

Quantum Computing Lectures for Nano and Quantum Workshop

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Solving quantum mechanical problems

1. Simple Hamiltonian, the Lipkin model
2. Introducing the Variational Quantum Eigensolver (VQE)
3. Additional material with technicalities

Simple Hamiltonian, the Lipkin model

We will study a schematic model (the Lipkin model, see Nuclear Physics **62** (1965) 188), for the interaction among 2 and more fermions that can occupy two different energy levels.

For four fermions, the case we consider first here, each level has degeneration $d = 4$, leading to different total spin values. The two levels have quantum numbers $\sigma = \pm 1$, with the upper level having $2\sigma = +1$ and energy $\varepsilon_1 = \varepsilon/2$. The lower level has $2\sigma = -1$ and energy $\varepsilon_2 = -\varepsilon/2$. That is, the lowest single-particle level has negative spin projection (or spin down), while the upper level has spin up. In addition, the substates of each level are characterized by the quantum numbers $p = 1, 2, 3, 4$.

Single-particle states

We define the single-particle states (for the four fermion case which we will work on here)

$$|u_{\sigma=-1,p}\rangle = a_{-p}^\dagger|0\rangle \quad |u_{\sigma=1,p}\rangle = a_{+p}^\dagger|0\rangle.$$

The single-particle states span an orthonormal basis.

The Hamiltonian

The Hamiltonian of the system is given by

$$\begin{aligned}\hat{H} &= \hat{H}_0 + \hat{H}_1 + \hat{H}_2 \\ \hat{H}_0 &= \frac{1}{2}\varepsilon \sum_{\sigma,p} \sigma a_{\sigma,p}^\dagger a_{\sigma,p} \\ \hat{H}_1 &= \frac{1}{2}V \sum_{\sigma,p,p'} a_{\sigma,p}^\dagger a_{\sigma,p'}^\dagger a_{-\sigma,p'} a_{-\sigma,p} \\ \hat{H}_2 &= \frac{1}{2}W \sum_{\sigma,p,p'} a_{\sigma,p}^\dagger a_{-\sigma,p'}^\dagger a_{\sigma,p'} a_{-\sigma,p}\end{aligned}$$

where V and W are constants. The operator H_1 can move pairs of fermions while H_2 is a spin-exchange term. The latter moves a pair of fermions from a state $(p\sigma, p' - \sigma)$ to a state $(p - \sigma, p'\sigma)$.

Rewrite in terms of quasispin operators

We are going to rewrite the above Hamiltonian in terms of so-called quasispin operators

$$\begin{aligned}\hat{J}_+ &= \sum_p a_{p+}^\dagger a_{p-} \\ \hat{J}_- &= \sum_p a_{p-}^\dagger a_{p+} \\ \hat{J}_z &= \frac{1}{2} \sum_{p\sigma} \sigma a_{p\sigma}^\dagger a_{p\sigma} \\ \hat{J}^2 &= J_+ J_- + J_z^2 - J_z\end{aligned}$$

We can in turn express \hat{H} in terms of the above quasispin operators and the number operator

$$\hat{N} = \sum_{p\sigma} a_{p\sigma}^\dagger a_{p\sigma}.$$

Rewriting the Hamiltonian

We can rewrite the Hamiltonian in terms of the above quasi-spin operators and the number operator. We have

$$H_0 = \varepsilon J_z. \tag{1}$$

Moving over to H_1 and using the anti-commutation relations (10) through (12) we obtain

$$H_1 = \frac{1}{2}V (J_+^2 + J_-^2). \tag{2}$$

Finally, we rewrite the last term

$$H_2 = \frac{1}{2}W(-N + J_+J_- + J_-J_+). \quad (3)$$

We have thus expressed the Hamiltonian in term of the quasi-spin operators. See additional material for more details.

Variational Quantum Eigensolver

One initial algorithm to estimate the eigenenergies of a quantum Hamiltonian was [quantum phase estimation](#). In it, one encodes the eigenenergies, one binary bit at a time (up to n bits), into the complex phases of the quantum states of the Hilbert space for n qubits. It does this by applying powers of controlled unitary evolution operators to a quantum state that can be expanded in terms of the Hamiltonian's eigenvectors of interest. The eigenenergies are encoded into the complex phases in such a way that taking the inverse quantum Fourier transformation (see material on Quantum Fourier Transforms) of the states into which the eigen-energies are encoded results in a measurement probability distribution that has peaks around the bit strings that represent a binary fraction which corresponds to the eigen-energies of the quantum state acted upon by the controlled unitary operators. While quantum phase estimation (QPE) is provably efficient, non-hybrid, and non-variational, the number of qubits and length of circuits required is too great for our NISQ era quantum computers. Thus, QPE is only efficiently applicable to large, fault-tolerant quantum computers that likely won't exist in the near, but the far future.

Therefore, a different algorithm for finding the eigen-energies of a quantum Hamiltonian was put forth in 2014 called the variational quantum eigensolver, commonly referred to as [VQE](#). The algorithm is hybrid, meaning that it requires the use of both a quantum computer and a classical computer. It is also variational, meaning that it relies, ultimately, on solving an optimization problem by varying parameters and thus is not as deterministic as QPE. The variational quantum eigensolver is based on the variational principle: The expectation value of a Hamiltonian H in a state $|\psi(\theta)\rangle$ parameterized by a set of angles θ , is always greater than or equal to the minimum eigen-energy E_0 . To see this, let $|n\rangle$ be the eigenstates of H , that is

$$H|n\rangle = E_n|n\rangle. \quad (4)$$

We can then expand our state $|\psi(\theta)\rangle$ in terms of said eigenstates

$$|\psi(\theta)\rangle = \sum_n c_n |n\rangle,$$

and plug this into the expectation value to yield

$$\langle\psi(\theta)|H|\psi(\theta)\rangle = \sum_{nm} c_m^* c_n \langle m|H|n\rangle = \sum_{nm} c_m^* c_n E_n \langle m|n\rangle = \sum_{nm} \delta_{nm} c_m^* c_n E_n = \sum_n |c_n|^2 E_n \geq E_0 \sum_n |c_n|^2 = E_0,$$

which implies that we can minimize over the set of angles θ and arrive at the ground state energy E_0

$$\min_{\theta} \langle \psi(\theta) | H | \psi(\theta) \rangle = E_0.$$

Using this fact, the VQE algorithm can be broken down into the following steps

1. Prepare the variational state $|\psi(\theta)\rangle$ on a quantum computer.
2. Measure this circuit in various bases and send these measurements to a classical computer
3. The classical computer post-processes the measurement data to compute the expectation value $\langle \psi(\theta) | H | \psi(\theta) \rangle$
4. The classical computer varies the parameters θ according to a classical minimization algorithm and sends them back to the quantum computer which runs step 1 again.

This loop continues until the classical optimization algorithm terminates which results in a set of angles θ_{\min} that characterize the ground state $|\phi(\theta_{\min})\rangle$ and an estimate for the ground state energy $\langle \psi(\theta_{\min}) | H | \psi(\theta_{\min}) \rangle$.

VQE and efficient computations of gradients

We start with a simple 2×2 Hamiltonian matrix expressed in terms of Pauli X and Z matrices, as discussed in the project text.

We define a symmetric matrix $H \in \mathbb{R}^{2 \times 2}$

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

We let $H = H_0 + H_I$, where

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

is a diagonal matrix. Similarly,

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

where V_{ij} represent various interaction matrix elements. We can view H_0 as the non-interacting solution

$$H_0|0\rangle = E_1|0\rangle, \tag{5}$$

and

$$H_0|1\rangle = E_2|1\rangle, \tag{6}$$

where we have defined the orthogonal computational one-qubit basis states $|0\rangle$ and $|1\rangle$.

We rewrite H (and H_0 and H_I) via Pauli matrices

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

and

$$H_I = cI + \omega_z\sigma_z + \omega_x\sigma_x,$$

with $c = (V_{11} + V_{22})/2$, $\omega_z = (V_{11} - V_{22})/2$ and $\omega_x = V_{12} = V_{21}$. We let our Hamiltonian depend linearly on a strength parameter λ

$$H = H_0 + \lambda H_I,$$

with $\lambda \in [0, 1]$, where the limits $\lambda = 0$ and $\lambda = 1$ represent the non-interacting (or unperturbed) and fully interacting system, respectively. The model is an eigenvalue problem with only two available states.

Here we set the parameters $E_1 = 0$, $E_2 = 4$, $V_{11} = -V_{22} = 3$ and $V_{12} = V_{21} = 0.2$.

The non-interacting solutions represent our computational basis. Pertinent to our choice of parameters, is that at $\lambda \geq 2/3$, the lowest eigenstate is dominated by $|1\rangle$ while the upper is $|0\rangle$. At $\lambda = 1$ the $|0\rangle$ mixing of the lowest eigenvalue is 1% while for $\lambda \leq 2/3$ we have a $|0\rangle$ component of more than 90%. The character of the eigenvectors has therefore been interchanged when passing $z = 2/3$. The value of the parameter V_{12} represents the strength of the coupling between the two states.

Setting up the matrix

```
from matplotlib import pyplot as plt
import numpy as np
dim = 2
Hamiltonian = np.zeros((dim,dim))
e0 = 0.0
e1 = 4.0
Xnondiag = 0.20
Xdiag = 3.0
Eigenvalue = np.zeros(dim)
# setting up the Hamiltonian
Hamiltonian[0,0] = Xdiag+e0
Hamiltonian[0,1] = Xnondiag
Hamiltonian[1,0] = Hamiltonian[0,1]
Hamiltonian[1,1] = e1-Xdiag
# diagonalize and obtain eigenvalues, not necessarily sorted
EigValues, EigVectors = np.linalg.eig(Hamiltonian)
permute = EigValues.argsort()
EigValues = EigValues[permute]
# print only the lowest eigenvalue
print(EigValues[0])
```

Now rewrite it in terms of the identity matrix and the Pauli matrix X and Z

```

# Now rewrite it in terms of the identity matrix and the Pauli matrix X and Z
X = np.array([[0,1],[1,0]])
Y = np.array([[0,-1j],[1j,0]])
Z = np.array([[1,0],[0,-1]])
# identity matrix
I = np.array([[1,0],[0,1]])

epsilon = (e0+e1)*0.5; omega = (e0-e1)*0.5
c = 0.0; omega_z=Xdiag; omega_x = Xnondiag
Hamiltonian = (epsilon+c)*I+(omega_z+omega)*Z+omega_x*X
EigValues, EigVectors = np.linalg.eig(Hamiltonian)
permute = EigValues.argsort()
EigValues = EigValues[permute]
# print only the lowest eigenvalue
print(EigValues[0])

```

Implementing the VQE

For a one-qubit system we can reach every point on the Bloch sphere (as discussed earlier) with a rotation about the x -axis and the y -axis.

We can express this mathematically through the following operations (see whiteboard for the drawing), giving us a new state $|\psi\rangle$

$$|\psi\rangle = R_y(\phi)R_x(\theta)|0\rangle.$$

We can produce multiple ansatzes for the new state in terms of the angles θ and ϕ . With these ansatzes we can in turn calculate the expectation value of the above Hamiltonian, now rewritten in terms of various Pauli matrices (and thereby gates), that is compute

$$\langle\psi|(c + \mathcal{E})\mathbf{I} + (\Omega + \omega_z)\boldsymbol{\sigma}_z + \omega_x\boldsymbol{\sigma}_x|\psi\rangle.$$

We can now set up a series of ansatzes for $|\psi\rangle$ as function of the angles θ and ϕ and find thereafter the variational minimum using for example a gradient descent method.

To do so, we need to remind ourselves about the mathematical expressions for the rotational matrices/operators.

$$R_x(\theta) = \cos \frac{\theta}{2} \mathbf{I} - i \sin \frac{\theta}{2} \boldsymbol{\sigma}_x,$$

and

$$R_y(\phi) = \cos \frac{\phi}{2} \mathbf{I} - i \sin \frac{\phi}{2} \boldsymbol{\sigma}_y.$$

```

# define the rotation matrices
# Define angles theta and phi
theta = 0.5*np.pi; phi = 0.2*np.pi
Rx = np.cos(theta*0.5)*I-1j*np.sin(theta*0.5)*X
Ry = np.cos(phi*0.5)*I-1j*np.sin(phi*0.5)*Y
#define basis states
basis0 = np.array([1,0])

```

```

basis1 = np.array([0,1])

NewBasis = Ry @ Rx @ basis0
print(NewBasis)
# Compute the expectation value
#Note hermitian conjugation
Energy = NewBasis.conj().T @ Hamiltonian @ NewBasis
print(Energy)

```

Not an impressive results. We set up now a loop over many angles θ and ϕ and compute the energies

```

# define a number of angles
n = 20
angle = np.arange(0,180,10)
n = np.size(angle)
ExpectationValues = np.zeros((n,n))
for i in range(n):
    theta = np.pi*angle[i]/180.0
    Rx = np.cos(theta*0.5)*I-1j*np.sin(theta*0.5)*X
    for j in range(n):
        phi = np.pi*angle[j]/180.0
        Ry = np.cos(phi*0.5)*I-1j*np.sin(phi*0.5)*Y
        NewBasis = Ry @ Rx @ basis0
        Energy = NewBasis.conj().T @ Hamiltonian @ NewBasis
        Edifference=abs(np.real(EigValues[0]-Energy))
        ExpectationValues[i,j]=Edifference

print(np.min(ExpectationValues))

```

Clearly, this is not the best way of proceeding. Rather, here we could try to find the optimal values for the parameters θ and ϕ through computation of their respective gradients and thereby find the minimum as function of the optimal angles $\hat{\theta}$ and $\hat{\phi}$.

Let us now implement a classical gradient descent algorithm to the computation of the energies. We will follow closely <https://journals.aps.org/prabstract/10.1103/PhysRevA.99.032331> in order to calculate gradients of the Hamiltonian.

Gradient descent and calculations of gradients

In order to optimize the VQE ansatz, we need to compute derivatives with respect to the variational parameters. Here we develop first a simpler approach tailored to the one-qubit case. For this particular case, we have defined an ansatz in terms of the Pauli rotation matrices. These define an arbitrary one-qubit state on the Bloch sphere through the expression

$$|\psi\rangle = |\psi(\theta, \phi)\rangle = R_y(\phi)R_x(\theta)|0\rangle.$$

Each of these rotation matrices can be written in a more general form as

$$R_i(\gamma) = \exp -(\imath \frac{\gamma}{2} \sigma_i) = \cos(\frac{\gamma}{2})\mathbf{I} - \imath \sin(\frac{\gamma}{2})\sigma_i,$$

where σ_i is one of the Pauli matrices $\sigma_{x,y,z}$.

It is easy to see that the derivative with respect to γ is

$$\frac{\partial R_i(\gamma)}{\partial \gamma} = -\frac{\gamma}{2} \sigma_i R_i(\gamma).$$

We can now calculate the derivative of the expectation value of the Hamiltonian in terms of the angles θ and ϕ . We have two derivatives

$$\frac{\partial}{\partial \theta} [\langle \psi(\theta, \phi) | \mathbf{H} | \psi(\theta, \phi) \rangle] = \frac{\partial}{\partial \theta} [\langle \mathbf{H}(\theta, \phi) \rangle] = \langle \psi(\theta, \phi) | \mathbf{H}(-\frac{i}{2} \sigma_x | \psi(\theta, \phi) \rangle + \text{h.c.},$$

and

$$\frac{\partial}{\partial \phi} [\langle \psi(\theta, \phi) | \mathbf{H} | \psi(\theta, \phi) \rangle] = \frac{\partial}{\partial \phi} [\langle \mathbf{H}(\theta, \phi) \rangle] = \langle \psi(\theta, \phi) | \mathbf{H}(-\frac{i}{2} \sigma_y | \psi(\theta, \phi) \rangle + \text{h.c.}$$

This means that we have to calculate two additional expectation values in addition to the expectation value of the Hamiltonian itself. If we stay with an ansatz for the single qubit states given by the above rotation operators, we can, following for example [the article by Maria Schuld et al](#), show that the derivative of the expectation value of the Hamiltonian can be written as (we focus only on a given angle ϕ)

$$\frac{\partial}{\partial \phi} [\langle \mathbf{H}(\phi) \rangle] = \frac{1}{2} [\langle \mathbf{H}(\phi + \frac{\pi}{2}) \rangle - \langle \mathbf{H}(\phi - \frac{\pi}{2}) \rangle].$$

To see this, consider again the definition of the rotation operators. We can write these operators as

$$R_i(\phi) = \exp -i(\phi \sigma_i),$$

with ***sigma*** $_i$, with σ_i being any of the Pauli matrices X , Y and Z . The latter can be generalized to other unitary matrices as well. The derivative with respect to ϕ gives

$$\frac{\partial R_i(\phi)}{\partial \phi} = -\frac{i}{2} \sigma_i \exp -i(\phi \sigma_i) = -\frac{i}{2} \sigma_i R_i(\phi).$$

Our ansatz for a general one-qubit state on the Bloch sphere contains the product of a rotation around the x -axis and the y -axis. In the derivation here we focus only on one angle however. Our ansatz is then given by

$$|\psi\rangle = R_i(\phi)|0\rangle,$$

and the expectation value of our Hamiltonian is

$$\langle \psi | \hat{H} | \psi \rangle = \langle 0 | R_i(\phi)^\dagger \hat{H} R_i(\phi) | 0 \rangle.$$

Our derivative with respect to the angle ϕ has a similar structure, that is

$$\frac{\partial}{\partial \phi} [\langle \psi(\theta, \phi) | \mathbf{H} | \psi(\theta, \phi) \rangle] = \langle \psi(\theta, \phi) | \mathbf{H}(-\frac{i}{2} \sigma_y | \psi(\theta, \phi) \rangle + \text{h.c.}$$

In order to rewrite the equation of the derivative, the following relation is useful

$$\langle \psi | \hat{A}^\dagger \hat{B} \hat{C} | \psi \rangle = \frac{1}{2} \left[\langle \psi | (\hat{A} + \hat{C})^\dagger \hat{B} (\mathbf{A} + \hat{C}) | \psi \rangle - \langle \psi | (\hat{A} - \hat{C})^\dagger \hat{B} (\mathbf{A} - \hat{C}) | \psi \rangle \right],$$

where \hat{A} , \hat{B} and \hat{C} are arbitrary hermitian operators. If we identify these operators as $\hat{A} = \mathbf{I}$, with \mathbf{I} being the unit operator, $\hat{B} = \hat{H}$ our Hamiltonian, and $\hat{C} = -i\sigma_i/2$, we obtain the following expression for the expectation value of the derivative (excluding the hermitian conjugate)

$$\langle \psi | \mathbf{I}^\dagger \hat{H} (-\frac{i}{2} \sigma_i | \psi \rangle = \frac{1}{2} \left[\langle \psi | (\mathbf{I} - \frac{i}{2} \sigma_i)^\dagger \hat{H} (\mathbf{I} - \frac{i}{2} \sigma_i) | \psi \rangle - \langle \psi | (\mathbf{I} + \frac{i}{2} \sigma_i)^\dagger \hat{H} (\mathbf{I} + \frac{i}{2} \sigma_i) | \psi \rangle \right].$$

If we then use that the rotation matrices can be rewritten as

$$R_i(\phi) = \exp(-i\frac{\phi}{2} \sigma_i) = \cos(\frac{\phi}{2}) \mathbf{I} - i \sin(\frac{\phi}{2}) \sigma_i,$$

we see that if we set the angle to $\phi = \pi/2$, we have

$$R_i(\frac{\pi}{2}) = \cos(\frac{\pi}{4}) \mathbf{I} - i \sin(\frac{\pi}{4}) \sigma_i = \frac{1}{\sqrt{2}} \left(\mathbf{I} - \frac{i}{2} \sigma_i \right).$$

This means that we can write

$$\langle \psi | \mathbf{I}^\dagger \hat{H} (-\frac{i}{2} \sigma_i | \psi \rangle = \frac{1}{2} \left[\langle \psi | R_i(\frac{\pi}{2})^\dagger \hat{H} R_i(\frac{\pi}{2}) | \psi \rangle - \langle \psi | R_i(-\frac{\pi}{2})^\dagger \hat{H} R_i(-\frac{\pi}{2}) | \psi \rangle \right] = \frac{1}{2} (\langle \hat{H}(\phi + \frac{\pi}{2}) \rangle - \langle \hat{H}(\phi - \frac{\pi}{2}) \rangle).$$

Additional material on the Lipkin model

Properties of the Lipkin model

We have the following quasispin operators

$$J_\pm = \sum_p a_{p\pm}^\dagger a_{p\mp}, \quad (7)$$

$$J_z = \frac{1}{2} \sum_{p,\sigma} \sigma a_{p\sigma}^\dagger a_{p\sigma}, \quad (8)$$

$$J^2 = J_+ J_- + J_z^2 - J_z, \quad (9)$$

and we want to compute the commutators

$$[J_z, J_\pm], \quad [J_+, J_-], \quad [J^2, J_\pm] \quad \text{og} \quad [J^2, J_z].$$

Let us start with the first one and inserting for J_z and J_\pm given by the equations (8) and (7), respectively, we obtain

$$\begin{aligned} [J_z, J_\pm] &= J_z J_\pm - J_\pm J_z \\ &= \left(\frac{1}{2} \sum_{p,\sigma} \sigma a_{p\sigma}^\dagger a_{p\sigma} \right) \left(\sum_{p'} a_{p'\pm}^\dagger a_{p'\mp} \right) - \left(\sum_{p'} a_{p'\pm}^\dagger a_{p'\mp} \right) \left(\frac{1}{2} \sum_{p,\sigma} \sigma a_{p\sigma}^\dagger a_{p\sigma} \right) \\ &= \frac{1}{2} \sum_{p,p',\sigma} \sigma \left(a_{p\sigma}^\dagger a_{p\sigma} a_{p'\pm}^\dagger a_{p'\mp} - a_{p'\pm}^\dagger a_{p'\mp} a_{p\sigma}^\dagger a_{p\sigma} \right). \end{aligned}$$

Using the commutation relations for the creation and annihilation operators

$$\{a_l, a_k\} = 0, \quad (10)$$

$$\{a_l^\dagger, a_k^\dagger\} = 0, \quad (11)$$

$$\{a_l^\dagger, a_k\} = \delta_{lk}, \quad (12)$$

in order to move the operators in the right product to be in the same order as those in the lefthand product

$$\begin{aligned} [J_z, J_\pm] &= \frac{1}{2} \sum_{p,p',\sigma} \sigma \left(a_{p\sigma}^\dagger a_{p\sigma} a_{p'\pm}^\dagger a_{p'\mp} - a_{p'\pm}^\dagger (\delta_{p'p} \delta_{\mp\sigma} - a_{p\sigma}^\dagger a_{p'\mp}) a_{p\sigma} \right) \\ &= \frac{1}{2} \sum_{p,p',\sigma} \sigma \left(a_{p\sigma}^\dagger a_{p\sigma} a_{p'\pm}^\dagger a_{p'\mp} - a_{p'\pm}^\dagger \delta_{p'p} \delta_{\mp\sigma} a_{p\sigma} + a_{p'\pm}^\dagger a_{p\sigma}^\dagger a_{p'\mp} a_{p\sigma} \right), \end{aligned}$$

which results in

$$\begin{aligned} [J_z, J_\pm] &= \frac{1}{2} \sum_{p,p',\sigma} \sigma \left(a_{p\sigma}^\dagger a_{p\sigma} a_{p'\pm}^\dagger a_{p'\mp} - a_{p'\pm}^\dagger \delta_{pp'} \delta_{\mp\sigma} a_{p\sigma} + a_{p\sigma}^\dagger a_{p'\pm}^\dagger a_{p\sigma} a_{p'\mp} \right) \\ &= \frac{1}{2} \sum_{p,p',\sigma} \sigma \left(a_{p\sigma}^\dagger a_{p\sigma} a_{p'\pm}^\dagger a_{p'\mp} - a_{p'\pm}^\dagger \delta_{pp'} \delta_{\mp\sigma} a_{p\sigma} + a_{p\sigma}^\dagger (\delta_{pp'} \delta_{\pm\sigma} - a_{p\sigma} a_{p'\pm}^\dagger) a_{p'\mp} \right) \\ &= \frac{1}{2} \sum_{p,p',\sigma} \sigma \left(a_{p\sigma}^\dagger \delta_{pp'} \delta_{\pm\sigma} a_{p'\mp} - a_{p'\pm}^\dagger \delta_{pp'} \delta_{\mp\sigma} a_{p\sigma} \right). \end{aligned}$$

The last equality leads to

$$\begin{aligned} [J_z, J_\pm] &= \frac{1}{2} \sum_p \left((\pm 1) a_{p\pm}^\dagger a_{p\mp} - (\mp 1) a_{p\pm}^\dagger a_{p\mp} \right) = \pm \frac{1}{2} \sum_p \left(a_{p\pm}^\dagger a_{p\mp} + (\pm 1) a_{p\pm}^\dagger a_{p\mp} \right) \\ &= \pm \sum_p a_{p\pm}^\dagger a_{p\mp} = \pm J_\pm, \end{aligned}$$

where the last results follows from comparing with Eq. (7).

We can then continue with the next commutation relation, using Eq. (7),

$$\begin{aligned}
[J_+, J_-] &= J_+ J_- - J_- J_+ \\
&= \left(\sum_p a_{p'+}^\dagger a_{p-} \right) \left(\sum_{p'} a_{p'-}^\dagger a_{p'+} \right) - \left(\sum_{p'} a_{p'-}^\dagger a_{p'+} \right) \left(\sum_p a_{p+}^\dagger a_{p-} \right) \\
&= \sum_{p,p'} \left(a_{p'+}^\dagger a_{p-} a_{p'-}^\dagger a_{p'+} - a_{p'-}^\dagger a_{p'+} a_{p+}^\dagger a_{p-} \right) \\
&= \sum_{p,p'} \left(a_{p'+}^\dagger a_{p-} a_{p'-}^\dagger a_{p'+} - a_{p'-}^\dagger \left(\delta_{++} \delta_{pp'} - a_{p+}^\dagger a_{p'+} \right) a_{p-} \right) \\
&= \sum_{p,p'} \left(a_{p'+}^\dagger a_{p-} a_{p'-}^\dagger a_{p'+} - a_{p'-}^\dagger \delta_{pp'} a_{p-} + a_{p'+}^\dagger a_{p+}^\dagger a_{p'+} a_{p-} \right) \\
&= \sum_{p,p'} \left(a_{p'+}^\dagger a_{p-} a_{p'-}^\dagger a_{p'+} - a_{p'-}^\dagger \delta_{pp'} a_{p-} + a_{p+}^\dagger a_{p'-}^\dagger a_{p-} a_{p'+} \right) \\
&= \sum_{p,p'} \left(a_{p'+}^\dagger a_{p-} a_{p'-}^\dagger a_{p'+} - a_{p'-}^\dagger \delta_{pp'} a_{p-} + a_{p+}^\dagger \left(\delta_{--} \delta_{pp'} - a_{p-} a_{p'-}^\dagger \right) a_{p'+} \right) \\
&= \sum_{p,p'} \left(a_{p+}^\dagger \delta_{pp'} a_{p'+} - a_{p'-}^\dagger \delta_{pp'} a_{p-} \right),
\end{aligned}$$

which results in

$$[J_+, J_-] = \sum_p \left(a_{p+}^\dagger a_{p+} - a_{p-}^\dagger a_{p-} \right) = 2J_z,$$

It is straightforward to show that

$$[J^2, J_\pm] = [J_+ J_- + J_z^2 - J_z, J_\pm] = [J_+ J_-, J_\pm] + [J_z^2, J_\pm] - [J_z, J_\pm].$$

Using the relations

$$[AB, C] = A[B, C] + [A, C]B, \quad (13)$$

$$[A, BC] = [A, B]C + B[A, C], \quad (14)$$

we obtain

$$[J^2, J_\pm] = J_+[J_-, J_\pm] + [J_+, J_\pm]J_- + J_z[J_z, J_\pm] + [J_z, J_\pm]J_z - [J_z, J_\pm].$$

Finally, from the above it follows that

$$\begin{aligned}
[J^2, J_+] &= -2J_+ J_z + J_z[J_z, J_+] + [J_z, J_+]J_z - [J_z, J_+] \\
&= -2J_+ J_z + J_z J_+ + J_+ J_z - J_+ \\
&= -2J_+ J_z + J_+ + J_+ J_z + J_+ J_z - J_+ = 0,
\end{aligned}$$

and

$$\begin{aligned}
[J^2, J_-] &= 2J_z J_- + J_z[J_z, J_-] + [J_z, J_-]J_z - [J_z, J_-] \\
&= 2J_z J_- - J_z J_- - J_- J_z + J_- \\
&= J_z J_- - (J_z J_- + J_-) + J_- = 0.
\end{aligned}$$

Our last commutator is given by

$$\begin{aligned}
[J^2, J_z] &= [J_+ J_- + J_z^2 - J_z, J_z] \\
&= [J_+ J_-, J_z] + [J_z^2, J_z] - [J_z, J_z] \\
&= J_+[J_-, J_z] + [J_+, J_z]J_- \\
&= J_+ J_- - J_+ J_- = 0
\end{aligned}$$

Summing up we have

$$[J_z, J_\pm] = \pm J_\pm, \quad (15)$$

$$[J_+, J_-] = 2J_z, \quad (16)$$

$$[J^2, J_\pm] = 0, \quad (17)$$

$$[J^2, J_z] = 0, \quad (18)$$

which are the standard commutation relations for angular (or orbital) momentum L_\pm , L_z og L^2 .

We can rewrite the Hamiltonian in terms of the above quasi-spin operators and the number operator

$$N = \sum_{p,\sigma} a_{p\sigma}^\dagger a_{p\sigma}. \quad (19)$$

Going through each term of the Hamiltonian and using the expressions for the quasi-spin operators we obtain

$$H_0 = \varepsilon J_z. \quad (20)$$

Moving over to H_1 and using the anti-commutation relations (10) through (12) we obtain

$$\begin{aligned}
H_1 &= \frac{1}{2}V \sum_{p,p',\sigma} a_{p\sigma}^\dagger a_{p'\sigma}^\dagger a_{p'-\sigma} a_{p-\sigma} \\
&= \frac{1}{2}V \sum_{p,p',\sigma} -a_{p\sigma}^\dagger a_{p'\sigma}^\dagger a_{p-\sigma} a_{p'-\sigma} \\
&= \frac{1}{2}V \sum_{p,p',\sigma} -a_{p\sigma}^\dagger \left(\delta_{pp'} \delta_{\sigma-\sigma} - a_{p-\sigma} a_{p'\sigma}^\dagger \right) a_{p'-\sigma} \\
&= \frac{1}{2}V \sum_{p,p',\sigma} a_{p\sigma}^\dagger a_{p-\sigma} a_{p'\sigma}^\dagger a_{p'-\sigma}
\end{aligned}$$

Rewriting the sum over σ we arrive at

$$\begin{aligned}
H_1 &= \frac{1}{2}V \sum_{p,p'} a_{p+}^\dagger a_{p-} a_{p'+}^\dagger a_{p'-} + a_{p-}^\dagger a_{p+} a_{p'-}^\dagger a_{p'+} \\
&= \frac{1}{2}V \left[\sum_p \left(a_{p+}^\dagger a_{p-} \right) \sum_{p'} \left(a_{p'+}^\dagger a_{p'-} \right) + \sum_p \left(a_{p-}^\dagger a_{p+} \right) \sum_{p'} \left(a_{p'-}^\dagger a_{p'+} \right) \right] \\
&= \frac{1}{2}V [J_+ J_+ + J_- J_-] = \frac{1}{2}V [J_+^2 + J_-^2],
\end{aligned}$$

which leads to

$$H_1 = \frac{1}{2}V (J_+^2 + J_-^2). \quad (21)$$

Finally, we rewrite the last term

$$\begin{aligned}
H_2 &= \frac{1}{2}W \sum_{p,p',\sigma} a_{p\sigma}^\dagger a_{p'-\sigma}^\dagger a_{p'\sigma} a_{p-\sigma} \\
&= \frac{1}{2}W \sum_{p,p',\sigma} -a_{p\sigma}^\dagger a_{p'-\sigma}^\dagger a_{p-\sigma} a_{p'\sigma} \\
&= \frac{1}{2}W \sum_{p,p',\sigma} -a_{p\sigma}^\dagger \left(\delta_{pp'} \delta_{-\sigma-\sigma} - a_{p-\sigma} a_{p'-\sigma}^\dagger \right) a_{p'\sigma} \\
&= \frac{1}{2}W \sum_{p,p',\sigma} -a_{p\sigma}^\dagger \delta_{pp'} a_{p'\sigma} + a_{p\sigma}^\dagger a_{p-\sigma} a_{p'-\sigma}^\dagger a_{p'\sigma} \\
&= \frac{1}{2}W \left(-\sum_{p,\sigma} a_{p\sigma}^\dagger a_{p\sigma} + \sum_{p,p',\sigma} a_{p\sigma}^\dagger a_{p-\sigma} a_{p'-\sigma}^\dagger a_{p'\sigma} \right)
\end{aligned}$$

Using the expression for the number operator we obtain

$$\begin{aligned}
\sum_{p,p',\sigma} a_{p\sigma}^\dagger a_{p-\sigma} a_{p'-\sigma}^\dagger a_{p'\sigma} &= \sum_{p,p'} a_{p+}^\dagger a_{p-} a_{p'+}^\dagger a_{p'-} + a_{p-}^\dagger a_{p+} a_{p'+}^\dagger a_{p'-} \\
&= \sum_p \left(a_{p+}^\dagger a_{p-} \right) \sum_{p'} \left(a_{p'+}^\dagger a_{p'-} \right) + \sum_p \left(a_{p-}^\dagger a_{p+} \right) \sum_{p'} \left(a_{p'+}^\dagger a_{p'-} \right) \\
&= J_+ J_- + J_- J_+,
\end{aligned}$$

resulting in

$$H_2 = \frac{1}{2}W (-N + J_+ J_- + J_- J_+). \quad (22)$$

We have thus expressed the Hamiltonian in term of the quasi-spin operators.

Commutation relations for the Hamiltonian

The above expressions can in turn be used to show that the Hamiltonian commutes with the various quasi-spin operators. This leads to quantum numbers which are conserved. Let us first show that $[H, J^2] = 0$, which means that J is a so-called *good* quantum number and that the total spin is a conserved quantum number.

We have

$$\begin{aligned} [H, J^2] &= [H_0 + H_1 + H_2, J^2] \\ &= [H_0, J^2] + [H_1, J^2] + [H_2, J^2] \\ &= \varepsilon[J_z, J^2] + \frac{1}{2}V[J_+^2 + J_-^2, J^2] + \frac{1}{2}W[-N + J_+J_- + J_-J_+, J^2]. \end{aligned}$$

We have previously shown that

$$[H, J^2] = \frac{1}{2}V([J_+^2, J^2] + [J_-^2, J^2]) + \frac{1}{2}W(-[N, J^2] + [J_+J_-, J^2] + [J_-J_+, J^2])$$

Using that $[J_\pm, J^2] = 0$, it follows that $[J_\pm^2, J^2] = 0$. We can then see that $[J_+J_-, J^2] = 0$ and $[J_-J_+, J^2] = 0$ which leads to

$$\begin{aligned} [H, J^2] &= -\frac{1}{2}W[N, J^2] \\ &= \frac{1}{2}W(-[N, J_+J_-] - [N, J_z^2] + [N, J_z]) \\ &= \frac{1}{2}W(-[N, J_+]J_- - J_+[N, J_-] - [N, J_z]J_z - J_z[N, J_z] + [N, J_z]). \end{aligned}$$

Combining with the number operator we have

$$\begin{aligned}
[N, J_\pm] &= NJ_\pm - J_\pm N \\
&= \left(\sum_{p,\sigma} a_{p\sigma}^\dagger a_{p\sigma} \right) \left(\sum_{p'} a_{p'\pm}^\dagger a_{p'\mp} \right) - \left(\sum_{p'} a_{p'\pm}^\dagger a_{p'\mp} \right) \left(\sum_{p,\sigma} a_{p\sigma}^\dagger a_{p\sigma} \right) \\
&= \sum_{p,p',\sigma} a_{p\sigma}^\dagger a_{p\sigma} a_{p'\pm}^\dagger a_{p'\mp} - a_{p'\pm}^\dagger a_{p'\mp} a_{p\sigma}^\dagger a_{p\sigma} \\
&= \sum_{p,p',\sigma} a_{p\sigma}^\dagger a_{p\sigma} a_{p'\pm}^\dagger a_{p'\mp} - a_{p'\pm}^\dagger (\delta_{\mp\sigma} \delta_{pp'} - a_{p\sigma}^\dagger a_{p'\mp}) a_{p\sigma} \\
&= \sum_{p,p',\sigma} a_{p\sigma}^\dagger a_{p\sigma} a_{p'\pm}^\dagger a_{p'\mp} - a_{p'\pm}^\dagger \delta_{\mp\sigma} \delta_{pp'} a_{p\sigma} + a_{p'\pm}^\dagger a_{p\sigma}^\dagger a_{p'\mp} a_{p\sigma} \\
&= \sum_{p,p',\sigma} a_{p\sigma}^\dagger a_{p\sigma} a_{p'\pm}^\dagger a_{p'\mp} + a_{p\sigma}^\dagger a_{p'\pm}^\dagger a_{p\sigma} a_{p'\mp} - \sum_p a_{p\pm}^\dagger a_{p\mp} \\
&= \sum_{p,p',\sigma} a_{p\sigma}^\dagger a_{p\sigma} a_{p'\pm}^\dagger a_{p'\mp} + a_{p\sigma}^\dagger (\delta_{pp'} \delta_{\pm\sigma} - a_{p\sigma} a_{p'\pm}^\dagger) a_{p'\mp} - \sum_p a_{p\pm}^\dagger a_{p\mp} \\
&= \sum_p a_{p\pm}^\dagger a_{p\mp} - \sum_p a_{p\pm}^\dagger a_{p\mp} = 0.
\end{aligned}$$

We obtain then

$$\begin{aligned}
[N, J_z] &= NJ_z - J_z N \\
&= \left(\sum_{p,\sigma} a_{p\sigma}^\dagger a_{p\sigma} \right) \left(\frac{1}{2} \sum_{p',\sigma} \sigma a_{p'\sigma}^\dagger a_{p'\sigma} \right) - \left(\frac{1}{2} \sum_{p',\sigma} \sigma a_{p'\sigma}^\dagger a_{p'\sigma} \right) \left(\sum_{p,\sigma} a_{p\sigma}^\dagger a_{p\sigma} \right) \\
&= \sum_{p,p',\sigma} \sigma a_{p\sigma}^\dagger a_{p\sigma} a_{p'\sigma}^\dagger a_{p'\sigma} - \sigma a_{p'\sigma}^\dagger a_{p'\sigma} a_{p\sigma}^\dagger a_{p\sigma} = 0,
\end{aligned}$$

which leads to

$$[H, J^2] = 0, \quad (23)$$

and J is a good quantum number.

Constructing the Hamiltonian matrix for $J = 2$. We start with the state (unique) where all spins point down

$$|2, -2\rangle = a_{1-}^\dagger a_{2-}^\dagger a_{3-}^\dagger a_{4-}^\dagger |0\rangle \quad (24)$$

which is a state with $J_z = -2$ and $J = 2$. (we label the states as $|J, J_z\rangle$). For $J = 2$ we have the spin projections $J_z = -2, -1, 0, 1, 2$. We can use the lowering and raising operators for spin in order to define the other states

$$J_+ |J, J_z\rangle = \sqrt{J(J+1) - J_z(J_z+1)} |J, J_z+1\rangle, \quad (25)$$

$$J_- |J, J_z\rangle = \sqrt{J(J+1) - J_z(J_z-1)} |J, J_z-1\rangle. \quad (26)$$

We can then construct all other states with $J = 2$ using the raising operator J_+ on $|2, -2\rangle$

$$\begin{aligned}
J_+|2, -2\rangle &= \sqrt{2(2+1) - (-2)(-2+1)}|2, -2+1\rangle = \sqrt{6-2}|2, -1\rangle = 2|2, -1\rangle, \\
\text{which gives} \\
|2, -1\rangle &= \frac{1}{2}J_+|2, -2\rangle \\
&= \frac{1}{2}\sum_p a_{p+}^\dagger a_{p-} a_{1-}^\dagger a_{2-}^\dagger a_{3-}^\dagger a_{4-}^\dagger |0\rangle \\
&= \frac{1}{2}\left(a_{1+}^\dagger a_{2-}^\dagger a_{3-}^\dagger a_{4-}^\dagger + a_{1-}^\dagger a_{2+}^\dagger a_{3-}^\dagger a_{4-}^\dagger + a_{1-}^\dagger a_{2-}^\dagger a_{3+}^\dagger a_{4-}^\dagger + a_{1-}^\dagger a_{2-}^\dagger a_{3-}^\dagger a_{4+}^\dagger\right)|0\rangle.
\end{aligned} \tag{27}$$

We can construct all the other states in the same way. That is

$$J_+|2, -1\rangle = \sqrt{2(2+1) - (-1)(-1+1)}|2, -1+1\rangle = \sqrt{6}|2, 0\rangle,$$

which results in

$$\begin{aligned}
|2, 0\rangle &= \frac{1}{\sqrt{6}}\left(a_{1+}^\dagger a_{2+}^\dagger a_{3-}^\dagger a_{4-}^\dagger + a_{1+}^\dagger a_{2-}^\dagger a_{3+}^\dagger a_{4-}^\dagger + a_{1+}^\dagger a_{2-}^\dagger a_{3-}^\dagger a_{4+}^\dagger + a_{1-}^\dagger a_{2+}^\dagger a_{3+}^\dagger a_{4-}^\dagger + \right. \\
&\quad \left. a_{1-}^\dagger a_{2+}^\dagger a_{3-}^\dagger a_{4+}^\dagger + a_{1-}^\dagger a_{2-}^\dagger a_{3+}^\dagger a_{4+}^\dagger\right)|0\rangle
\end{aligned} \tag{28}$$

The two remaining states are

$$|2, 1\rangle = \frac{1}{2}\left(a_{1+}^\dagger a_{2+}^\dagger a_{3+}^\dagger a_{4-}^\dagger + a_{1+}^\dagger a_{2+}^\dagger a_{3-}^\dagger a_{4+}^\dagger + a_{1+}^\dagger a_{2-}^\dagger a_{3+}^\dagger a_{4+}^\dagger + a_{1-}^\dagger a_{2+}^\dagger a_{3+}^\dagger a_{4+}^\dagger\right). \tag{29}$$

and

$$|2, 2\rangle = a_{1+}^\dagger a_{2+}^\dagger a_{3+}^\dagger a_{4+}^\dagger |0\rangle. \tag{30}$$

These five states can in turn be used as computational basis states in order to define the Hamiltonian matrix to be diagonalized. The matrix elements are given by $\langle J, J_z | H | J', J_z' \rangle$. The Hamiltonian is hermitian and we obtain after all this labor of ours

$$H_{J=2} = \begin{bmatrix} -2\varepsilon & 0 & \sqrt{6}V & 0 & 0 \\ 0 & -\varepsilon + 3W & 0 & 3V & 0 \\ \sqrt{6}V & 0 & 4W & 0 & \sqrt{6}V \\ 0 & 3V & 0 & \varepsilon + 3W & 0 \\ 0 & 0 & \sqrt{6}V & 0 & 2\varepsilon \end{bmatrix} \tag{31}$$

We can now select a set of parameters and diagonalize the above matrix. We select $\varepsilon = 2$, $V = -1/3$, $W = -1/4$ and our matrix becoes

$$H_{J=2}^{(1)} = \begin{bmatrix} -4 & 0 & -\sqrt{6}/3 & 0 & 0 \\ 0 & -2 - 3/4 & 0 & -1 & 0 \\ -\sqrt{6}/3 & 0 & -1 & 0 & -\sqrt{6}/3 \\ 0 & -1 & 0 & 2 + -3/4 & 0 \\ 0 & 0 & -\sqrt{6}/3 & 0 & 4 \end{bmatrix},$$

which gives the eigenvalue

$$D = \begin{bmatrix} -4.21288 & 0 & 0 & 0 & 0 \\ 0 & -2.98607 & 0 & 0 & 0 \\ 0 & 0 & -0.91914 & 0 & 0 \\ 0 & 0 & 0 & 1.48607 & 0 \\ 0 & 0 & 0 & 0 & 4.13201 \end{bmatrix}.$$

The lowest state has an admixture of basis states given by

$$|\psi_0\rangle = 0.96735|2, -2\rangle + 0.25221|2, 0\rangle + 0.02507|2, 2\rangle,$$

with energy $E_0 = -4.21288$.

We can now change the parameters to $\varepsilon = 2$, $V = -4/3$, $W = -1$. Our matrix reads then

$$H_{J=2}^{(2)} = \begin{bmatrix} -4 & 0 & -4\sqrt{6}/3 & 0 & 0 \\ 0 & -5 & 0 & -4 & 0 \\ -4\sqrt{6}/3 & 0 & -4 & 0 & -4\sqrt{6}/3 \\ 0 & -4 & 0 & -1 & 0 \\ 0 & 0 & -4\sqrt{6}/3 & 0 & 4 \end{bmatrix},$$

with the following eigenvalues

$$D = \begin{bmatrix} -7.75122 & 0 & 0 & 0 & 0 \\ 0 & -7.47214 & 0 & 0 & 0 \\ 0 & 0 & -1.55581 & 0 & 0 \\ 0 & 0 & 0 & 1.47214 & 0 \\ 0 & 0 & 0 & 0 & 5.30704 \end{bmatrix}.$$

The new ground state (lowest state) has the following admixture of computational basis states

$$|\psi_0\rangle = 0.64268|2, -2\rangle + 0.73816|2, 0\rangle + 0.20515|2, 2\rangle,$$

with energy $E_0 = -7.75122$.

For the first set of parameters, the likelihood for observing the system in the computational basis state $|2, -2\rangle$ is rather large. This is expected since the interaction matrix elements are smaller than the single-particle energies. For the second case, with larger matrix elements, we see a much stronger mixing of the other states, again as expected due to the ratio of the interaction matrix elements and the single-particle energies.

Quantum Circuit, rewriting the Lipkin model in terms of Pauli matrices

To solve the Lipkin model on a quantum computer we have to solve Schrodinger's equation. To achieve this, we will use the Variational Quantum Eigensolver (VQE) discussed above

Before we proceed however, we need to rewrite the quasispin operators in terms of Pauli spin matrices/operators.

We take the liberty here of reminding you of some of the derivations done previously. We defined the number operator as

$$N = \sum_{n\sigma} a_{n\sigma}^\dagger a_{n\sigma},$$

which commutes with the Lipkin Hamiltonian. This can be seen by examining the Lipkin model Hamiltonian and noticing that the one-body part simply counts particles while the two-body term moves particles in pairs. Thus, the Hamiltonian conserves particle number. To find more symmetries we rewrote the Lipkin Hamiltonian in terms of $SU(2)$ quasispin operators

$$H = \epsilon J_z + \frac{1}{2} V (J_+^2 + J_-^2), \quad (32)$$

via the mappings

$$J_z = \sum_n j_z^{(n)},$$

and

$$J_\pm = \sum_n j_\pm^{(n)},$$

where we have the onebody operators

$$j_z^{(n)} = \frac{1}{2} \sum_\sigma \sigma a_{n\sigma}^\dagger a_{n\sigma},$$

and

$$j_\pm^{(n)} = a_{n\pm}^\dagger a_{n\mp}.$$

These operators obey the $SU(2)$ commutation relations

$$[J_+, J_-] = 2J_z,$$

and

$$[J_z, J_\pm] = \pm J_\pm.$$

Here the ladder operators are defined as $J_\pm = J_x \pm iJ_y$. With this rewriting, we can see that the total spin operator J^2 , which is defined as

$$J^2 = J_x^2 + J_y^2 + J_z^2 = \frac{1}{2} \{J_+, J_-\} + J_z^2,$$

commutes with the Hamiltonian since the Hamiltonian. We note also that the rotation operator

$$R = e^{i\phi J_z},$$

commutes with the Hamiltonian, which can be explained as follows. Writing J_z as

$$J_z = \frac{1}{2} (N_+ - N_-),$$

where $N_{\pm} = \sum_{n\pm} a_{n\pm}^\dagger a_{n\pm}$, allows us to see that it measures half the difference between the number of particles in the upper and lower levels. Thus, the possible eigenvalues r of the signature operator are

$$r = +1, j_z = 2n \quad (33)$$

$$r = +i, j_z = 2n + \frac{1}{2} \quad (34)$$

$$r = -1, j_z = 2n + 1 \quad (35)$$

$$r = -i, j_z = 2n + \frac{3}{2} \quad (36)$$

$$(37)$$

for $n \in \mathbb{Z}$. Note that r is real or imaginary if the number of particles N is even or odd, respectively. Since, as discussed above, the Lipkin Hamiltonian conserves N , r cannot jump between being real and imaginary. Additionally, because particles must be moved in pairs, and J_z measures half the difference between particles in the upper and lower levels, j_z can only change by as

$$j_z \rightarrow \frac{1}{2}[(N_+ \pm 2n) - (N_- \mp 2n)]$$

or $j_z \rightarrow J_z \pm 2n$.

To solve the Lipkin model with a quantum computer, the first step is to map the system to a set of qubits. We will restrict ourselves here to the half-filled case where the number of particles N equals the degeneracy of the states Ω . One could assign each possible state (n, σ) a qubit such that the qubit being in the state $|1\rangle$ or $|0\rangle$ would imply that the state (n, σ) is occupied or unoccupied, respectively. This mapping scheme (which we will call occupation mapping) requires 2Ω qubits.

The Hamiltonian takes the form

$$H = \epsilon J_z + \frac{1}{2} V (J_+^2 + J_-^2). \quad (38)$$

Plugging the mapping from the total J operators to the individual one-body j operators yields

$$H = \epsilon \sum_n j_z^{(n)} + \frac{1}{2} V \left[\left(\sum_n j_+^{(n)} \right)^2 + \left(\sum_n j_-^{(n)} \right)^2 \right] \quad (39)$$

$$= \epsilon \sum_n j_z^{(n)} + \frac{1}{2} V \sum_{n,m} \left(j_+^{(n)} j_+^{(m)} + j_-^{(n)} j_-^{(m)} \right) \quad (40)$$

$$= \epsilon \sum_n j_z^{(n)} + 2V \sum_{n < m} \left(j_x^{(n)} j_x^{(m)} - j_y^{(n)} j_y^{(m)} \right), \quad (41)$$

where we have used the definitions

$$j_{\pm}^{(n)} = j_x^{(n)} \pm ij_y^{(n)}.$$

To convert to Pauli matrices, we make the transformations

$$j_x^{(n)} \rightarrow X_n/2,$$

and

$$j_y^{(n)} \rightarrow Y_n/2,$$

and finally

$$j_z^{(n)} \rightarrow Z_n/2,$$

which preserve the above $SU(2)$ commutation relations. The factor of $1/2$ is due to the eigenvalues of the Pauli matrices being ± 1 while we are dealing with spin $1/2$ particles.

This transforms our Hamiltonian into

$$H = \frac{1}{2}\epsilon \sum_{k=1}^n Z_k + \frac{1}{2}V \sum_{n \neq j=1}^N (X_k X_j - Y_k Y_j).$$

With this form, we can clearly see that the first (one-body) term in the Hamiltonian returns the energy $-\epsilon/2$ or $+\epsilon/2$ if the qubit representing the particle of a doublet is in the ground ($|1\rangle$) or excited ($|0\rangle$) state, respectively. The action of the second (two-body) term in the Hamiltonian can be determined by noting that

$$\frac{1}{2}(XX - YY)|00\rangle = |11\rangle, \quad (42)$$

$$\frac{1}{2}(XX - YY)|01\rangle = 0, \quad (43)$$

$$\frac{1}{2}(XX - YY)|10\rangle = 0, \quad (44)$$

$$\frac{1}{2}(XX - YY)|11\rangle = |00\rangle. \quad (45)$$

That is, the two-body term moves a pair of particles between the ground states $|00\rangle$ and the excited states $|11\rangle$ of their respective doublets.

To construct an efficient ansatz, we must determine the subspace within which the Hamiltonian lives. To begin, note that particles are only ever moved between energy levels in pairs. Further, note that the Hamiltonian's coefficients (ϵ and V) are state independent (do not depend on the indices n or m) as the states labeled by these indices are degenerate and thus have the same energy level. Thus, the Hamiltonian treats all states with the same number of excited particles (Hamming weight of the state) as the same. Therefore, the following ansatz forms exactly cover the subspace within which the N -degenerate Hamiltonian explores:

$$|\psi_{\text{even}}\rangle = \sum_{k=0}^{\lfloor n/2 \rfloor} c_{2k} |D_{2k}^n\rangle, \quad (46)$$

$$|\psi_{\text{odd}}\rangle = \sum_{k=0}^{\lfloor n/2 \rfloor} c_{2k+1} |D_{2k+1}^n\rangle. \quad (47)$$

Here $|D_k^n\rangle$ represents a Dicke state which is defined as equal superposition of all n -qubit states with Hamming weight k . That is

$$|D_k^n\rangle = \frac{1}{\sqrt{\binom{n}{k}}} \sum_{x \in h_k^n} |x\rangle, \quad (48)$$

where $h_k^n = \{|x\rangle \mid l(x) = n, \text{wt}(x) = k\}$. There are two ways we can think of to prepare such ansatz: The first is to prepare them exactly as it is known how to deterministically prepare Dicke states with linear depth. The reference provides an algorithm for preparing a set of gates U_k^n that prepares a Dicke state from a product state of Hamming weight k ; that is

$$U_k^n |1\rangle^{\otimes k} |0\rangle^{\otimes n-k} = |D_k^n\rangle. \quad (49)$$

It then describes how to one can create an arbitrary superposition of Dicke states, which we modify here to restrict ourselves to a Hamming weight of constant parity. The circuit to construct such a state (for the $k = 6$ case, as an example) is discussed next week.