Variational Approaches to Transitions in Non-Hermitian Quantum Spin Models

James Hancock[1*], Matthew Craven[1], Craig McNeile[1], Davide Vadacchino[1]

[1]School of Engineering, Computing and Mathematics
University of Plymouth
*james.hancock@plymouth.ac.uk

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Summary

1. **Non-Hermitian Quantum Mechanics**
2. **The Variational Quantum Method**
3. **The Quantum Spin Models**
4. **Conclusions**

- Developing quantum computing methods.
- The method offers a solid way to generate groundstates
- This work is linked to work done for the Lattice Conference proceedings: (Hancock et al. 2025) [https://arxiv.org/abs/2501.17003]

Quantum Field Theory in Constant Background Fields

- QCD has an interesting phase structure in background magnetic fields with potential applications to heavy ion collisions. But what happens with background electric fields?
- There is a sign problem with QCD in a background electric field

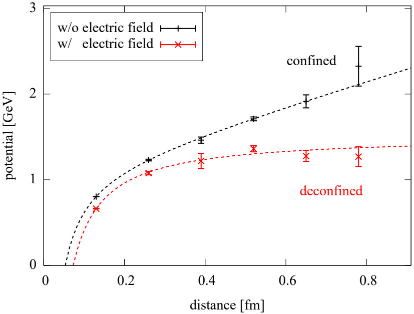


Figure: Heavy quark potential in constant electric field (special case: isospin electric charge)

- See the review by Yamamoto [`https://arxiv.org/abs/2103.00237`]
- Start by studying a simpler, but similar, system

Non-Hermitian Quantum Mechanics

- Hermicity normally means the probability is conserved and $|\phi_L\rangle = |\phi_R\rangle$
- Non-Hermitian terms break this

$$U(t) = e^{-iHt} = e^{-i(H_0+iH_1)} = e^{H_1 t} e^{-iH_0 t} = A(t) e^{-iH_0 t}, \tag{1}$$

  where $A(t)$ is not unitary and $|\phi_L\rangle \neq |\phi_R\rangle$
- Can encapsulate loss/gain to an environment
- Could have applications in the study of quantum channels
- Monte Carlo and VQE struggle with complex energy
- Applications to optics[1] and condensed matter[2]

[1] Wang et al. 2023.
[2] Okuma and Sato 2023.

$\mathcal{PT}$-Symmetic Quantum Mechanics

- Special case with two phases: broken and unbroken
  - In the unbroken phase, eigenvalues are all real - meaning probability is preserved
  - In the broken phase this is no longer true, but they appear in conjugate pairs
  - Transition occurs at *exceptional points* - coalescence of eigenpairs
- Applications to lasers[3]
- In the discussion of $\mathcal{PT}$-symmetric quantum mechanics, must mention Carl Bender[4]

[3] Praveena and Senthilnathan 2023.

[4] Bender 2005; Bender 2007.

Cost Function

- Given a Hamiltonian of the form

$$H = H_0 + iH_1 = \sum_{\alpha} h_\alpha P_\alpha + i \sum_{\beta} g_\alpha P_\beta, \tag{2}$$

  where P_α are Pauli strings - suitable for quantum algorithms
- Produce new matrices[5]

$$\begin{aligned} M(E) &= (H^\dagger - E^*)(H - E) \\ M'(E) &= (H - E)(H^\dagger - E^*), \end{aligned} \tag{3}$$

  for finding right and left eigenpairs, respectively
- Our cost is

$$C(\theta, E) = \langle \phi(\theta) | M(E) | \phi(\theta) \rangle , \tag{4}$$

  suitable for use on a quantum computer

[5] Xie, Xue, and Zhang 2024.

Optimization Strategy

- Initial guess for $\mathrm{Re}(E) = E_R$ and $\mathrm{Im}(E) = E_I$ are E_R^0 and E_I^0

$$E_R^0 = -\sum_{\alpha} |h_\alpha| \text{ , when looking for groundstate} \tag{5}$$

$$E_I^0 = \sum_{\alpha} |g_\alpha| \text{ , when looking for spectral state} \tag{6}$$

- Three stages (slight modification of original):
  1. Optimize just θ
  2. Optimize over E_R and θ
  3. Optimize over E_R, E_I and θ

Model Definitions

- We test three models:
  1. Transverse Ising model
  2. Transverse Ising model with complex magnetic field
  3. Kitaev honeycomb model with small real field and $\mathcal{PT}$-symmetric
- The Ising models can be defined by their respective Hamiltonians

$$H_{Ising} = -\sum_{j=0}^{n-1} \left[\sigma_z^j \sigma_z^{j+1} + \Gamma \sigma_x^j\right] \quad (7)$$

$$\mathcal{H}_{Ising} = -\sum_{j=0}^{n-1} \left[\sigma_z^j \sigma_z^{j+1} + i\gamma \sigma_x^j\right] \quad (8)$$

Kitaev Honeycomb Model

- The Kitaev model is of more physical relevance
- Defined by the Hamiltonian

$$\begin{aligned} H_{Kitaev} &= -\sum_{\langle j,k\rangle_x} J_x \sigma_x^j \sigma_x^k - \sum_{\langle j,k\rangle_y} J_y \sigma_y^j \sigma_y^k - \sum_{\langle j,k\rangle_z} J_z \sigma_z^j \sigma_z^k \\ &= -\sum_{\alpha\in\{x,y,z\}} \sum_{\langle j,k\rangle_\alpha} J_\alpha \sigma_\alpha^j \sigma_\alpha^k \end{aligned} \tag{9}$$

- This model can support Abelian *anyons* in the gapped sector, $|J_\alpha| > |J_\beta| + |J_\gamma|$, for $\alpha, \beta, \gamma \in \{x, y, z\}$, meaning one term dominates.

$\mathcal{PT}$-Symmetry of Kitaev Model

- The $\mathcal{T}$-symmetry is defined as

$$\mathcal{T} = i\sigma_y K, \tag{10}$$

where K is complex conjugation

- Terms transform as

$$\begin{aligned} \mathcal{T}\sigma_\alpha^j\mathcal{T}^{-1} &= -\sigma_\alpha^j \\ \mathcal{T}i\mathcal{T}^{-1} &= -i \end{aligned} \tag{11}$$

- The $\mathcal{P}$-symmetry can be defined as

$$\mathcal{P} = U_\pi \prod_j R_j, \tag{12}$$

where U_π is a reflection along a σ_z bond and $R_j = e^{-i\pi/4\sigma_x^j}$

- Terms transform as

$$\begin{aligned} \mathcal{P}\sigma_x^j\mathcal{P}^{-1} = \sigma_y^k \qquad \mathcal{P}\sigma_y^j\mathcal{P}^{-1} = -\sigma_x^k \\ \mathcal{P}\sigma_z^j\mathcal{P}^{-1} = \sigma_z^k \end{aligned} \tag{13}$$

where the k's are determined by the specific site, on which we mirror

Non-Hermitian Kitaev Honeycomb Model

- With the introduction of a small external field, the Kitaev model can support non-Abelian in the gapless sector, where $|J_\alpha| \approx |J_\beta| \approx |J_\gamma|$
- This is relevant to topological quantum computers
- We can perturb this with a small real field and $\mathcal{PT}$-symmetric complex field
- This has the Hamiltonian

$$\mathcal{H}_{Kitaev} = -\sum_{\alpha\in\{x,y,z\}} \left[\sum_{\langle j,k\rangle_\alpha} \left[\sigma_\alpha^j \sigma_\alpha^k \right] - B_R \sum_j \sigma_\alpha^j \right] + iB_I \sum_j \sigma_z^j \tag{14}$$

where $|B_R| \ll 1$

$\mathcal{PT}$-Symmetry Breaking

- This is $\mathcal{PT}$-symmetric for $B_R = 0$, $B_R \neq 0$ breaks $\mathcal{T}$-symmetry
- $\mathcal{PT}$-symmetry is broken for $B_I \neq 0$, groundstate energy stays real (non-degenerate)

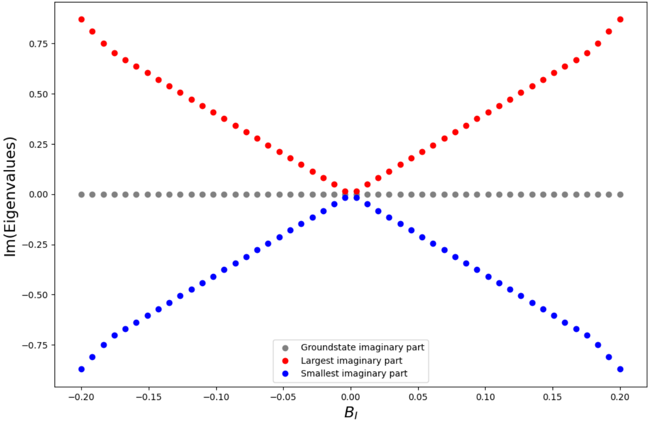


Figure: Largest, smallest and groundstate imaginary parts for a range of B_I values, with $B_R = 0$.

Quantum Phase Transition

- A distinct discontinuous change in the form of the groundstate of the system
- Occurs at zero temperature - at finite temperature thermal fluctuations dominate
- An order parameter can be used to characterize these; often represented as an operator we measure on the groundstate

Order Parameters

- For the transverse and complex Ising models, we use the σ_x-magnetization

$$\langle M_x \rangle = \sum_j \langle \sigma_x^j \rangle \tag{15}$$

- To truly encapsulate the topological behavior of the Kitaev model, we look at the Wilson loop over one hexagon

$$\langle W_p \rangle = \langle \sigma_x^1 \sigma_y^2 \sigma_z^3 \sigma_x^4 \sigma_y^5 \sigma_z^6 \rangle, \tag{16}$$

  counted around anti-clockwise around the plaquette
- In the non-Abelian phase, $\langle W_p \rangle \approx 1$ for the groundstate and $\langle W_p \rangle \approx -1$ for the first three excited states. The value will stray from this if the external field is too strong

Non-Hermitian Order Parameter

- When dealing with the $\mathcal{PT}$-symmetric, non-Hermitian version of the Kitaev model, we must use a different order parameter
- We must consider *biorthogonal* measurements of observables on the groundstate

$$\langle O \rangle_{NH} = \langle \phi_0^L | O | \phi_0^R \rangle, \tag{17}$$

  where $|\phi_0^L\rangle$ and $|\phi_0^R\rangle$ are the left and right groundstates, respectively
- $\langle W_p \rangle_{NH} \in \mathbb{C}$, and so we instead opt for $|\langle W_p \rangle_{NH}|$
- As a non-local operator, it does not meet the normal definition of order parameter, but does track a topological change in the groundstate structure

Ising Model Results

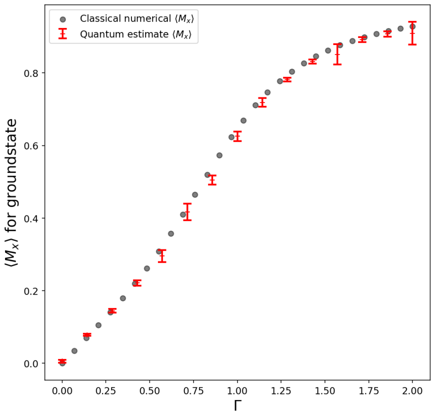


Figure: $\langle \hat{M}_x \rangle$ over a change in real magnetic field (Γ) in the transverse Ising model.

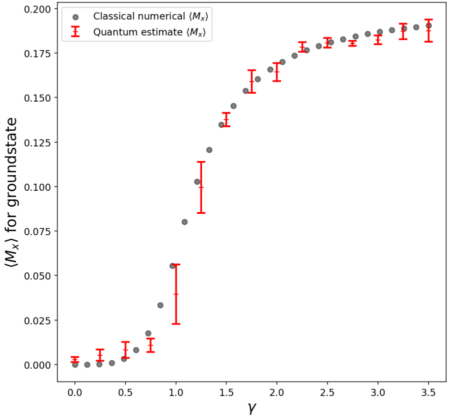


Figure: $\langle \hat{M}_x \rangle$ over a change in complex magnetic field (γ) in the transverse Ising model.

Kitaev Model Results

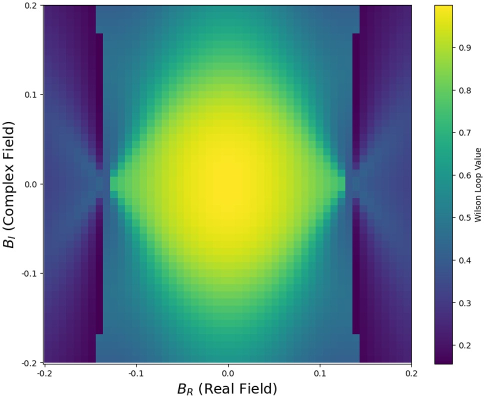


Figure: $|\langle W_p \rangle_{NH}|$ on the complex plane for the $\mathcal{PT}$-symmetric Kitaev model, results found using dense eigensolvers

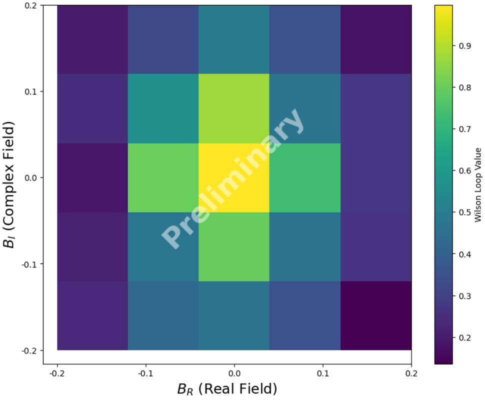
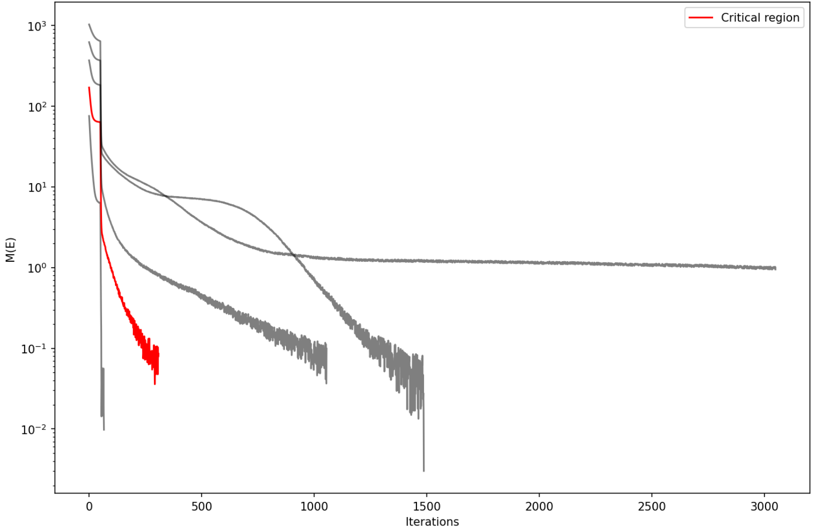


Figure: $|\langle W_p \rangle_{NH}|$ on the complex plane for the $\mathcal{PT}$-symmetric Kitaev model, results found using the variational quantum method

Optimization Performance



Conclusions

- The variational approach offers a quantum way to create these states and take measurements on them
- Initial conditions are key to success
- Kitaev model has a rich phase structure with a $\mathcal{PT}$-symmetric magnetic field
- Looking forward:
  - Simulation of finite-lifetime anyons
  - Link models with complex or background fields

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Bonus: Technical Details of Simulation

- Ising model results are from a system of five spins
- Kitaev model was for a system of eight total spins, arranged in a honeycomb lattice - this allows for one plaquette
- The Wilson loop operator in this arrangement is

$$W_p = \sigma_x^2 \sigma_z^3 \sigma_y^4 \sigma_y^5 \sigma_z^6 \sigma_x^7 \tag{18}$$

- Simulations were run with a quantum simulator in C++ for the noisy results, with a shot count of $O(2000) \sim$ uniformly distributed in the range $(-\epsilon, \epsilon)$, $\epsilon = 0.04$

Bonus: Modification for Finding Excited States

- This algorithm searches for *any* eigenpair - very dependent on initial guesses
- To find the groundstate, we try to best guess the lowest energy
- Once we have found an eigenpair, $C(\theta, E) \approx 0$, we store that θ as θ_0^*
- Introduce new term[6]

$$\langle \phi(\theta) | \phi(\theta_0^*) \rangle \tag{19}$$

  to encourage a new eigenpair (VQD)
- Moreoever, for finding the j^{th} eigenpair

$$C_j(\theta, E) = \langle \phi(\theta) | M(E) | \phi(\theta) \rangle + \sum_{k=0}^{j-1} |\langle \phi(\theta) | \phi(\theta_k^*) \rangle|^2 \tag{20}$$

[6] This can become expensive quickly on real hardware

Bonus: Measuring Non-Hermitian Observables

- To measure states in a non-Hermitian setting, we use the left and right states, i.e.

$$\langle O \rangle_{NH} = \langle \phi^L | O | \phi^R \rangle \tag{21}$$

- We must use a Hadamard test, similar to VQD

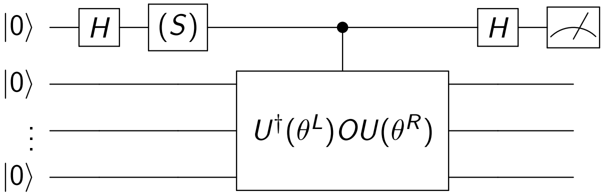


Table: Hadamard test circuit for measuring O on the left and right states. We apply the S gate for the imaginary part and don't for the real part

Bonus: Circuit Design

- To encapsulate the state structure with minimal parameters, we opt for a highly entangled physics-inspired ansatz

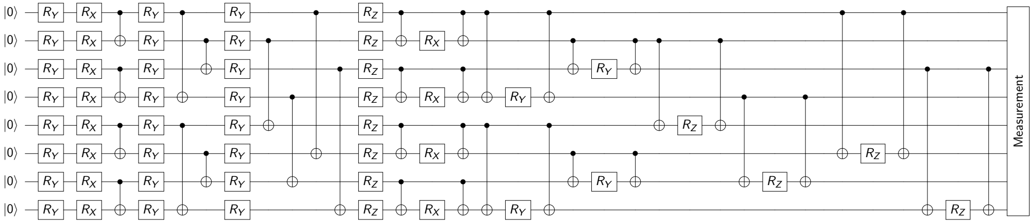
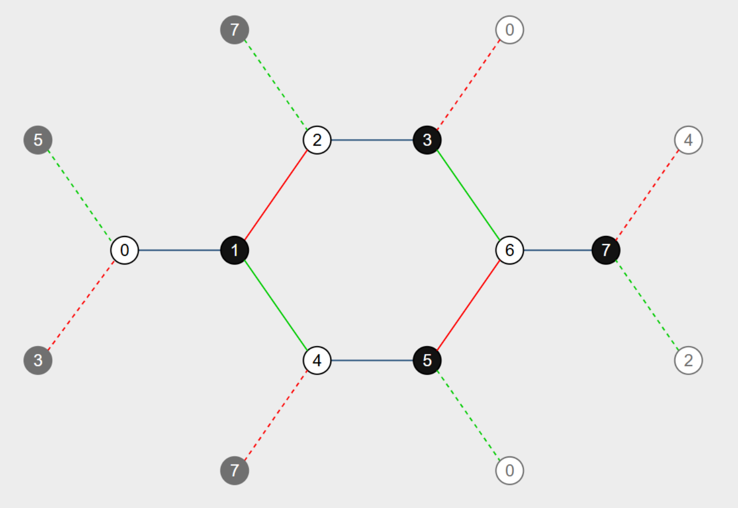


Table: Parametric circuit used for studying the Kitaev honeycomb spin model

Bonus: Lattice Diagram



- Blue bonds are σ_x, red are σ_y and green are σ_z
- Solid points are in lattice A, white ones are from lattice B
- Solid lines are model bonds, dashed are boundary conditions