Quantum Phase Transition of Non-Hermitian Systems

Using Variational Quantum Techniques

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Introduction to Non-Hermitian Systems

Normally in quantum theory, we study Hermitian Hamiltonians, which lead to unitary time evolution. We are interested in studying the effects of adding non-Hermitian portions to Hamiltonians,

$$\hat{\mathcal{H}} = \hat{H} + i\hat{\eta}, \tag{1}$$

where both $\hat{H}$ and $\hat{\eta}$ are Hermitian. Note that $\hat{\eta}$ is not a perturbation, and may be of similar or even larger size than $\hat{H}$.

The time evolution of these Hamiltonians is non-unitary

$$M(t) = e^{-it\hat{\mathcal{H}}} = e^{t\hat{\eta}}e^{-it\hat{H}}, \tag{2}$$

this means that the non-Hermitian portion of the Hamiltonian can drive *growth* or *decay* of states.

In this regime, we lose the notion of the eigenstates of the Hamiltonian being orthonormal. We instead now have that the left and right eigenvectors are biorthonormal.

For further details on non-Hermitian quantum mechanics see Ref. [1].

Motivation for Studying Non-Hermitian Systems

By extending normal quantum mechanics to allow non-Hermitian Hamiltonians, we are offered a way to study *open systems*, *dissipation*, and *decay processes*. This means that we can study systems that exhibit features such as *decoherence* through loss to the environment or with apparatus. This prescription offers possible improvement in our understanding of fields such as quantum optics, condensed matter, and nuclear physics.

We are studying these imaginary potential systems to develop methodologies on quantum computers for simulation when there is a **sign problem classically**, such as when there is a constant background electric field.

Introduction to $\mathcal{PT}$-Symmetry

As a looser restriction on our system than requiring Hermiticity, we instead enforce $\mathcal{PT}$-symmetry. This means that our Hamiltonian must remain invariant under simultaneous *parity* and *time* reversals. We can check that our model exhibits this symmetry by ensuring

$$\left[\hat{\mathcal{H}}, \mathcal{PT}\right] = 0. \tag{3}$$

We often study the two phases of this system: *unbroken* and *broken* $\mathcal{PT}$-symmetry. In the unbroken phase $\lambda_i \in \mathbb{R}$ for all $\lambda_i \in \text{spec}(\hat{\mathcal{H}})$; this is broken when this is no longer true. The points in parameter space where the symmetry breaking occurs are known as *exceptional points* - here we have a coalition of eigenstates. Another way we can ensure that our system has $\mathcal{PT}$-symmetry is by seeing that the eigenvalues appear in conjugate pairs in the broken phase.

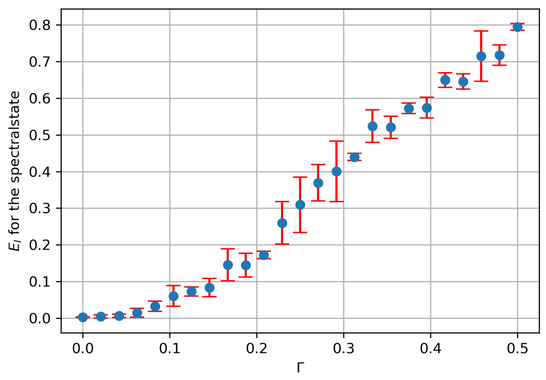

Figure 1: Largest imaginary part of an eigenvalue from the non-Hermitian QHO (Eq. 11). The phase is unbroken when $E_I = 0$ and broken when $E_I \neq 0$.

Introduction to Quantum Computing

In our studies, we are particularly interested in *variational quantum algorithms (VQAs)*, wherein we apply entangling and parameterized rotational gates to our state and then calculate the expected value with respect to some Hamiltonian. Typically this expected value is optimized using a classical routine. The solution to our problem is encoded in the final state or output value. An example of a VQA is the Variational Quantum Eigensolver (VQE). The VQE works by breaking the Hamiltonian into *Pauli strings*, and then calculating the expectation value of that particular string with respect to a variational state. We use a classical optimizer to minimize a cost function comprised of these expectation values.

Variational Quantum Algorithm for Scanning the Spectrum of Non-Hermitian Hamiltonians

The VQA for non-Hermitian systems was introduced in Ref. [2]. The algorithm centers around finding the zero-variance points of the non-Hermitian Hamiltonian. We define the cost function to be

$$C = \langle 0|U^\dagger(\theta)M(\theta, E)U(\theta)|0\rangle, \tag{4}$$

where

$$M(\theta, E) = \left(M^\dagger - E^*\right)(H - E)\,. \tag{5}$$

If we find θ_* and E_* such that $C = 0$, then

$$H\left[U(\theta_*)|0\rangle\right] = E_*\left[U(\theta_*)|0\rangle\right], \tag{6}$$

and thus we have found an eigenpair of the Hamiltonian. With this setup, we find the right eigenstates; to study the left eigenstates, we instead minimize a similar cost function C', where the operator is instead

$$M'(\theta, E) = (H - E)\left(M^\dagger - E^*\right). \tag{7}$$

The results on this poster focus on the right-hand eigenvectors of the Hamitlonian. Similar work can be done with respect to the lef-hand eigenvectors; we instead look at $M' = (M - E)(M^\dagger - E^*)$

The optimization of this cost function is carried out in two phases - these are defined depending on which eigenpair you are looking for.

The groundstate (state with the smallest real part) allows us to study quantum phase transitions and the spectralstate (the state with the largest imaginary component) shows when $\mathcal{PT}$-symmetry is broken.

Quantum Phase Transition

A *quantum phase transition (QPT)* is when we see a distinct change in the form of the groundstate. These occur at zero temperature for an infinite system size. Due to technical limitations of quantum simulations, we fall short of this - to help we impose periodic boundary conditions. The zero temperature requirement means that we can see the full effects by studying just the groundstate and do not need to build up ensembles.

Non-Hermitian Ising Model

We have been studying a non-Hermitian variation of the transverse field Ising model, defined by the Hamiltonian

$$\hat{\mathcal{H}} = -\sum_{j=0}^{n-1} Z_j Z_{j+1} - \sum_{j=0}^{n-1}\left[Z_j + i\Gamma X_j\right], \tag{8}$$

where X_j and Z_j are the Pauli spin matrices acting on qubit j. This Hamiltonian is non-Hermitian for $\Gamma \neq 0$. We study the QPT of this system as we change Γ. We quantify this by measuring M_x on the found groundstate,

$$M_x = \frac{1}{n}\sum_{j=0}^{n-1} X_j. \tag{9}$$

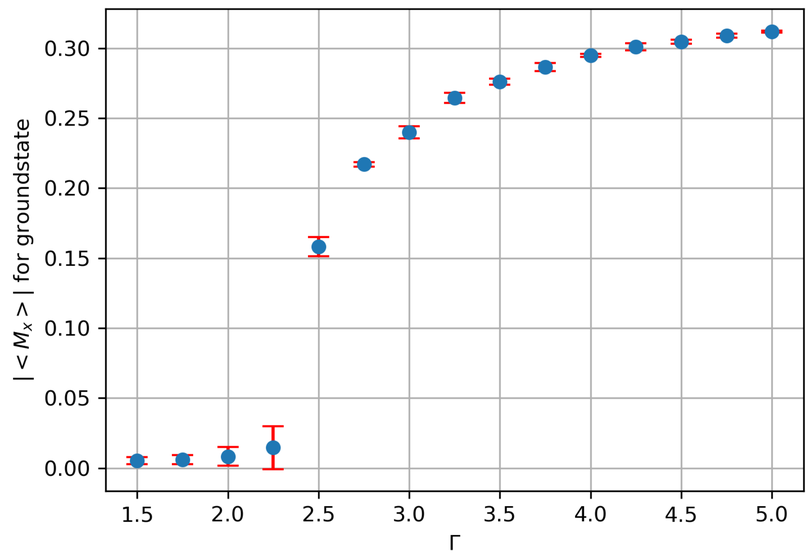

Figure 2: Absolute value of magnetization in X-direction over a change in imaginary field strength. These results were collected using noisy state-vector simulations. Each data point is an average over four runs, on a five qubit system. These simulations were run locally on my laptop.

Non-Hermitian Quantum Harmonic Oscillator

The Hamiltonian of the non-Hermitian quantum harmonic oscillator is given by

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2} + \frac{1}{2}\hat{x}^2 + i\Gamma\hat{x}^3, \tag{10}$$

this Hamiltonian is non-Hermitian for $\Gamma \neq 0$. After making use of fermionic ladder operators and the Jordan-Wigner transformation, we can map this to a system of n-qubits as

$$\hat{\mathcal{H}} = \sum_{j=0}^{n-1}\left[I - \frac{1}{2}Z_j + i\frac{\Gamma}{\sqrt{2}}X_j\left(\prod_{k<j} Z_k\right)\right]. \tag{11}$$

We quantify the QPT of this system in a similar way to the Ising model, by measuring M_x on the found groundstate.

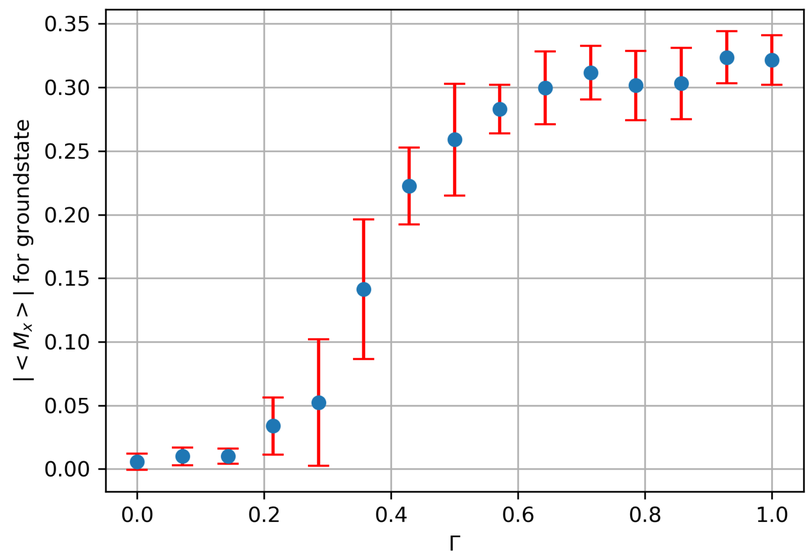

Figure 3: Absolute value of magnetization in X-direction over a change in imaginary field strength. These results were collected using noisy state-vector simulations. Each data point is an average over four runs, on a five qubit system. These simulations were run locally on my laptop.

Conclusion and future work

In this work, we have explored the applicability of a variational quantum algorithm for simulating systems that we cannot simulate effectively with usual Monte Carlo methods. We are porting our codes to HPC and GPU based systems, so we can simulate larger systems. In the future, we hope to explore more complex systems, in particular systems in a background electric field.

References

[1] Carl M Bender. Making sense of non-hermitian hamiltonians. *Reports on Progress in Physics*, 70(6):947–1018, May 2007.

[2] Xu-Dan Xie, Zheng-Yuan Xue, and Dan-Bo Zhang. Variational quantum algorithms for scanning the complex spectrum of non-hermitian systems. *Frontiers of Physics*, 19(4), February 2024.