

1 Results and discussion

1.0.1 Making measurements

Before we move on to construct the VQE algorithm, we firstly test our implementation of the computational basis as well as the gates we need (and some more). As we've previously mentioned, an important task for us is to make measurements of expectation values. By following the methodology in the theory section for making measurements and building a quantum circuit, we construct the ϕ_+ Bell state and make spin Z measurements of the two qubits.

Doing this for 1000 shots, yields the following histogram (of what states have been measured)

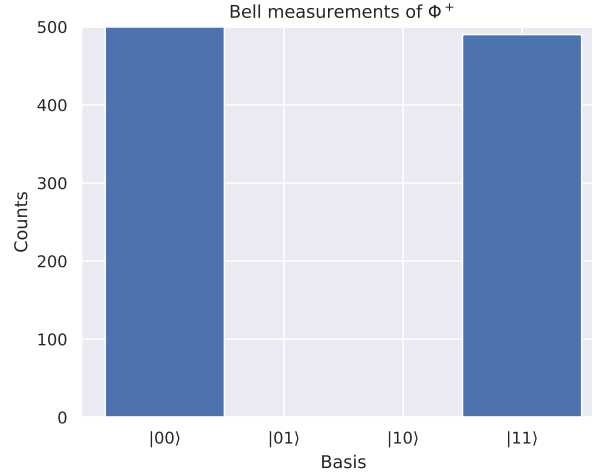


Figure 1: Histogram of the measured states of the ϕ_+ Bell state.

The histogram shows that the states $|00\rangle, |11\rangle$ are measured with (almost) equal occurrence, which is expected since the ϕ_+ state is a superposition of $|00\rangle$ and $|11\rangle$. If we've done this for more shots, the histogram would have been more even. This is a good indication that our implementation of the computational basis and the gates are correct.

Now we can apply the Hadamard gate to the first qubit and make measurements of the two qubits. This will yield the following histogram in figure (??):

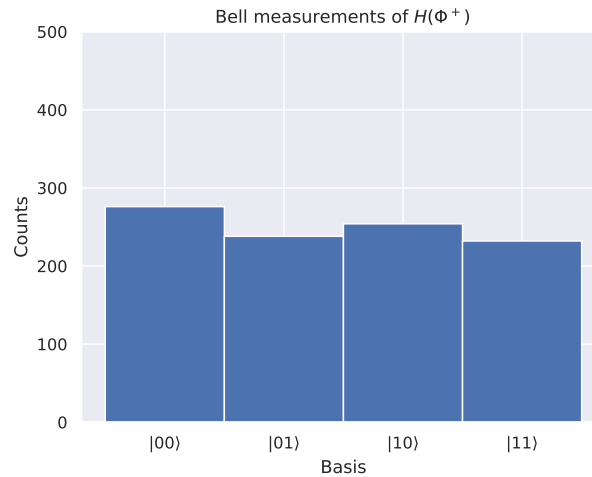


Figure 2: Histogram of the measured states of the ϕ_+ Bell state after applying the Hadamard gate to the first qubit.

Here we see that the state is an (almost) equal superposition of the basis states, which is to be expected when we apply the Hadamard gate. Again, with more shots, we'd achieve a more even distribution of the states - but this figure shows that our Hadamard gate implementation works as intended by mixing the states. It would be interesting to compare our own qubit measurement code with the framework provided by QisKit, but as of March 22nd, there seems to be some issues with the code we've previously written (as QisKit was recently updated), so this comparison will be done at a later time.

1.0.2 Simple one-qubit system

As stated in the previous sections, we build our code from the bottom by first looking at a simplified, one-qubit hamiltonian system. Implementing, and solving by diagonalization, the Hamiltonian for a single qubit system (??) gives us the following energy spectrum (??) for the ground state and the first excited state for increasing interaction strength λ :

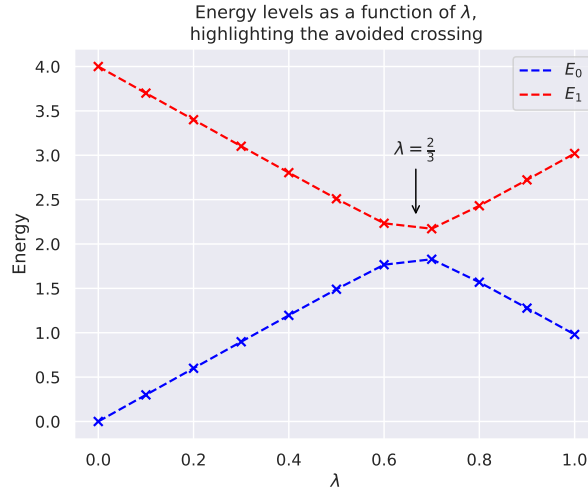


Figure 3: Energy spectrum for the ground state and the first excited state for increasing interaction strength λ .

Here we clearly see the avoided crossing occur for $\lambda = \frac{2}{3}$, where the ground state and the first excited state "repel" each other due to the interaction term in the Hamiltonian.

This is an important feature in our system, which we will need to take into account when we now want to solve for the ground state using a VQE algorithm.

Implementing this one-qubit Hamiltonian in our VQE algorithm, using GD optimization, with the Pauli basis encoding presented in the theory and method sections, we can compute an estimate for the ground state energy. This energy estimate is shown in the following figure (??) for increasing interaction strength λ :

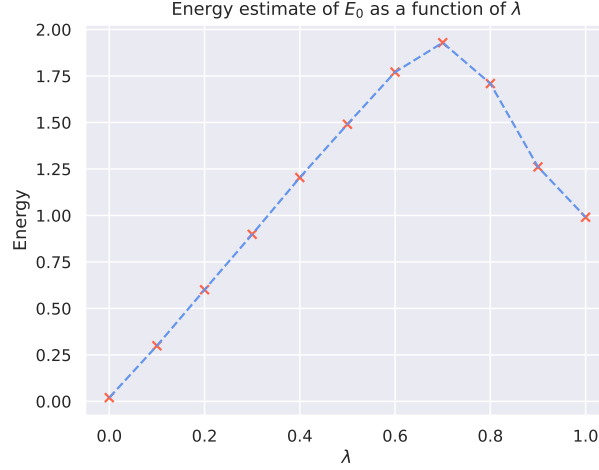


Figure 4: Energy estimate for the ground state for increasing interaction strength λ computed with the VQE algorithm.

In this plot we can clearly see again the avoided crossing, where the ground state energy estimate "turns around" and starts to decrease, after a steady increase up until $\lambda = \frac{2}{3}$, and our VQE algorithm seems to properly capture the entanglement in the system. This should indicate that we've made a good choice for our ansatz, and that our optimization algorithm is indeed working as intended.

1.0.3 Two-qubit system

Now we are ready to extend our program with another qubit, and implement the two-qubit Hamiltonian (??). Again we diagonalize the Hamiltonian to obtain the energy eigenvalues, presented in the following figure (??):

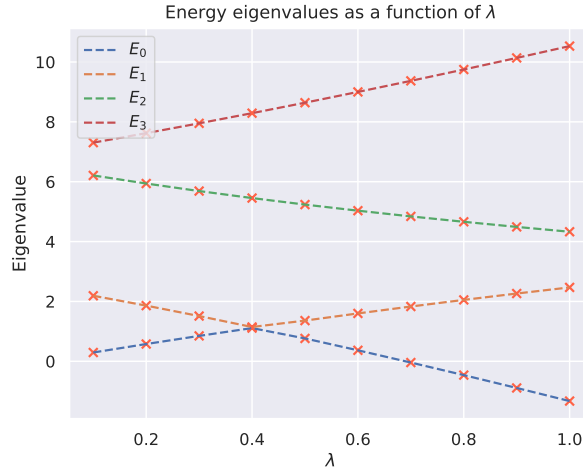


Figure 5: Energy spectrum for the 4 lowest energy states for increasing interaction strength λ in a two-qubit system.

Here we can again see an avoided crossing occur, but at $\lambda = 0.4$. This implies some form of entanglement in the energy eigenstates of our system when the interaction becomes non-negligible.

We can make a study of this entanglement by computing the Von Neumann entropy for one of the subsystems, and the results are presented in the following figure (??):

In figure (??) we can see a clear spike in entanglement entropy when we reach the avoided crossing, as expected.

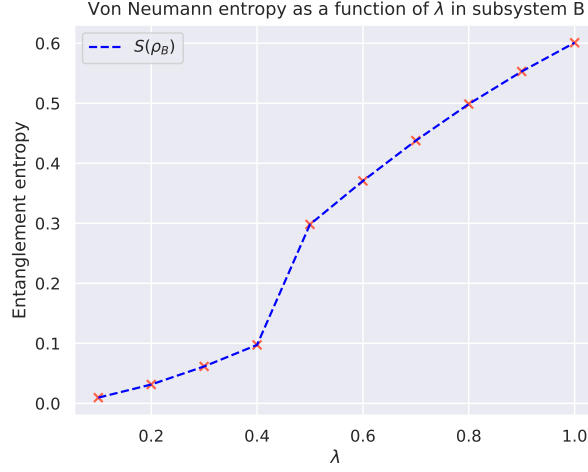


Figure 6: Von Neumann entropy for the two-qubit system for increasing interaction strength λ .

As before, we are also interested in computing the eigenvalues using the VQE algorithm - and the results are presented in the following figure (??):

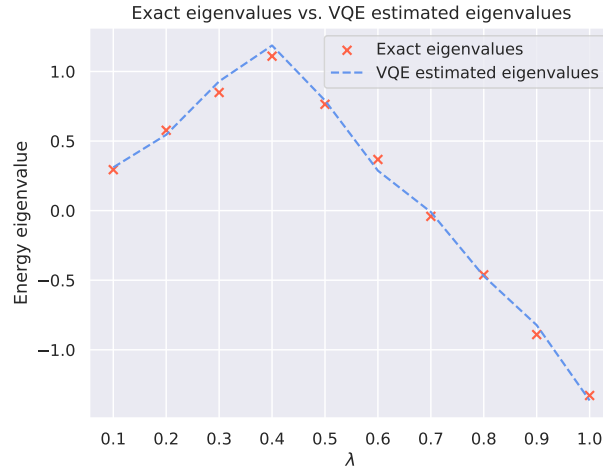


Figure 7: Energy estimate for the ground state for increasing interaction strength λ computed with the VQE algorithm against the exact values.

Here we've plotted the VQE estimates against the exact values found by diagonalization to illustrate an interesting point on the VQE algorithm. As it is a variational method, one would expect to never "undershoot" the ground state energy - however, due to the nature of the energy measurements (presented previously), the states are not measured exactly. This is a source of error in the VQE algorithm, and we can see that the VQE estimates are not always above the exact values.

1.0.4 Lipkin model

Finally, we are ready to implement the Lipkin model Hamiltonian (??). For the various encoding schemes we will reference multiple times to the article in **PhysRevC.106.024319** where the Lipkin model is studied in detail. We do this for $J = 1$ and $J = 2$, i.e 2 and 4 particle systems respectively.

We follow the methodology presented in the theory section and method section to again express the Lipkin hamiltonian in the Pauli basis which we can easily implement numerically. The results from diagonalization, for rising interaction parameter V is presented in figure (??): We see here a clear decrease

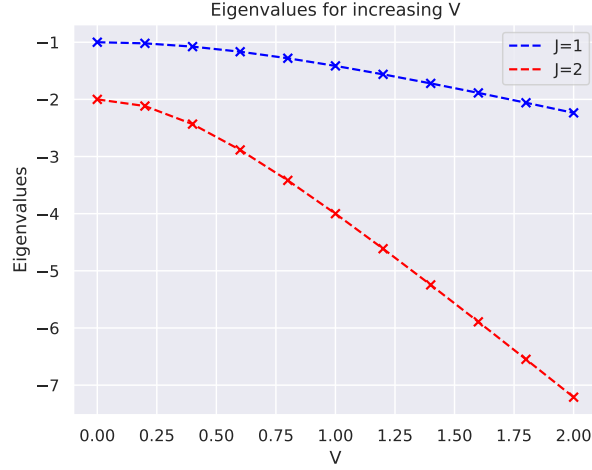


Figure 8: Ground state energy for increasing interaction strength V in the Lipkin model, for $J = 1$ and $J = 2$.

in the energy for the ground state as the interaction strength increases, which is expected for the Lipkin model due to the nature of the Hamiltonian.

Next we will make an estimate of the ground state energy using the VQE algorithm, for both the $J = 1$ and $J = 2$ systems. We will first study the simple $J = 1$ system, where with clever manipulation (as seen in the article), we can, for $N = 2$ use a single-qubit basis system (when we are only interested in the ground state that is). As seen in the appendix (A4) the Hamiltonian becomes a 4x4 matrix (see eq. (46) in the article), and we have a very simple ansatz for the wavefunction in this case (see fig. 12 in appendix A) - and the results are presented in the following figure

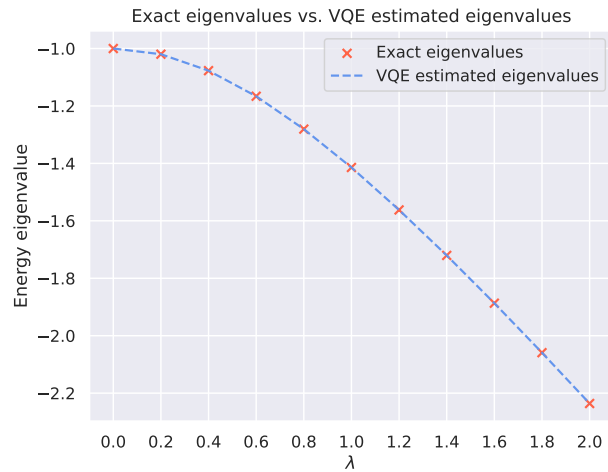


Figure 9: Ground state energy estimate for increasing interaction strength V in the Lipkin model, for $J = 1$ computed with the VQE algorithm.

We can see in that our VQE algorithm, with a single qubit, manages to capture the exact ground state energy extremely well - even for very high levels on interaction. This is a remarkable result, that with a clever encoding we (with good help from our friends in the Physics Review article) managed to reduce the $N = 2$ Lipkin model to a very simple Hamiltonian, and with a simple ansatz we find a (near) perfect estimate for the ground state energy.

Moving on, we'd like to study the $J = 2$ system, with $N = 4$ particles. Here we will also use a clever encoding presented to us by our friends in the Physics Review, where the 4 particle system can be reduced to a 2-qubit system, with $W = 0$, since there will effectively only be 3 interacting states that contributes in the ground state. The pauli expansion of the reduced Hamiltonian can be seen in eq. (62) in the article, where the exact eigenstates are also presented.

The ansatz we will need to use for the VQE algorithm for the $J = 2$ system can be found in figure 1 in the article, and with this ansatz, and the methodology presented in the theory section, we can compute the ground state of the system for increasing interaction strength V . The results are presented in the following figure:

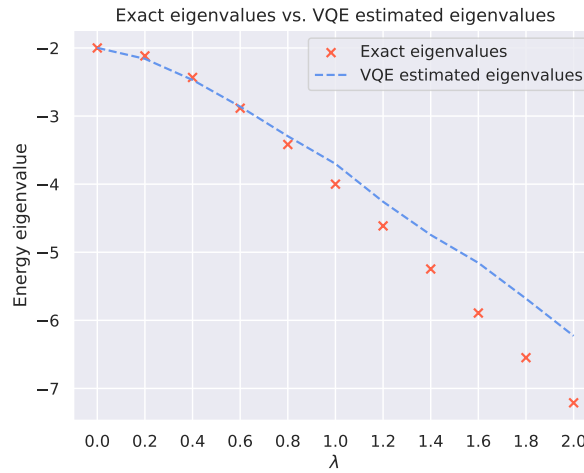


Figure 10: Ground state energy estimate for increasing interaction strength V in the Lipkin model, for $J = 2$ computed with the VQE algorithm.

In this plot we can clearly see that our VQE algorithm mimics the ground state energy, and makes good estimates for low levels of interaction. It seems to struggle more and more as we turn the interaction parameter up, and there may be many reasons for this. One major issue could lie in how we make the energy measurements, since we make a finite amount of shots, the expectation values used to compute the Hamiltonian will not be exact. Furthermore, as can be seen from the article in Physical Review C volume 106, the encoding of the $J = 2$ Hamiltonian with the ansatz we've used deviates from the true ground state energy for higher interaction strengths.

This means, that our (simplified) VQE algorithm captures much of the same properties in the system as the actual quantum computer that was used in the article, but it is not perfect, nor did we expect it to be.