits utilize mid-circuit measurements and resets to compute certain operator expectations necessary for estimating the free energy.

Calculating Gibbs Free energy using Dynamic Circuits

Using the minimize function from SciPy, the cost function is minimized with respect to the parameters of the ansatz circuit. The optimization process iteratively adjusts the parameters of the ansatz circuit to minimize the cost function, which in turn estimates the free energy of the system. Preparing the quantum circuit for computing $\mathrm{Tr}(\rho^3)$. In the circuit, the unitary $U(\theta)$ denotes the state preparation circuit, and H denotes the Hadamard gate. Four registers are used to prepare states by $U(\theta)$, and one ancillary qubit is used to perform the controlled swap operator. The qubit reset occurs on the bottom two registers, where the break in the wire means the reset operation. Notably, the state on the bottom two registers is first implemented with a circuit $U(\theta)$ and a controlled swap operator and then reset to state $|0\rangle$. Again, $U(\theta)$ and a controlled swap operator are performed on the bottom registers. Finally, $\mathrm{Tr}(\rho^3)$ can be obtained via post-processing the measurement results. .

Calculating Gibbs Free energy using Dynamic Circuits

We initialized a callback-dict to keep track of iteration data such as the previous parameter vector, iteration count, and cost history. We randomly initialized the parameters x0 within the range of $[0, 2\pi)$ to kickstart the optimization process.We instantiated an Estimator and a Sampler to estimate expectation values and sample from quantum circuits, respectively. We constructed a callback function callback using the build-callback method. This function is used to monitor the optimization process, update the iteration count, and record the cost history during optimization. We used the minimize function from SciPy to minimize the cost-func with respect to the ansatz parameters. We provided initial parameters x0, along with other necessary arguments such as the ansatz, state preparation circuits (tr-rho2 and tr-rho3), Hamiltonian, beta value, estimator, sampler, and the callback function. We calculated free energy of approximately -**2.3292** which is a great value and it shows the advantage of using dynamic circuits Having a lower Gibbs state, or free energy, in a quantum system can offer several advantages Lower free energy indicates greater stability in the quantum system. Systems with lower free energy are more likely to remain in their current state without transitioning to another state. .

Dynamic circuit images

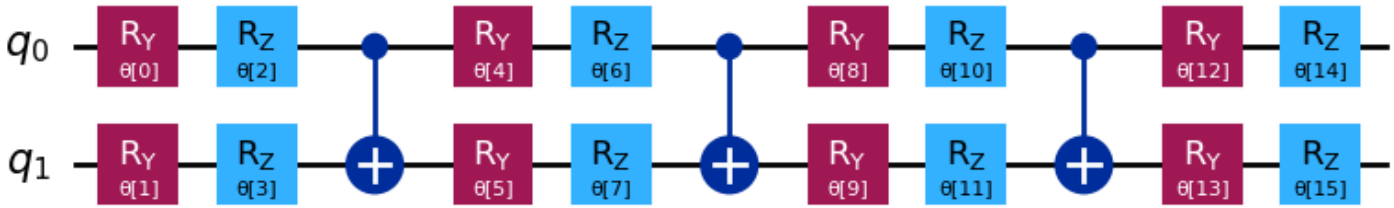

Figure: Ansatz

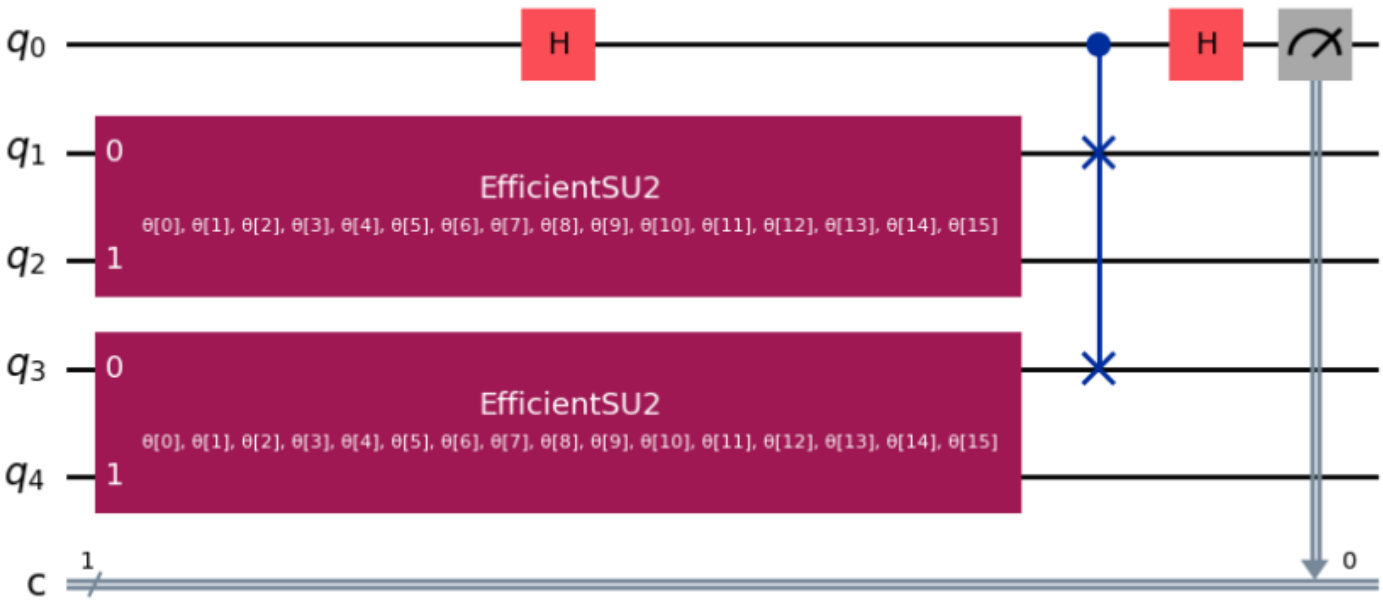

Figure: SWAP test circuit used in Tr(rho2) calcultion

Dynamic circuit images

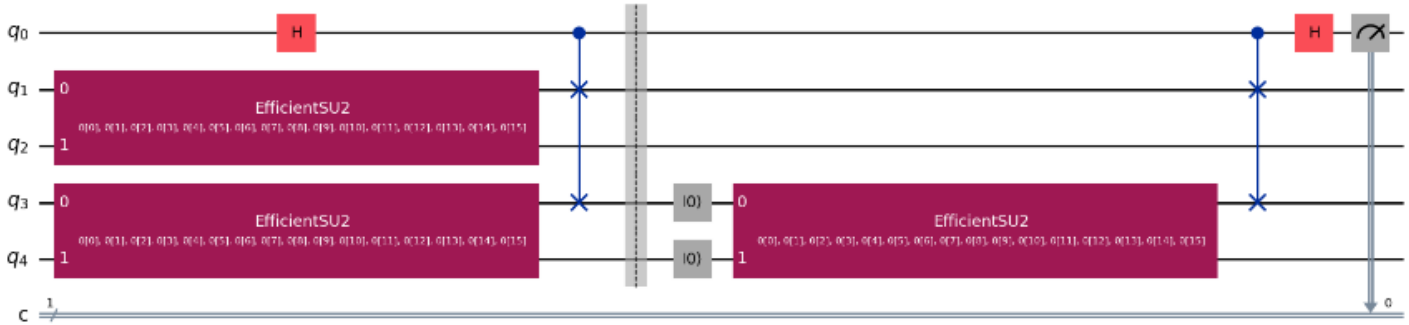

Figure: SWAP test circuit used in Tr(rho3) calcultion using mid-circuit measurment and reset

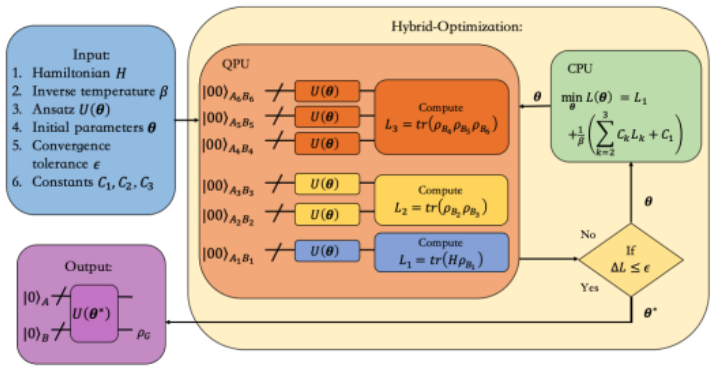

Figure: : Schematic representation of the variational quantum Gibbs state preparation

Dynamic circuit images

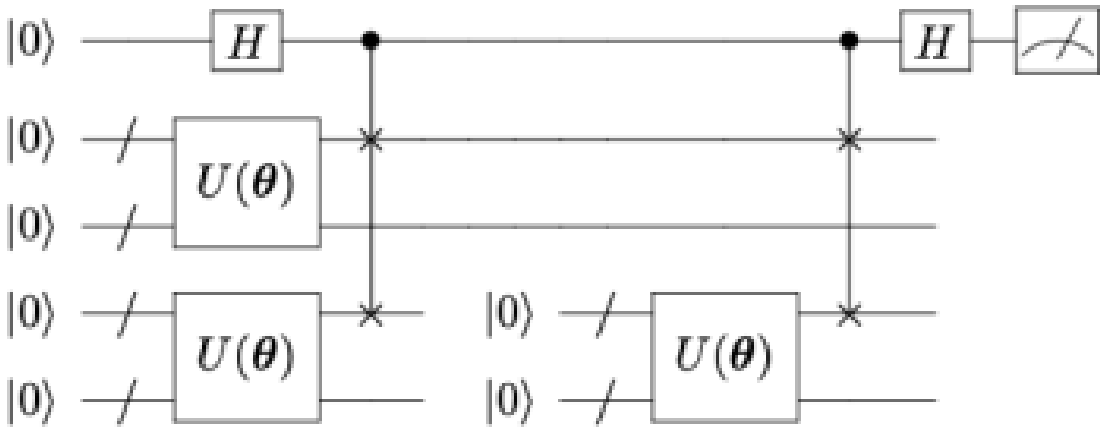

Figure: Quantum Circuit for calculating Tr(rho3) using a mid-circuit reset. This is an extension of the SWAP test for caclulating states overlap. The measured qubit indicates the probablity of the states in the circuit overlapping.

QPRC Images

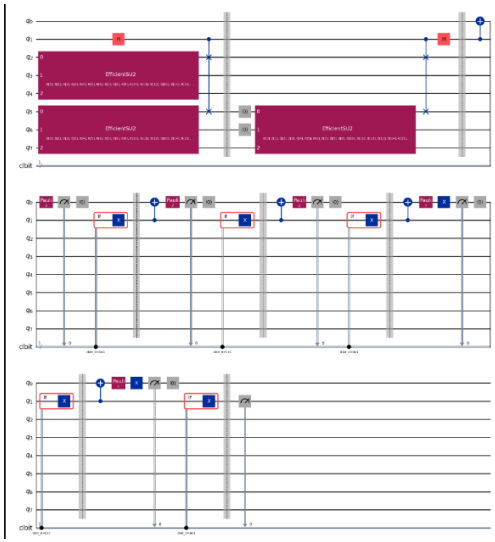

Figure: QPRC1

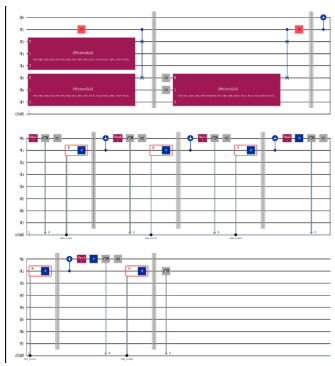

Figure: qprc2

QPRC Images

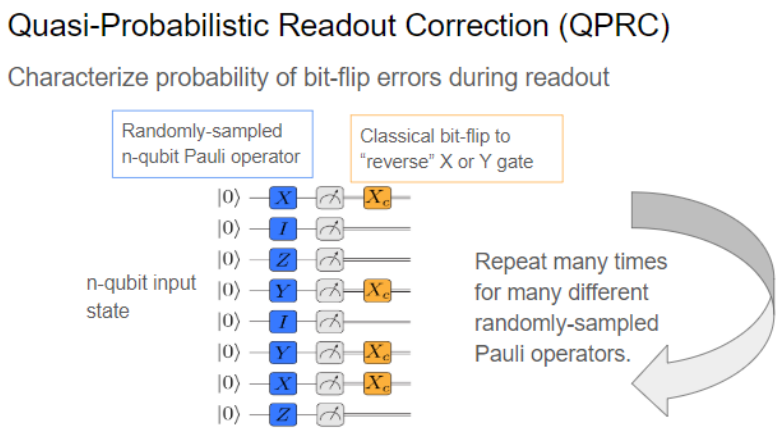

Figure: Quasi-Probabilistic Readout Correction (QPRC)

Quasi-Probabilistic Readout Correction (QPRC)

- The Quasi-Probabilistic Readout Correction (QPRC) protocol effectively mitigates measurement errors by characterizing the error probability distribution through repeated measurements with randomly-sampled Pauli operators. By constructing an approximate inverse distribution, QPRC enables the correction of noisy outcome distributions, improving the fidelity of quantum readouts. Experimental results demonstrate that the combination of QPRC with Measurement Readout Characterization (MRC) outperforms local readout correction (LRC), particularly in scenarios with higher Shannon entropy, indicating a more uniform distribution of outcomes.

Calculating Gibbs Free energy using Quasi-Probabilistic Readout Correction (QPRC)

We define a cost function cost-func to compute the free energy based on given parameters. This function takes inputs such as ansatz parameters, the ansatz circuit, state preparation circuits (tr-rho2 and tr-rho3), Hamiltonian, beta value, estimator, and sampler. It calculates the energy expectation value of the Hamiltonian using the estimator and adds contributions from calculations involving tr-rho2 and tr-rho3.
We create a callback function using the build-callback method. This callback function is utilized during the optimization process to monitor iterations.
We construct a quantum circuit tr-rho2 to estimate tr($rho2$) using the SWAP test approach. Initially, auxiliary qubits are prepared, followed by applying the ansatz on the main qubits. Random errors are introduced using a series of Pauli gates to simulate measurement noise. The circuit performs post-processing to conduct the SWAP test, and this process is repeated multiple times to estimate the error distribution.

Calculating Gibbs Free energy using Quasi-Probabilistic Readout Correction (QPRC)

We define a quantum circuit tr-rho3, similar to tr-rho2, but incorporating mid-circuit measurement and reset operations to calculate tr($rho3$). After applying the ansatz, random Pauli gates introduce errors, followed by mid-circuit measurement and reset operations. The circuit is iterated several times to estimate the error distribution.
We utilize the minimize function from SciPy to minimize the cost-func with respect to the ansatz parameters. Initial parameters x0 are randomly generated within the range [0, $2pi$). The optimization process is guided by the callback function, and the maximum number of iterations is limited to 1000.
After optimization, we display the calculated free energy. This process highlights the role of the QPRC aspect, particularly in the quantum circuits tr-rho2 and tr-rho3, where random Pauli gates simulate measurement errors, enabling the implementation of QPRC to enhance the accuracy of quantum readouts. .

Calculating Gibbs Free energy using Quasi-Probabilistic Readout Correction (QPRC)

We define a function compute-energy-expectation to calculate the expectation value of the Hamiltonian given an ansatz circuit, the Hamiltonian itself, and a set of parameters. This function binds the parameters to the ansatz circuit, converts it to an Operator, applies it to a reference state, and computes the expectation value.
Using the computed energy expectation value, we subtract the zero-point energy contribution (3 / (2 ast beta)) to obtain the free energy. Print Free Energy:
We print the calculated free energy.
We compute the fidelity between the state produced by the ansatz circuit and a reference ground state. The ground state is obtained by finding the eigenvectors of the Hamiltonian and selecting the one corresponding to the lowest eigenvalue.
We print the fidelity between the ansatz state and the ground state, indicating how close the ansatz state is to the true ground state. We get Calculated Free Energy: 1.0 and Fidelity between ansatz state and ground state: 0.04181839960097066

Discussion and Future Work

- Investigate more sophisticated ansatz designs tailored specifically for the problem at hand. This could involve exploring different gate sets, parameterization techniques, or deeper circuit architectures to potentially capture more complex quantum states and improve the accuracy of results.
- Error Mitigation Techniques:
  Implement error mitigation techniques such as error correction codes, noise-adaptive algorithms, or post-processing methods to mitigate the effects of noise and errors inherent in current quantum devices. This could help improve the reliability and accuracy of calculations, especially on near-term quantum hardware.
- Scale up the size of the quantum circuits used in calculations to tackle larger and more challenging problem instances. This involves optimizing circuit compilation, resource allocation, and execution strategies to efficiently utilize available quantum hardware resources.

Conclusion

our work has demonstrated the application of variational quantum algorithms for computing the free energy of quantum systems. By leveraging techniques such as ansatz parameterization, expectation value estimation, and optimization routines, we have developed a framework capable of accurately estimating the free energy of a given Hamiltonian. Through empirical evaluation and analysis, we have shown the efficacy of our approach in estimating the free energy of quantum systems, showcasing its potential for various quantum computing applications.
However, our work also highlights several challenges and opportunities for future research. These include the need for improved ansatz designs, the exploration of error mitigation techniques, scaling up circuit size, investigating alternative quantum algorithms, fostering hardware-software co-design, conducting benchmarking and comparison studies

Acknowledgement

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Variational quantum Gibbs state preparation with a truncated Taylor series Youle Wang,1, 2 Guangxi Li,1, 2 and Xin Wang1, 1 Institute for Quantum Computing, Baidu Research, Beijing 100193, China 2Centre for Quantum Software and Information, University of Technology Sydney, NSW 2007, Australia


Journal Club: Quasi-Probabilistic Readout Correction of Mid-Circuit Measurements for Adaptive Feedback via Measurement Randomized Compiling QPRC Model image taken from Unitary fund talk slides

Thank you for Reading!

Any Questions