Exploring the Variational Quantum Eigensolver through an application on the Lipkin Model

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Motivations

Motivations

Many-Body Problems

- Want to find eigenvalues of Hamiltonian.
- Hilbert space of complex quantum systems grow exponentially with the number of particles.

Current Solutions

- Exact diagonalization: Limited to small system sizes due to computational complexity.
- Classical algorithms suffer from the exponential increase in Hilbert space as the system size increase.

Variational Quantum Eigensolver (VQE)

- Uses variational methods for finding the ground state energy of a system: $E_0 \leq \langle\psi|\hat{H}|\psi\rangle$
- Allows the representation of quantum systems using limited number of qubits.
- Realisable in our noisy intermediate scale quantum computing (NISQ) era due its low depth circuit.

The Lipkin Model

- Simple but non-trivial, has analytical solutions.
- A testbed for quantum simulation algorithms such as VQE

Quantum Computing

Basis

We choose the single qubit computational basis to be the eigenbasis of the Pauli Z matrix,

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Multiqubit basis are tensor products of single qubits basis,

$$\begin{aligned} |00\rangle &= |0\rangle \otimes |0\rangle \\ |01\rangle &= |0\rangle \otimes |1\rangle \\ |10\rangle &= |1\rangle \otimes |0\rangle \\ |11\rangle &= |1\rangle \otimes |1\rangle \end{aligned}$$

Gates

One Qubit Gates

- X-gate$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
- Y-gate $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
- Z-gate $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
- Hadamard gate: $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$
- Phase gate $S^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}$
- Rotation gates:
  $R_x(\theta) = \cos\frac{\theta}{2} I - \imath \sin\frac{\theta}{2} X$, $R_y(\phi) = \cos\frac{\phi}{2} I - \imath \sin\frac{\phi}{2} X$.

Two Qubit Gates

- $CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
- $SWAP = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

Von Neumann entropy

It's a measure of entanglement

$$S(A, B) = -\mathrm{Tr}\left(\rho_{A,B} \log_2(\rho_{A,B})\right).$$

Measurements

- Computational basis is in the Z basis $\implies$ must apply the appropriate uniform transformation to rotate the basis
- Measurement is a non-reversible operation $\implies$ a new copy of the system must be prepared before each measurement.
- Measurement collapses the state onto one of the eigenstates $\implies$ measure N times then divide by N to reconstruct the coefficients following.

Change of Basis

Since we write Hamiltonian in terms of the Pauli matrices, and the computational basis are in the $Z, ZI, ZIII$ basis, measuring in other basis requires us to rotate the our computational basis to the appropriate basis, given by the unitary transformation below.

$$X = HZH$$

$$Y = HS^{\dagger}ZHS$$

Models

One-Qubit System

The Hamiltonian is given by:

$$H = H_0 + \lambda H_I$$

where H_0 and H_I can be written in terms of the Pauli matrices as:

$$H_I = cI + \omega_z Z + \omega_x X,$$
$$H_0 = \mathcal{E} I + \Omega Z$$

with $c = (V_{11} + V_{22})/2$, $\omega_z = (V_{11} - V_{22})/2$, $\omega_x = V_{12} = V_{21}$ and $\Omega = \frac{E_1 - E_2}{2}$, We choose $E_1 = 0$, $E_2 = 4$, $V_{11} = -V_{22} = 3$ and $V_{12} = V_{21} = 0.2$.

Two Qubit System

Hamiltonian is again:

$$H = H_0 + \lambda H_I$$

where H_0 and H_I can be written in terms of the Pauli matrices as

$$H_0 = aI \otimes I + bI \otimes Z + cZ \otimes I + dZ \otimes Z$$

with $a = 4, b = -0.75, c = -2.75, d = -0.5$

$$H_I = H_x \; X \otimes X + H_z \; Z \otimes Z,$$

with $Hx = 2.0, Hz = 3.0$

The Lipkin Model

J=1

- N fermions distributed in two levels each having an N-fold degeneracy and separated by an energy ϵ.
- Each state describe by $|n, \sigma\rangle$
- Can be written in terms of quasispin operators $J_{\pm}$ and J_z.

The Lipkin Hamiltonian is

$$H = H_0 + H_1(V) + H_2(W)$$

We will assume now $W = 0$ and $H_2 = 0$

In matrix representation, the Hamiltonian is:

$$H = \begin{pmatrix} -\epsilon & 0 & v \\ 0 & 0 & 0 \\ v & 0 & \epsilon \end{pmatrix}$$

Or in terms of Pauli matries:

$$H = \frac{\epsilon}{2}(ZI + IZ) + \frac{1}{2}V(XX - YY)$$

The Lipkin Model

J=2

In matrix representation, the Hamiltonian is:

$$H = \begin{pmatrix} -2\varepsilon & 0 & \sqrt{6}V & 0 & 0 \\ 0 & -\varepsilon + 3W & 0 & 3V & 0 \\ \sqrt{6}V & 0 & 4W & 0 & \sqrt{6}V \\ 0 & 3V & 0 & \varepsilon + 3W & 0 \\ 0 & 0 & \sqrt{6}V & 0 & 2\varepsilon \end{pmatrix}$$

For $W = 0$ in terms of Pauli matries:

$$\begin{aligned} H = {} & \epsilon(ZIII + IZII + IIZI + IIIZ) \\ & + \frac{V}{2}(XXII + XIXI + XIIX + IXXI + IXIX + IIXX) \\ & - \frac{V}{2}(YYII + YIYI + YIIY + IYYI + IYIY + IIYY) \end{aligned}$$

Level Mapping

How to map the Fermions to qubits?

Direct Mapping

Map each state $|n, \sigma\rangle$ by a qubit, with $|0\rangle$ and $|1\rangle$ representing the unoccupied state and occupied state respectively.

- Requires $2N$ qubits for a system of N particle.

Level Mapping

Instead map

$$|0\rangle \longleftrightarrow |n, -1\rangle$$
$$|1\rangle \longleftrightarrow |n, +1\rangle \, .$$

- Requires only N qubits for a system of N particle.

The W Term

We rewrote H_2 in terms of the Pauli matrices and obtained:

$$H_2 = \frac{1}{2}W(4IIII + 2(XXII + XIXI + XIIX + IXXI + IXIX + IIXX \\ + YYII + YIYI + YIIY + IYYI + IYIY + IIYY))$$

where we represented the $\hat{N}$ (particle number operator) by $4IIII$ since there are 4 particles in this system.

VQE

VQE

The hybrid variational algorithm follows the following steps:

1. Prepare a parameterised quantum circuit (the ansatz) $|\Psi(\vec{\theta})\rangle$.
2. Measure the expectation value $E(\vec{\theta})$.
3. Use a classical optimization algorithm (gradient based or not) to update the parameters $\vec{\theta}$.
4. Repeat the above steps until the change in $E(\vec{\theta})$ is below a certain threshold.

Implementation

Quantum Computing (`base.py`)

- Three classes: `Qubit`, `Qubits_2(Qubit)`, `Qubits(Qubits_2)`
- All single and two qubit gates mentioned above for any combination of qubits in the circuit.
- Measurement is done by calling `Qubits.measure(n_shots)` which returns the counts of all states.

VQE

- Class: `VQE(ansatz,expectation)`
- Minimisation algorithm: `scipy.optimize.minimise(method=‘‘Powell’’)`

Ansatz

One-Qubit

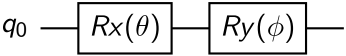


Figure: One-qubit ansatz

Two-Qubit

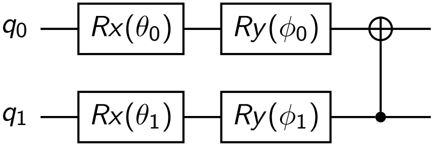


Figure: Two-qubit ansatz

Four-Qubit

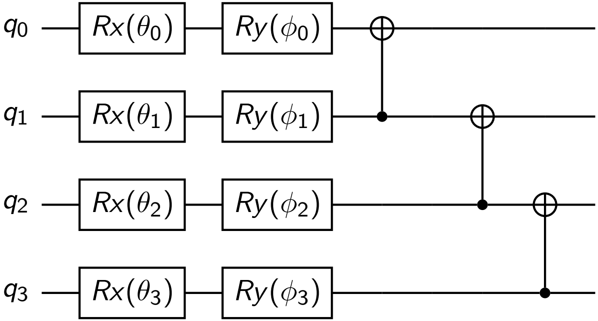
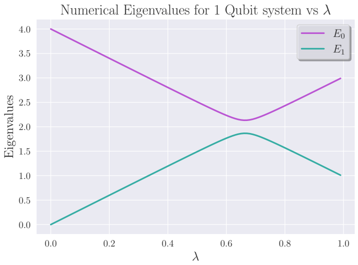


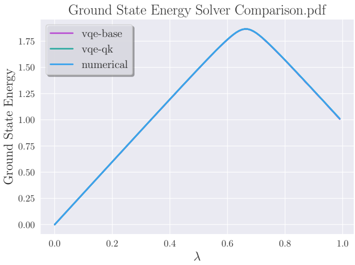
Figure: Four-qubit ansatz

Results

One-Qubit

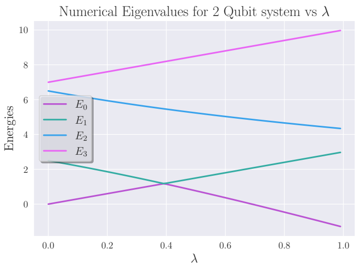


(a) Classical eigenvalues as a function of the interaction strength λ , with colours denoting different energy levels.

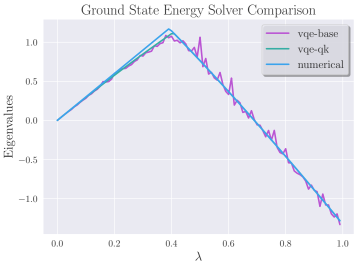


(b) Ground state energy calculated using VQE for a one-qubit system as a function of λ , from both our implementation and Qiskit.

Two-Qubit



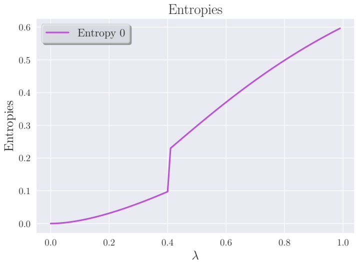
(a) Numerical eigenvalues for a two-qubit system, with colours indicating distinct energy levels.



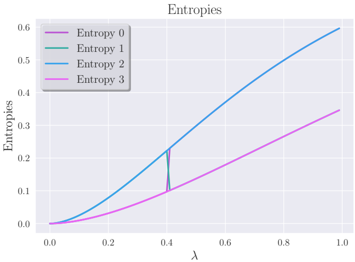
(b) Ground state energy determined with VQE for a two-qubit system as a function of interaction strength λ, from both our implementation and Qiskit.

Two-Qubit

Von Neumann Entropy



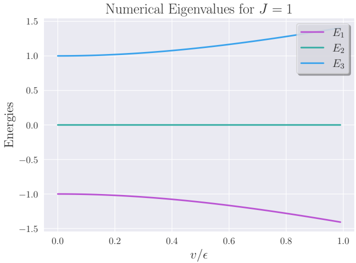
(a) Von Neumann entropy of the ground state for a simple two-qubit system as a function of interaction strength.



(b) Von Neumann entropy of the ground state for a simple two-qubit system as a function of interaction strength.

Lipkin

J=1



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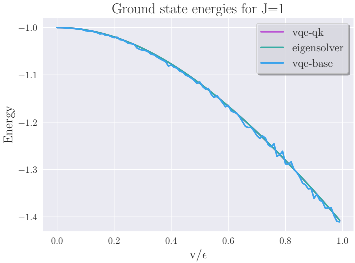

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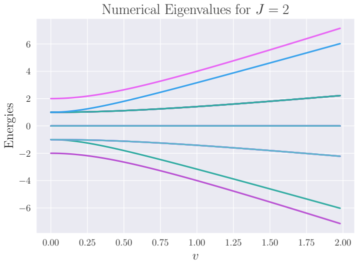
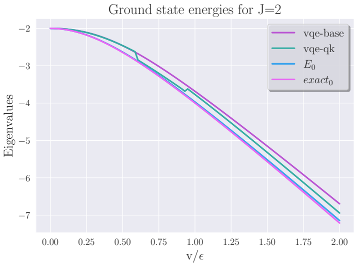
Lipkin

J=2



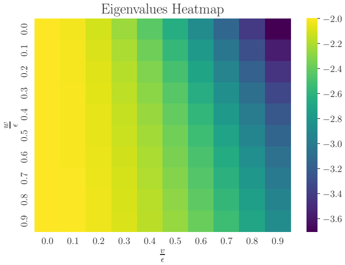
(a) Numerical results for the Lipkin Model with $J = 2$, utilising the full Hamiltonian with size 16×16, where all energies have a degeneracy of 2.



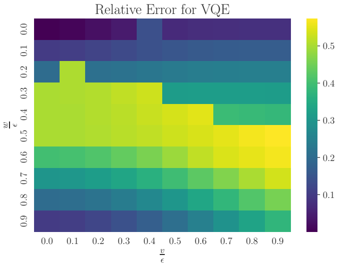
(b) Ground state energy determined with VQE for a two-qubit system as a function of interaction strength λ, from both our implementation and Qiskit.

Lipkin

J=2, with W



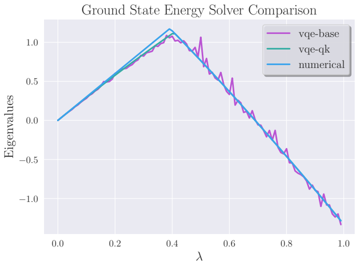
(a) Numerical results for the Lipkin Model for $J = 2$ with the W term.



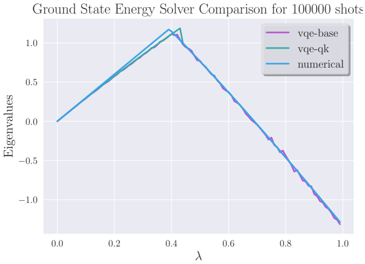
(b) Relative Error for Lipkin model for $J = 2$ with W using qiskit.

Discussion

Increasing number of shots

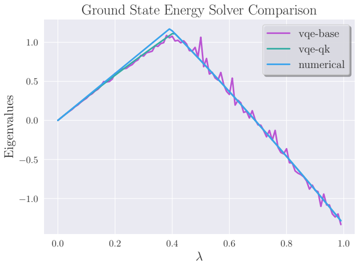


(a) round state energy determined with VQE for a two-qubit system as a function of interaction strength λ, from both our implementation and Qiskit.



(b) Ground state energy determined with VQE for a two-qubit system as a function of interaction strength λ, with 100000 shots gate.

The Importance of Entanglement



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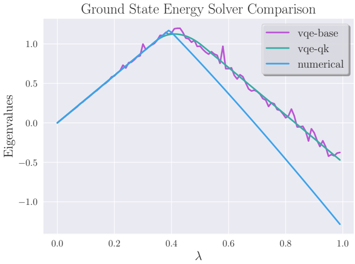
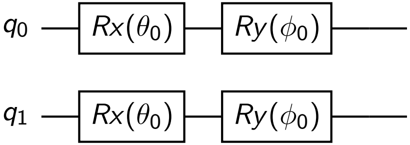


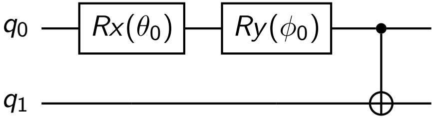
(b) Ground state energy determined with VQE for a two-qubit system as a function of interaction strength λ, without the CNOT gate.

Choice of Ansatz

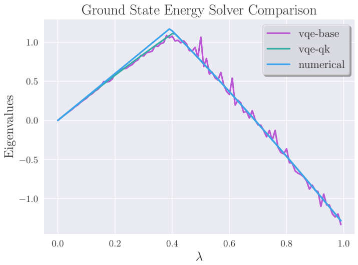
There is no universal way to choose an ansatz, and there is no unique ansatz.

Bad ansatzs





Choice of Ansatz



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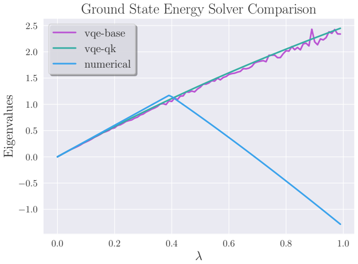


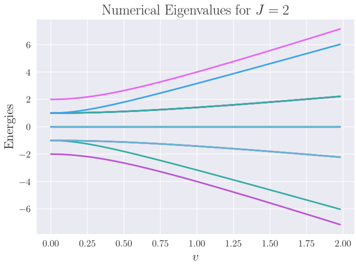
(b) Ground state energy determined with VQE for a two-qubit system as a function of interaction strength λ, without the CNOT gate.

Ansatz Initialisation

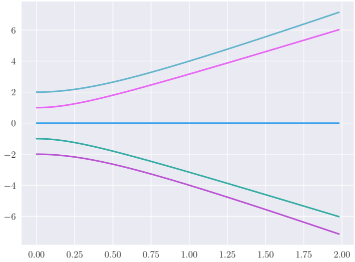
- Random
- Hartree Fock state [1]

[1] Jules Tilly, Hongxiang Chen, Shuxiang Cao, Dario Picozzi, Kanav Setia, Ying Li, Edward Grant, Leonard Wossnig, Ivan Rungger, George H. Booth, Jonathan Tennyson, "The Variational Quantum Eigensolver: a review of methods and best practices," arXiv:2111.05176 [quant-ph] (2021), accessed June 21, 2023, https://arxiv.org/abs/2111.05176.

How Many Eigenvalues?



(a) Energy eigenvalues for $J = 2$ using the full Hamiltonian in terms of Pauli matrices



(b) Ground state energy for $J = 2$ determined using the 5x5 matrix.

- Different Encoding Scheme
- Non-allowed eigenenergies?

Performance

- Same ansatz $\implies$ converges to the same values (correct or not).
- Qiskit is faster and produces smoother graphs.
- Non-gradient based methods (SLSQP, COBYLA, Powell) are faster than gradient based methods.

Conclusion

Conclusion

- Simulation showed that the VQE is a promising algorithm for studying the ground state energy problem for the Lipkin Model.
- Including entanglement is essential for obtaining the correct results especially for when the ground state is highly entangled.
- Non-gradient based methods are faster than gradient based methods
- Our implementation performs similar to the VQE from qiskit

Future Work

- Run on real quantum computers instead of a simulator.
- Compare the result from VQE with classical methods like HF or RPA.
- Implement general method for calculating expectation value through measurement.
- Test differential methods to initialise the ansatz
- Investigate the ground state energy for other systems.
- Investigate other choices of ansatz such as inclusion of multiple layers of gates.

Thank you!

Questions?