# Exploring the Variation Quantum Eigensovler: through an application in the Lipkin Model

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This report is a study on the Variational Quantum Eigensolver, with a focus on theory, its implementation and a comparison of its performance on the different model to that of a high-level library, classical eigensolvers and exact solutions. The results are optimistic for the simpler models but the $J = 2$ case does not converge exactly. We concluded that it should be reasonable solved by trying different classical optimisation methods, experimenting ansatz and initialisations of the parameters.

## I. INTRODUCTION

The development of quantum computing presents an alternative ways to simulate quantum problems. Among various applications of quantum computing, its potential in simulating quantum many-body systems with the Variational Quantum Eigensolver (VQE) is one of the promising near-term application we can achieve. [1]

The study of quantum many-body systems has been a fundamental aspect of quantum physics. Understanding these systems requires the ability to model the system and solve the Hamiltonian. Finding the ground state energy in a given Hamiltonian is one of the most essential problem to, for instance, condensed matter physics. It is, however, also a task that is computationally intensive, particularly as the system size grows. The VQE method, an algorithm that combines both classical and quantum schemes, promises the potential for solving complex systems with polynomial time. [1] Inspired by Hlatshwayo's article on *simulating excited states of Lipkin model on a quantum computer* [2], this study is heavily focused on trying to study the Lipkin model.

The Lipkin-Meshkov-Glick (LMG) model, or Lipkin model for short, is one of the paradigms for studying quantum many-body physics. It is a relatively simple model consist of $N$ fermions in a two level system with $N$ degeneracy. One of the advantage to the Lipkin model is that it can be easily expressed using the quasispin operators. [3]

In this report a study of the fundamentals in quantum computations with the focus of implementing basic quantum circuits and the VQE methods for solving the Lipkin model with $J = 1$ and $J = 2$. We first implemented a fully functional quantum computer simulator which works similar to qiskit, we then implemented the VQE methods and compare the results we obtained using numerical eigensolvers and the VQE algorithm from qiskit. We started by solving a simple one qubit system then a two qubit system. Through which we also computed the Von Neumann entropy and the role of entanglement. We'll first present the theory needed and the design of the quantum circuits, followed by presenting results for the different systems using various methods and a discussion of the results thereafter, before finally concluding our findings.

## II. THEORY

We'll first describe the basics of quantum computing, followed by the models being studied and finally the VQE algorithm.

### A. Quantum Computing

As an analogy to the classical "bits", the heart of quantum computer is "qubits". To distinguish them from "bits", we represent them as kets.

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

These are also our computational basis for the one qubit system. As a convention, the computational basis are usually the eigenbasis for the Pauli Z operator, $\sigma_z$ or $Z$, the latter is used for simplicity.

For multiple qubits, the computational basis is defined by tensor products of the single-qubit states, such as $|0\rangle \otimes |0\rangle$ as the 0 state for a two qubit (bipartite). The $\otimes$ sign is often omitted, for example, the basis for a bipartite system are written as $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$ for two qubits.

#### 1. Gates

#### 2. One Qubit Gates

Quantum gates are operators that change qubit states in order to perform an operation. The ones that most essential to this article are listed below

- X-gate (NOT gate): Maps $|0\rangle$ to $|1\rangle$ and vice versa. It's the Pauli-X matrix.

$$X|0\rangle = |1\rangle \tag{1}$$

$$X|1\rangle = |0\rangle \tag{2}$$

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{3}$$

- Y-gate: It flips the bit and multiply the phase by $i$. It's the Pauli-Y matrix.

$$Y|0\rangle = i|1\rangle \tag{4}$$

$$Y|1\rangle = -i|0\rangle \tag{5}$$

$$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{6}$$

- Z-gate (phase-flip gate): This gate flips the phase of the $|1\rangle$ state.

$$Z|0\rangle = |0\rangle \tag{7}$$

$$Z|1\rangle = -|1\rangle \tag{8}$$

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{9}$$

- Hadamard gate: This gate creates entanglement.

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \tag{10}$$

$$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \tag{11}$$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{12}$$

- $S^\dagger$ (S-dagger or S-inverse): This gate applies a $-90$ phase shift to the $|1\rangle$ state.

$$S^\dagger|0\rangle = |0\rangle \tag{13}$$

$$S^\dagger|1\rangle = -i|1\rangle \tag{14}$$

$$S^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} \tag{15}$$

- Rotation gates. Rx, Ry gates rotate the qubit around the x and y axis of the Bloch sphere by $\theta$ respectively.

$$Rx(\theta)|\psi\rangle = e^{-i\frac{\theta}{2}X}|\psi\rangle \tag{16}$$

$$Rx(\theta)|\psi\rangle = e^{-i\frac{\theta}{2}X}|\psi\rangle \tag{17}$$

where $|\psi\rangle$ is the initial state of the qubit and $\theta$ is the angle for the rotation.

- CNOT (Controlled NOT) gate: This gate applies a NOT gate to the second qubit (target) only if the first qubit (control) is in the state $|1\rangle$.

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{18}$$

- SWAP gate: This gate exchanges the states of two qubits.

The Von Neumann entropy is given by

$$S(A,B) = -\operatorname{Tr}\left(\rho_{A,B}\log_2(\rho_{A,B})\right). \tag{19}$$

It measure the degree of entanglement of the system.

$$SWAP = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{20}$$

### B. Simple Models

We studied the ground state energy for two simple Hamiltonians first. They can both be represented by

$$H = H_0 + \lambda H_1 \tag{21}$$

where $H_0$ is the non-interacting term, $H_1$ is the interacting term and $\lambda$ is the interaction strength which takes values $[0, 1]$.

#### 1. One-Qubit System

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix},$$

$$H_0 = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix}, \tag{22}$$

$$H_I = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix}, \qquad (23)$$

They can be rewrite using Pauli matrices ( in order to do quantum computation with )

$$H_0 = \mathcal{E}I + \Omega\sigma_z, \quad \mathcal{E} = \frac{E_1 + E_2}{2}, \ \Omega = \frac{E_1 - E_2}{2}, \quad (24)$$

and

$$H_I = c\boldsymbol{I} + \omega_z\sigma_z + \omega_x\sigma_x, \qquad (25)$$

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

### 2. Two-Qubit System

$$H_0 = \begin{bmatrix} \epsilon_{00} & 0 & 0 & 0 \\ 0 & \epsilon_{10} & 0 & 0 \\ 0 & 0 & \epsilon_{01} & 0 \\ 0 & 0 & 0 & \epsilon_{11} \end{bmatrix} \qquad (26)$$

$$H_{\mathrm{I}} = H_x\sigma_x \otimes \sigma_x + H_z\sigma_z \otimes \sigma_z, \qquad (27)$$

We choose $Hx = 2.0$, $Hz = 3.0$ and $\epsilon = [0.0, 2.5, 6.5, 7.0]$.

Rewrite $H_0$ in terms of the computational basis $Z$ and $I$.

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

Solving the above equations, we get[1]

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

and using the gates we have to switch to the computational basis $Z \otimes I$ we have:

Let the swap gate be denoted by $\mathcal{S}$, and cnot gate with control on qubit 1 and target on qubit 0 be $\mathcal{CN}$.

$$H_0 = 4I \otimes I + -0.75(\mathcal{S}Z \otimes I\mathcal{S}) - 2.75Z \otimes I + -0.5(\mathcal{CN}(1,0)Z \otimes I\mathcal{CN}(1,0))$$

$$H_{\mathrm{I}} = H_x\sigma_x \otimes \sigma_x + H_z\sigma_z \otimes \sigma_z,$$

Rewrite $X$ into $I \otimes Z$

$$H_I = H_x(I \otimes \sigma_z)(\sigma_z \otimes I) + H_z(\sigma_z \otimes I)(I \otimes \sigma_z)$$

$$H_I = \lambda(Hx\mathcal{S}Z \otimes I\mathcal{S}) + \lambda(Hz\mathcal{CN}(1,0)Z \otimes I\mathcal{CN}(1,0))$$

$$\begin{aligned} H = H_0 + H_I = &4\, I \otimes I \\ &+ (-0.75 + \lambda Hx)\,(\mathcal{S}Z \otimes I\mathcal{S}) \\ &+ -2.75\, Z \otimes I \\ &+ (-0.5 + \lambda Hz)\,(\mathcal{CN}(1,0)Z \otimes I\mathcal{CN}(1,0)) \end{aligned}$$

[1] How to solve this type equation are in Appendix ??.

### C. Lipkin Model

According to the original paper, the Lipkin model was proposed to be simple enough to solve analytically, and yet non-trival. "The model considers a situation where N fermions distributed in two levels each having an N-fold degeneracy and separated by an energy $\epsilon$. Each described by a quantum number $\sigma$ which has the value +1 in the upper shell and $-1$ in the lower shell, and a quantum number p specifying the particular degenerate state within the shell.For each value of p there are two corresponding states, one in the lower shell and one in the upper shell. Interactions can scatter these fermions in pairs between the 2 levels without changing the values of $p$. Let $\alpha_{p\sigma}^{\dagger}$ be the creation operator for a particle in the p state of the $\sigma$ level [3]. The Hamiltonian is given by

$$\begin{aligned} H_0 &= \varepsilon J_z, \\ H_1 &= \frac{1}{2}V \sum_{p,p',\sigma} a_{p\sigma}^{\dagger}a_{p'\sigma}^{\dagger}a_{p'-\sigma}a_{p-\sigma}, \\ H_2 &= \frac{1}{2}W \sum_{p,p',\sigma} a_{p\sigma}^{\dagger}a_{p'-\sigma}^{\dagger}a_{p'\sigma}a_{p-\sigma}. \end{aligned} \qquad (28)$$

In the lectures it was shown that the Lipkin Hamiltonian can be written as

$$\begin{aligned} H_0 &= \varepsilon J_z, \\ H_1 &= \frac{1}{2}V\left(J_+^2 + J_-^2\right) \\ H_2 &= \frac{1}{2}W\left(-N + J_+J_- + J_-J_+\right) \end{aligned} \qquad (29)$$

where the $J_+, J_-$ are quasispin ladder operators, and $J_z$ is the quasispin projection operator in the $Z$ direction and the total Hamiltonian is

$$H = H_0 + H_1 + H_2.$$

### 1. $J = 1$

Staring from relations involving the quasispin operators:

$$\begin{aligned} J_+|J, J_z\rangle &= \sqrt{J(J+1) - J_z(J_z+1)}|J, J_z+1\rangle, \\ J_-|J, J_z\rangle &= \sqrt{J(J+1) - J_z(J_z-1)}|J, J_z-1\rangle. \end{aligned} \qquad (30)$$

Acting $J_+$ and $J_-$ on all possible states to get the matrix elements:

$$J_+|1, -1\rangle = \sqrt{2}\,|1, 0\rangle$$

$$J_+|1, 0\rangle = \sqrt{2}\,|1, 1\rangle$$

$$J_+|1, 1\rangle = 0$$

We can obtain a set of similar relations for $J_-$. Obtaining the matrix form of the operators:

$$J_z = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$J_+^2 = \begin{bmatrix} 2 & 2 & 0 \\ 2 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{31}$$

$$J_-^2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 2 & 2 \\ 0 & 2 & 2 \end{bmatrix}$$

Substitute back into Equation (29), we obtain

$$\begin{bmatrix} -\epsilon & 0 & v \\ 0 & 0 & 0 \\ v & 0 & \epsilon \end{bmatrix} \tag{32}$$

We now want to rewrite the Hamiltonian in terms of Pauli matrices,

$$J_z = \sum_n j_z^{(n)} = \frac{1}{2}(Z_1 + Z_2)$$

$$\implies H_0 = \epsilon J_z = \frac{\epsilon}{2}(Z_1 + Z_2)$$

$$H_1 = \frac{1}{2}v(J_+^2 + J_-^2)$$

$$= \frac{1}{2}V \left[ (\sum_n j_+^{(n)})^2 + (\sum_n j_-^{(n)})^2 \right]$$

$$= \frac{1}{2}v \left( \sum_{nm} \left( j_+^{(n)} j_+^{(m)} + j_-^{(n)} j_-^{(m)} \right) \right) \tag{33}$$

$$= \frac{1}{2}v \sum_{nm} (j_x + ij_y)^{(n)} (j_x + ij_y)^{(m)}$$

$$+ (j_x - ij_y)^{(n)} (j_x - ij_y)^{(m)}$$

$$= \frac{1}{2}v \sum_{nm} (j_x^{(n)} j_x^{(m)} + ij_y^{(n)} j_x^{(m)} - j_y^{(n)} j_y^{(n)}$$

$$+ j_x^{(n)} j_x^m - ij_y^n j_x^{(m)} - j_y^{(n)} j_y^{(m)})$$

Since

$$j_x = \frac{X}{2}$$

$$j_y = \frac{Y}{2}$$

$$j_z = \frac{Z}{2}$$

Equation (33) becomes

$$v \sum_{nm} \left( j_x^{(n)} j_x^{(m)} - j_y^{(n)} j_y^{(m)} \right)$$

$$= 2v \sum_{n<m} \left( \frac{X_n}{2} \frac{X_m}{2} - \frac{Y_n}{2} \frac{Y_m}{2} \right)$$

$$\implies H_1 = \frac{1}{2}V(X_1 \otimes X_2 + Y_1 \otimes Y_2) \tag{34}$$

Combining $H_0$ and $H_1$

$$H = \frac{\epsilon}{2}(Z_1 + Z_2) + \frac{1}{2}V(X_1 \otimes X_2 + Y_1 \otimes Y_2) \tag{35}$$

### 2. $J = 2$

Using again Equation (30), we obtain the Hamiltonian matrix for $J = 2$.

$$H_{J=2} = \begin{pmatrix} -2\varepsilon & 0 & \sqrt{6}V & 0 & 0 \\ 0 & -\varepsilon+3W & 0 & 3V & 0 \\ \sqrt{6}V & 0 & 4W & 0 & \sqrt{6}V \\ 0 & 3V & 0 & \varepsilon+3W & 0 \\ 0 & 0 & \sqrt{6}V & 0 & 2\varepsilon \end{pmatrix} \tag{36}$$

Since this case follows the same Hamiltonian, upon inspection, we can rewrite the Hamiltonian in terms of the quasispin operators now for the $J = 2$ case. Note that the $H_0$ is a one body term, we take all linearly combination of the $Z$ and $I$, the identity operator with one $Z$, the $X$ and $Y$ terms both act on two bodies, so we need to take all combination of $XX$ (or $YY$) and $II$. The tensor product $\otimes$ sign is omitted for simplicity.

$$H = \epsilon(ZIII + IZII + IIZI + IIIZ)$$

$$+ \frac{v}{2}(XXII + XIXI + XIIX + IXXI + IXIX + IIXX)$$

$$- \frac{v}{2}(YYII + YIYI + YIIY + IYYI + IYIY + IIYY) \tag{37}$$

Again, rewriting the Hamiltonian in terms of Pauli matrices allows us to perform quantum computation with them.

We could also rewrite $H_2$ in terms of the Pauli matrices. Since $\hat{N}$ acting on any of the four qubit state must give $4|\psi\rangle$, we can represent it $4IIII$. The second term can be rewritten in similar ways to $H_1$

$$\implies H_2 = \frac{1}{2}W(4IIII + 2(XXII + \cdots IIXX$$

$$+ YYII \cdots IIYY)) $$

### D. Variational Quantum Eigensolver (VQE)

The Variational Quantum Eigensolver (VQE) is a quantum algorithm that employs a hybrid approach, combining quantum and classical processes, in order to find the ground state energy of a Hamiltonian. This algorithm is based on the Variational Principle, which states that the expectation value of the Hamiltonian, evaluated in any state, will always be greater than or equal to the ground state energy [4].

Mathematically,

$$E(\vec{\theta}) = \langle \Psi(\vec{\theta})|\hat{H}|\Psi(\vec{\theta})\rangle \geq E_0 \qquad (38)$$

where $|\Psi(\vec{\theta})\rangle$ is any state of a quantum system parameterised by a set of parameters $\vec{\theta}$, $\hat{H}$ is the Hamiltonian operator of the system and $E_0$ is the ground state energy.

The VQE algorithm follows these 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.

Unlike some of the other quantum algorithms, such as the quantum phase estimation algorithms (QPE), which is in theory more efficient, non-hybrid and non-variational but only applicable to large-scale fault tolerant quantum computers, VQE is viable in the current Noisy Intermediate-Scale Quantum (NISQ) computers [5, 6].

## III. METHODS

### A. Level Mapping

The fermions in the lipkin model needs to be mapped to qubits, one way, perhaps the more natural way, to map the fermions is using each qubit to represent a state $(n, \sigma)$ where $n$ is the particle slot and $\sigma$ is the level (either spin up or down). In this mapping it requires $2N$ qubits since there are 2 levels.

However, we know also that the Lipkin model do not permit the shift between particle slots, hence given an $n$, it's not possible that both $\sigma$'s are occupied at the same time. By taking advantage of this situation, we could consider the "level mapping", where we associate a qubit with a doublet, with

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

[5, 7]

### B. Ansatz

In the context of VQE, "ansatz" refers to the parametrised quantum circuit which performs a preset set a operations, with certain unbound parameters.

There is unique ansatz. If $Rx$ and $Ry$ represent the rotation gate in the $x$ and $y$ direction respectively, and $\theta, \phi$ represent the angle arguments within domain $[-\pi, \pi]$ they take: for the one qubit model, the ansatz we used is:
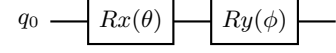


FIG. 1. One-qubit ansatz

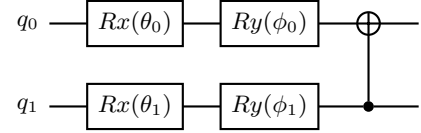For the two-qubit case, we used The CNOT gate at



FIG. 2. Two-qubit ansatz

the end entangles the two qubit.

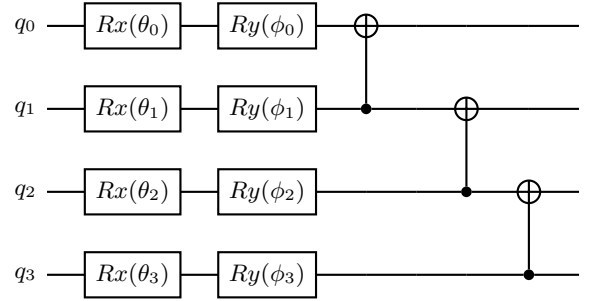The four-qubit ansatz is: Although, in general, the



FIG. 3. Four-qubit ansatz

ground state will be a superposition of the state with all quasispins down and all states with any number pairs of quasispins flipped up. Therefore it is also possible to reduce the cost of preparing a variational state and requiring only a single variational parameter due to the parity symmetry [7].

### C. Measurements

As mentioned in Section II A, our computational basis is in the $Z$ basis, and by extension the $ZI$ and $ZIII$ basis etc. in higher dimension. Therefore, in order to obtain the correct result for the other basis, we must rotate our circuit before taking measurements to the respective basis. When expectation values are calculated by taking repeated measurements, the number of shots was 10000

per measurement.

$$X = HZH.$$
$$Y = HS^{\dagger}ZHS \tag{39}$$

For example, if one were to measure in the $XIXI$ basis, one must apply the Hadamard gate on the $0th$ and $2nd$ qubit to rotate the system to the $XIXI$ basis. Note that measurement destroys the state and therefore a copy of the state must be obtained before each change of basis. To obtain the correct coefficients, we need to repeat each measurement $N$ times, where $N$ needs to be sufficiently larger. The measurement result is then the total number of counts divided by the number of shots, following

$$P(|\psi\rangle \to |x\rangle) \approx \sum_{n=0}^{N} \frac{x_n}{n} \tag{40}$$

For a precision of $\epsilon$ it requires $\mathcal{O}(1/\epsilon^2)$ samples for a circuit with depth $\mathcal{O}(1)$ [5].

## IV. RESULTS

Each result was produced by running different eigensolvers (both numerical and the VQE) for 100 different interaction strength ($\lambda$ or $v$).

### A. One Qubit

Figure 4

### B. Two Qubits

Figure 5 6.

### C. Lipkin Model: J=1

Figure 7

### D. Lipkin Model: J=2

Figure 8

## V. DISCUSSION

The implementation of a general $N$ qubit quantum computer simulator is difficult, especially for multi-qubit gates that needs to take into consideration all possible combinations and generalised the matrix (operator) accordingly. There the general $N$ qubit class *Qubits* finds the corresponding indices for certain gates, specifically
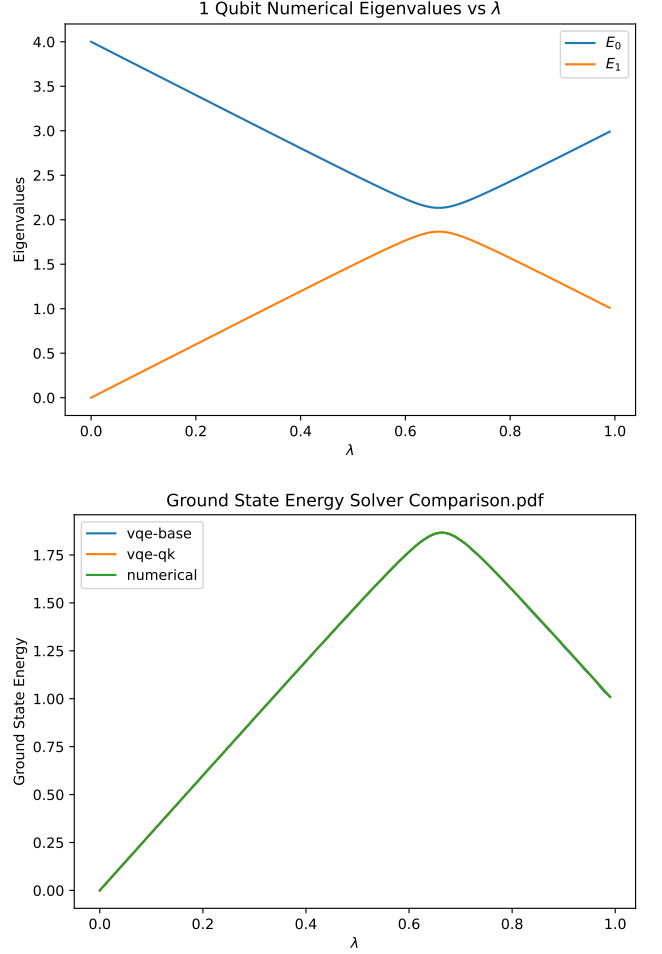




FIG. 4. Ground state for one qubit plotted against interacting strength $\lambda$.

the CNOT and SWAP gates, instead of making a general $N$ qubit operator. This has proven to be effective.

For our own VQE methods, we chose not to implement our own minimisation methods since we noticed the gradient based methods from 'Qiskit' (ADAM) is a lot slower than the non-gradient based methods, (Sequential Least Squares Programming (SLSQP), Constrained Optimization BY Linear Approximations (COBYLA)).The classical optimisation was therefore done using functionalities from 'Scipy.optimize.minimise'.

For the one qubit case, as seen in Figure 4, all three methods produced results that are next to identical. For the two qubit system, both VQE methods produced good results. However, the VQE method from Qiskit gave more outliers (from multiple runs) but a more precise result, while the VQE of our implementation has more 'bumps'. Given that the bumps seem to be uniformly distributed around the correct value, it's possibly due to the errors from measurement when calculating the expectation values. Indeed, when increase the number of shots to 100000, the 'bumps' smoothed out (Figure 10),
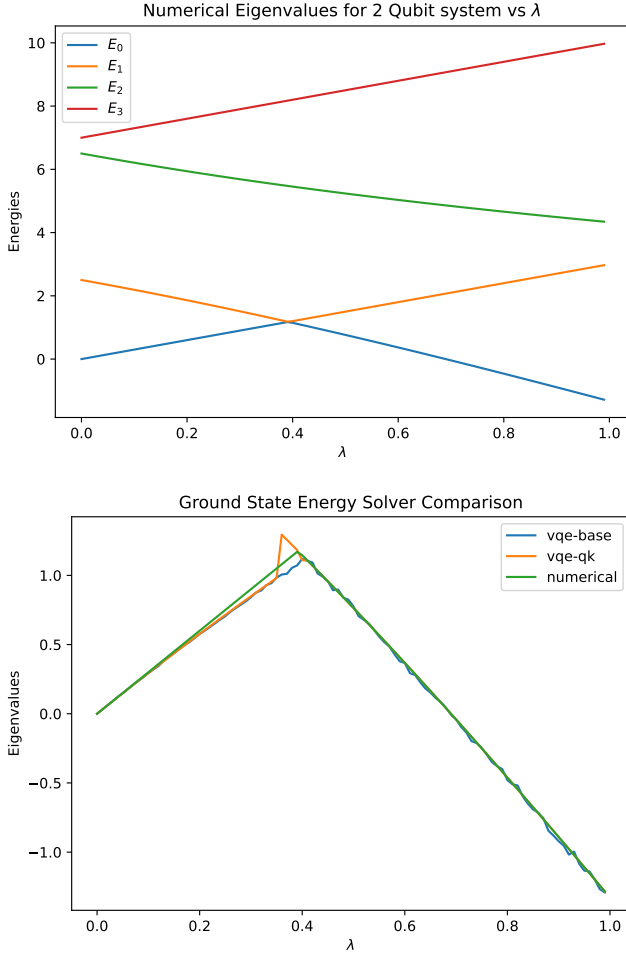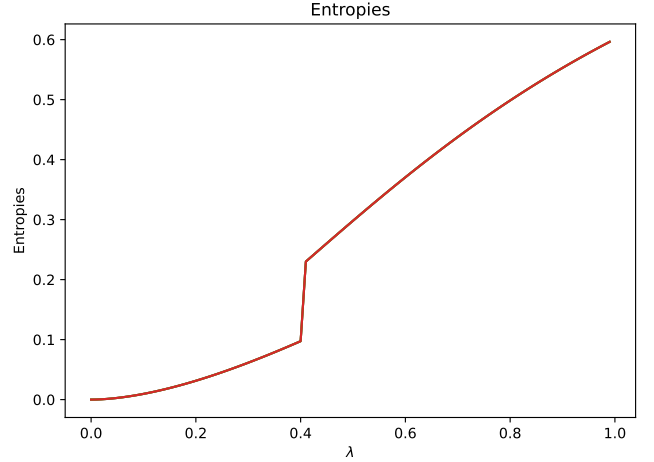
FIG. 6. The Von Neumann entropy for the ground state of the simple 2 qubit system.

contained results from computing the expectation values exactly by taking:
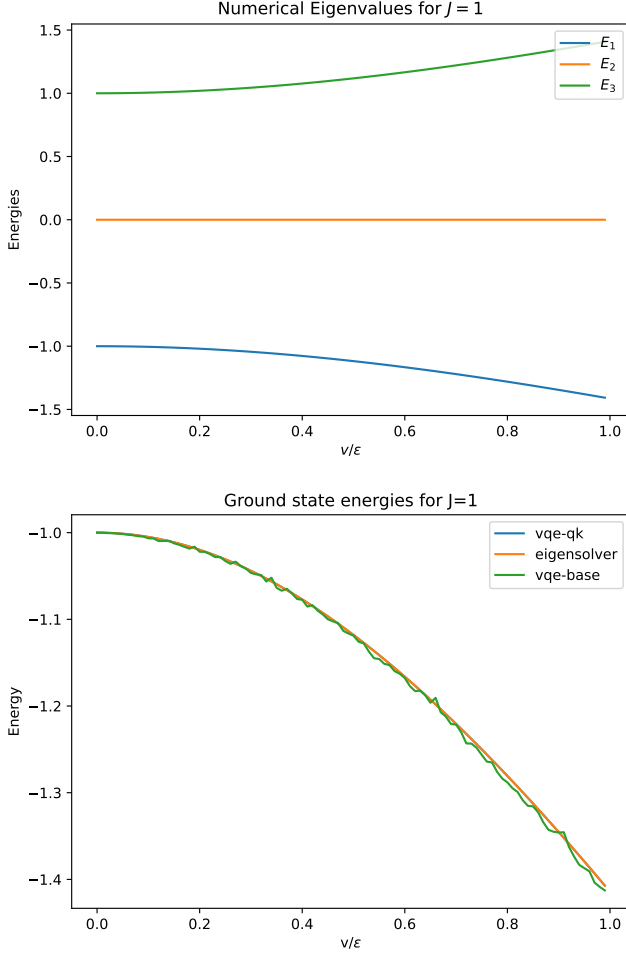
$$\langle\psi|H|\psi\rangle$$

This could be a result of unwise choice of ansatz, however, this ansatz gave the best results amongst many others which included more CNOT gates for non-neighbouring qubits or Toffoli (CCNOT) gate(s). One could also consider using an Hartree Fock ansatz [8]. Since the numerical eigenvalue solver underperformed in this task, it could also be simply due to the lack of computational power, which could potentially be improved by setting a lower tolerance rate or increase the maximum iteration steps. Another possibility of the cause of this problem is the parameters' initialisation. One could initialise using pretrained parameters which might increase the convergence rate.

## VI. CONCLUSION

Throughout this study, we have delved into the investigation of the Lipkin model with the Variational Quantum Eigensolver (VQE) method, implemented in a simulated quantum computing environment. We started with a simple one and two-qubit model and then for more complex models, specifically focusing on a Lipkin model.

Our implementation demonstrated the potential of such a hybrid algorithm in solving many body physics problems. Both the VQE methods, one from Qiskit and our own, delivered compelling results for the one and two qubit simple cases. Despite certain inconsistencies in the two-qubit systems, both the simple and Lipkin, our implementation achieved a performance comparable to that of Qiskit.
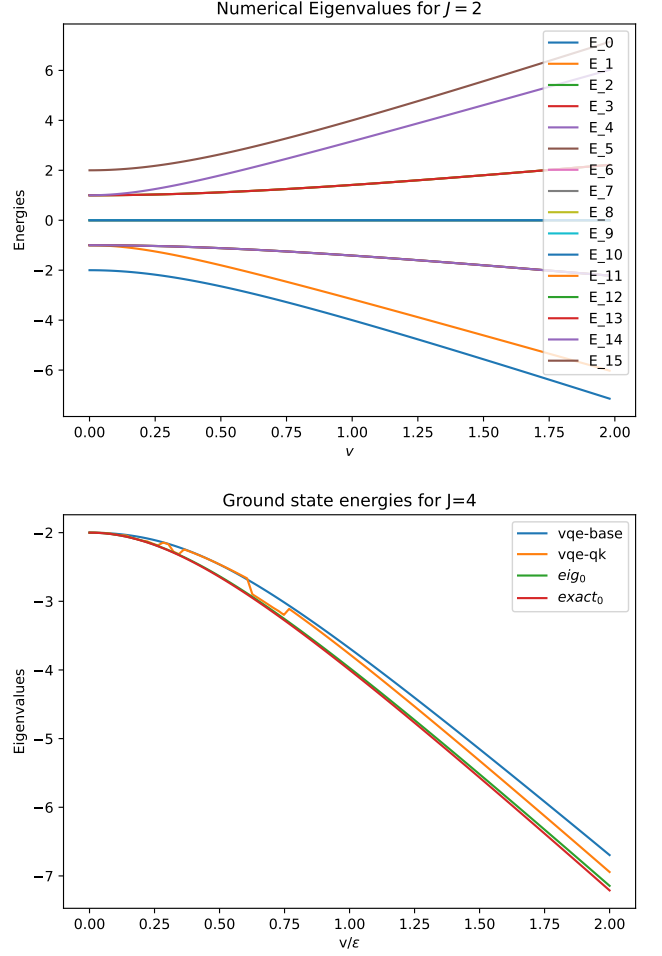
However, the results for $J = 2$ showed some discrepancies from the exact value and the expectation value cal-



FIG. 5. Ground state Hamiltonian for two qubit system plotted against interaction strength $\lambda$.

but the circuit runs extremely slowly, therefore they are not repeated for more complicated circuits. The Von Neumann entropy of the ground state is also interacting, we see a general increase in entropy but at the level crossing we see a huge leap of the entropy, signifying a drastic increase in entanglement.

The inclusion of the final CNOT gate in the ansatz as shown in Figure 2 was essential as it introduced entanglement to the circuit, the results obtained without the CNOT gate was not impressive, as in Figure 9. The circuit was able to predict the ground state before the level crossing, but both failed and converged to an incorrect state afterwards.

The results for the $J = 1$ has performance similar to the simple two qubit system. For $J = 2$ however, both the VQE methods from Qiskit and our own has some visble discrepancies from the exact value. Even the numerical eigenvalue solver wasn't able to obtain the result with high enough accuracy, as seen in Figure 8. We failed to compute the expectation value correctly, despite following the same procedure as section III C. This figure

FIG. 7. Lipkin Model with $J = 1$



FIG. 8. Ground state energy for the Lipkin model with different values of $v$ using ansatz with rep=2.

culation appears to be faulty. This could be attributed to multiple factors like the choice of ansatz or the initialisation of parameters. Adjustments in these aspects may improve the accuracy of the results.

For future work, improvements could be made in all aspects. Perhaps the most obvious choice being extending the VQE study to include the $H_2$ term in the Lipkin model and exploring different ansatzs using the parity symmetry mentioned in papers [7]. On top of that, our base quantum computer simulator could be improved to include a generic function to rotate the basis. This would eliminate the need for setting up an expectation value each time we use a different Hamiltonian, reduce the likelihood of introducing errors.

In summary, our study again showed the promising potential for the Variational Quantum Eigensolver. Despite requiring refinements, our understanding in quantum computing and the VQE method has deepened. We believe this will act as a stepping stone for future work.

## APPENDIX A: REWRITE A MATRIX IN TERMS OF ANOTHER ABSIS

1. Consider the general 4x4 matrix M:

$$M = \begin{bmatrix} m_{11} & m_{12} & m_{13} & m_{14} \\ m_{21} & m_{22} & m_{23} & m_{24} \\ m_{31} & m_{32} & m_{33} & m_{34} \\ m_{41} & m_{42} & m_{43} & m_{44} \end{bmatrix}$$

2. Express the tensor products of I and $\sigma_z$:

$$M = (a \cdot I \otimes I) + (b \cdot I \otimes \sigma_z) + (c \cdot \sigma_z \otimes I) + (d \cdot \sigma_z \otimes \sigma_z)$$

$$I \otimes I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

responding elements of M and the tensor product combinations:

$$I \otimes \sigma_z = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

$$m_{11} = a + b + c + d$$
$$m_{12} = 0$$
$$m_{13} = \cdots$$
$$\cdots$$

$$\sigma_z \otimes I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

4. Solve the system of equations to find the values of the coefficients a, b, c and d.

By determining the specific values of the coefficients a, b, c, and d, we can then rewrite any 4x4 matrix in the form:

$$\sigma_z \otimes \sigma_z = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$M = (a \cdot I \otimes I) + (b \cdot I \otimes \sigma_z) + (c \cdot \sigma_z \otimes I) + (d \cdot \sigma_z \otimes \sigma_z)$$

**APPENDIX B: OTHER RESULTS**

3. Set up a system of equations by equating the cor-

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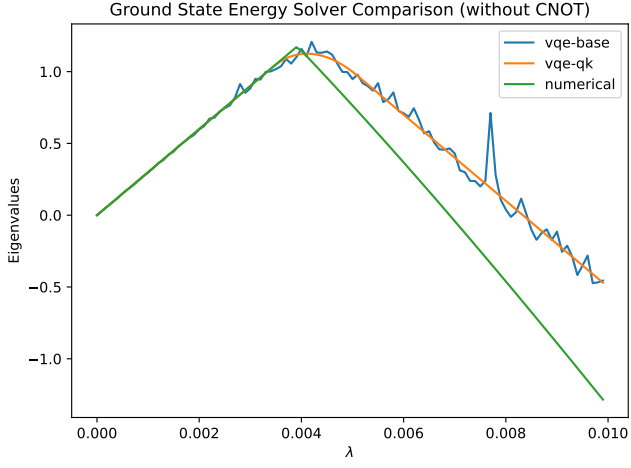
FIG. 9. Two Qubit results without CNOT gate in the sansatz.
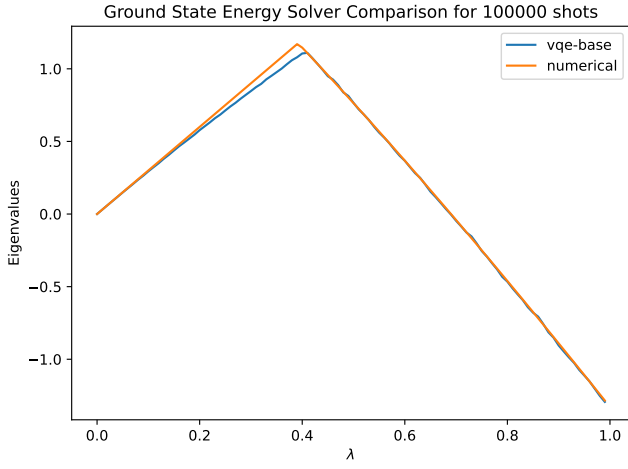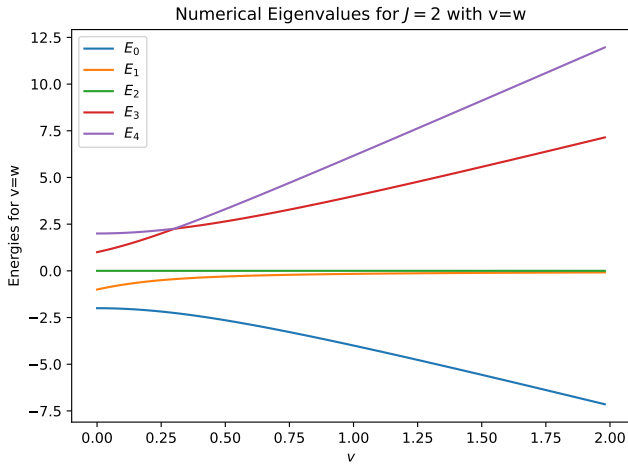


FIG. 10. Two qubit system with 100000 shots.



FIG. 11. Eigenvalues obtained by classical eigensolver included $H_2$, for $v = w$.