Undergraduate Computational Physics Projects on Quantum Computing

Andrew Fournier

Faculty Adviser: David Heddle

Abstract:

For this project I simulated a quantum computer that would simulate Hadamard gates and phase shift gates and use those to run Grover's search algorithm. This algorithm would search through the diagonal of an 8x8 matrix to find an answer. The answer could be in any of the locations on the diagonal. I had to achieve a 95% accuracy with 2.22 iterations. This result would be far superior to the accuracy of a normal classical computer searching through eight possibilities with only 2.22 iterations, which only had a 27.75% accuracy. When Grover's search had completed, with 10000 trials it returned the correct answer 94% - 95% of the time. This confirmed that a quantum computer is far more accurate in less steps than a classical computer.

Introduction:

The objective of this capstone is write a quantum computer simulation for three qubits which requires 8D quantum vectors and is large enough to solve a real search problem, but is small enough to be doable. This capstone will show, on a small scale, the power and speed of a quantum computer. The first program is that of a classical computer. It will read in a simulated phonebook and, given a certain amount of names, it will search through the phonebook and print out the time taken. The second program is in three parts. I will code three programs that will implement Grover's search algorithm to achieve the same as the previous program.

Upon completion I will run a classical computer program and a simulated quantum computer that will implement Grover's search algorithm. These programs will be run many times. After each program has completed, it will print out the time taken to complete. Then I will plot the data given form each program. The final objective is to prove that, for a given N, the iterations it takes for the quantum computer to achieve 95% accuracy will be $(N^{1/2})/4$ compared to the iterations taken for a classical computer, which is N. The following graph simulates the data we hope to achieve.

Theory:

One of the most commonly used quantum gates is the Hadamard gate, symbolized by a box with an H in it. This gate acts on a single qubit and, given a single basis state, which are $|0\rangle = [1,0]$ and $|1\rangle = [0,1]$, returns a superposition of both basis states. A Hadamard gate can also take a superposition of the basis states and "put it back together" into a single basis state.

Another important one-qubit gate is the phase shift gate. This gate is symbolized by a box with Θ in it. Usually Θ has a specified value like $\frac{\pi}{4}$ or π, which will replace Θ in the box. This phase shift will have an effect if further quantum gate operations are applied to the qubit before it is measured.

I coded three programming projects. The first simulated the measurement of the N-qubit register. The computer program had to be able perform three tasks. First it must allocate a column vector with 2^N (in this case, N = 3, there will be eight complex entries) and set it to the desired initial state $|\Psi\rangle$. Secondly needed to produce a result by making a simulated measurement of S_z for the three qubits. The result will be random, but the probability of getting each result must follow the quantum mechanics of expressing a state vector Ψ as a linear sum. If $\Psi = a\,|000\rangle + b\,|001\rangle + c\,|010\rangle + d\,|011\rangle + e\,|100\rangle + f\,|101\rangle + g\,|110\rangle + h\,|111\rangle$ then the probability of a measurement resulting in $|110\rangle$ is $|g|^2$.

The result should be one of the eight basis states $|000\rangle$….$|111\rangle$ and should print out the result in this form. Finally the last step is repeating the second step many times to see how variable the results are.

The second programming project was set up to run the four quantum computations shown in the following image.

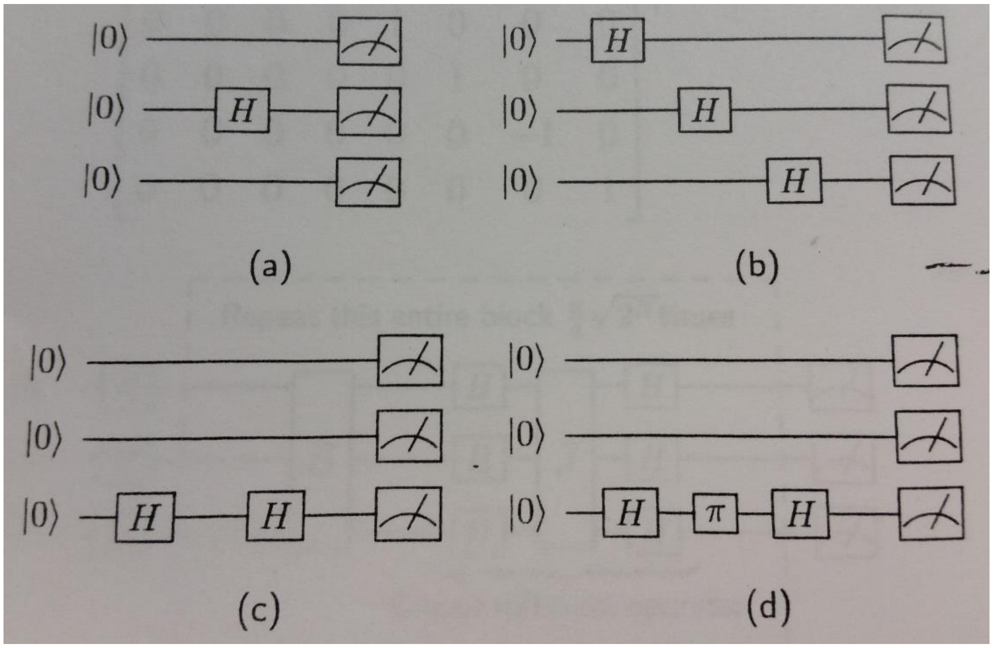


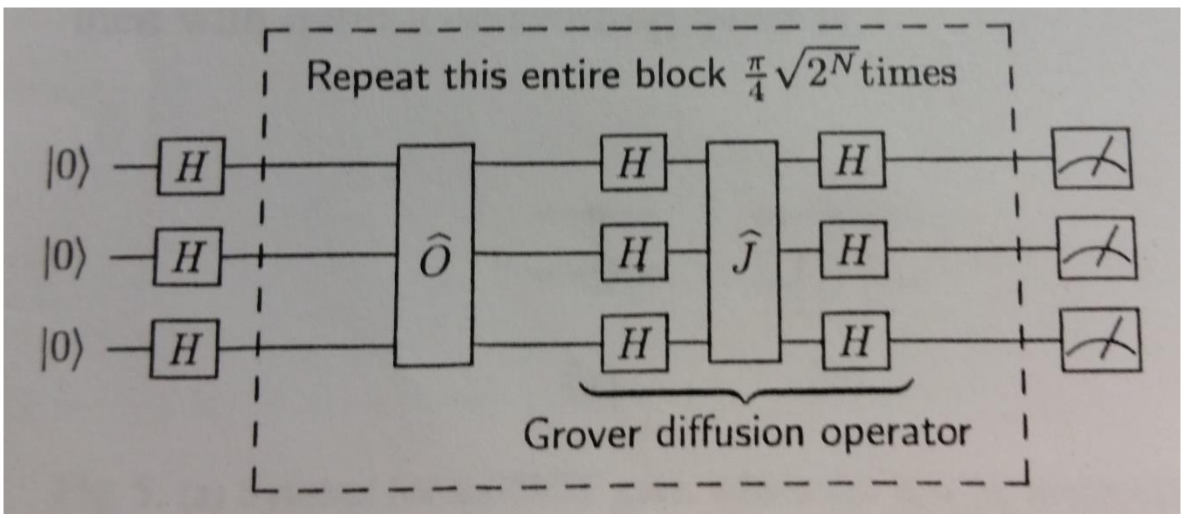
Figure (a) applies a Hadamard gate to qubit 2 which puts it into an equal superposition $|0\rangle$ and $|1\rangle$. Therefore, the result of the calculation should vary randomly between the two possibilities, $|000\rangle$ and $|010\rangle$.

Figure (b) applies a Hadamard gate to qubits 1, 2, and 3. Which puts each qubits into an equal superposition $|0\rangle$ and $|1\rangle$, with no correlations between the qubits. Knowing the state of qubit 1 gives no information about the states of 2 or 3. The result of this calculation should vary randomly between all eight possibilities, $|000\rangle$, $|001\rangle$, …, $|111\rangle$. Putting the N-qubit register into an equal superposition of all 2^N basis states is one of the important building blocks of many quantum algorithms.

Figure (c) applies 2 Hadamard gates to the same qubit. Since the Hadamard Gate puts a superposition back into a single basis state, the result of the calculation should always be $|000\rangle$.

Figure (d) also applies two Hadamard gates to the same qubit, but this time with a phase shift gate with $\Theta = \pi$. The result of this calculation will be perfectly definite, but now with the result always being $|001\rangle$. The net effect of these three gates was to flip qubit 3 from $|0\rangle$ to $|1\rangle$. This shows that using a phase-shift gate to change the phase of quantum amplitudes can indeed change the results of the calculation.

The third program I coded implemented Grover's quantum search.



The first set of Hadamard gates in the image above creates an equal superposition of all 2^N basis states. Which is then passed to the Oracle, an 8x8 diagonal matrix of 1's except where the answer of -1 is placed, also along the diagonal. The oracle asks all of the 2^N questions of where the answer is at the same time and flips the sign of the amplitude for the correct question. The "Grover Diffusion Operator" converts the phase difference in a magnitude difference that can be measured. The J operator is like the oracle but the -1 element is always in the first position along the diagonal.

Using Grover's search algorithm I searched through the Oracle to determine where along the diagonal our answer was located. Instead of the number of iterations it took for a classical computer to find the answer, which is on average 2^N, It took the quantum computer using Grover's algorithm only $(2^N)^{1/2} / 4$ iterations, with N being the number of qubits, 3, it took 2 iterations.

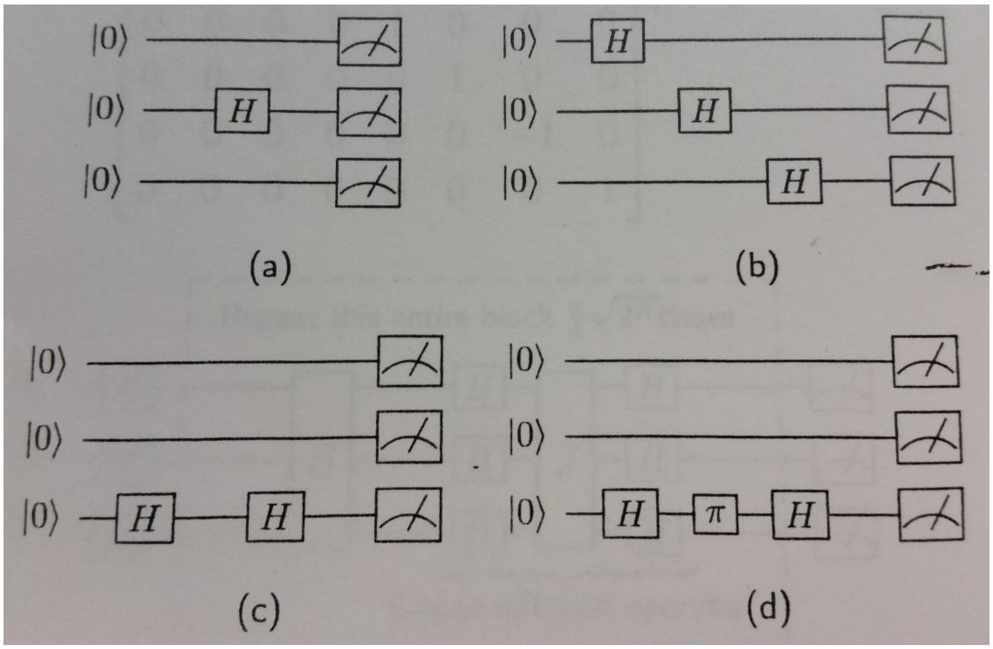
Methods:

The first step in coding these programs was to construct basis classes to implement. I defined the 8 basis states, $|000\rangle$, $|001\rangle$, …, $|111\rangle$, as strings. Then I created a complex number class that defined complex numbers and implemented three methods. The first would receive a complex number, $(a + ib)$, and return the magnitude. This was achieved by taking the square root of the real number squared plus the imaginary squared, $(a \times a + b \times b)^{1/2}$. The second method would receive two complex numbers multiply them together and return and the resulting complex number, $a_3 = (a_1 \times a_2 - b_1 \times b_2)$, $b_3 = (a_1 \times b_2 + a_2 \times b_1)$. The final would receive a complex number and return its complex conjugate, $(a + ib)^* = (a - ib)$. The final basis state program was a state vector class that would receive an 8x1 complex number vector, compute the magnitude of each complex number and normalize each value, so that the sum of each magnitude would equal 1.

Using these programs I was able to implement the Hadamard gates and the phase shift gates. Then I was able to combine those gates with the oracle matrix and the J matrix to implement Grover's Search Algorithm. I coded the search to run 10000 trials with 2 iterations each run through and return the amount of times it resulted in each answer as well as the percentage of each answer.

Data:

For each test of the Hadamard gates and the phase shift gates I ran each program many times with 10000 trials and recorded each result and the percentage of each result. I tested each program for the following figure.



Expected:

- One Hadamard gate (a)
  - 50% |000> and 50% |010>
- Three Hadamard gates (b)
  - equal mix of all basis states
- Two Hadamard gates on one qubit (c)
  - 100% |000>
- Phase Shift (d)
  - 100% |001>

Recorded:

- One Hadamard gate (a)
  - 49% - 51% |000> and 49% - 50% |010>
- Three Hadamard gates (b)
  - 11% - 13% of each state
- Two Hadamard gates on one qubit (c)
  - 100% |000>
- Phase Shift (d)
  - 100% |001>

After testing the data for the data for the Hadamard and Phase shift gates, I moved onto Grover's Search. I changed the number of iterations to determine how accurate the Quantum computer would be. In addition to that I changed the positioning of the answer in the Oracle.

Grover's Search (quantum computer)

- π(8^1/2)/4 = 2.22 iterations (Optimal)
  - 94% - 95% accuracy
- π(4^1/2)/4 = 1.57 iterations
  - 77% - 79% accuracy
- π(16^1/2)/4 = 3.14 iterations
  - 32% - 34% accuracy

Classical Computer

- 2.22 iterations
  - 27.75% accuracy
- 1.57 iterations
  - 19.63% accuracy
- 3.14 iterations
  - 39.25% accuracy

Discussion and Conclusion:

As shown by the data above, the Hadamard and phase shifts gates gave the expected results. The only discrepancy being 1% in either direction for the one Hadamard gate and the three Hadamard gates. This is to be expected from the gates due to the probabilities of each result. It will sometimes not be evenly split between the states. Grover's Search Algorithm was expected to be 95% accurate with the optimal number of iteration. Which is what was achieved. When the iterations decreased to 1.57 or increased to 3.14 the accuracy of the search decreased dramatically. Due to the algorithm, this is to be expected.

I determined the accuracy of the classical computer through simple probability. When give 2.22 iterations it had a 27.75% of finding the answer in the first 2.22 states. If the answer was in a state past those, it would be unable to find it.

These results show that a quantum computer is capable of performing actions much quicker and with less iterations than a classical computer.

Bibliography:

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