Tutorial Problems for Quantum Computing

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RUNNING CIRCUITS ON THE IBM QUANTUM PLATFORM

IBM allows anyone to run quantum circuits on some of their digital quantum computers, as well as quantum simulators, for free. In order to do so, you will need to register via IBM's Quantum Experience. Once you do so, you can run up to 10minutes of circuits per month.

The language that IBM uses to construct and communicate with their machine is Qiskit. You can find documentation here: Introduction to Qiskit. Qiskit is a Python-based software specifically built to write machine code for quantum computers. To learn how to write circuits, the tutorial on circuit construction is quite useful: Constructing Circuits.

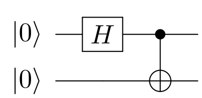
I provide hints to the problems on the very last page (after an empty page). Feel free to refer to this, though I encourage you to do so only after giving yourself a day to ruminate on the problems.

I. GHZ STATE

Recall from Monday's lecture that it is possible to construct an entangled state on a quantum computer. In particular, we constructed a **Bell State**, a two-qubit entangled state,

$$|\psi\rangle_{Bell} = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \tag{1}$$

This was done via the following circuit



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In this problem, you will construct the **Greenberger–Horne–Zeilinger (GHZ) state**, a three-particle entangled state and run it on a quantum computer, to determine the effects of noise.

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1. Construct a circuit that creates the GHZ state,

$$|\psi\rangle_{GHZ} = \frac{|000\rangle + |111\rangle}{\sqrt{2}} \tag{3}$$

   Is there an alternative circuit that can create this state?

   Bonus question: can you generalize this to a GHZ state with an arbitary number of qubits, ie

$$|\psi\rangle^{(n)}_{GHZ} = \frac{|0\rangle \otimes |0\rangle \otimes |0\rangle \cdots \otimes |0\rangle + |1\rangle \otimes |1\rangle \otimes |1\rangle \cdots \otimes |1\rangle}{\sqrt{2}} \tag{4}$$

   where n is the total number of qubits.

2. For three qubits, what are the eight states that fully span the Hilbert space? What is the probability of measuring these states?

3. Now, run this circuit on a (real) quantum device. Remember to repeat the circuit sufficiently many times to have your result be statistically sufficient (this is controlled by altering the number of *shots*). What are the measured probabilities of each of the states from above? Do they match your prediction? Why or why not?

II. QUANTUM SIMULATION OF THE QUANTUM HARMONIC OSCILLATOR

Whenever I begin working with a new tool or technique, I find it incredibly illuminating to first apply it to a situation where I already know what the answer should be. Often times, the quantum harmonic oscillator is perfect for this. The goal of this problem is to help you start thinking about Hamiltonian formulations, the connections between matrix representations and quantum circuits and the various considerations you must weigh when trying to simulate quantum field theories on quantum computers.

1. Recall that the Hamiltonian for a Quantum Harmonic Oscillator (QHO) can be written in one of two forms

$$\begin{aligned} \hat{H} &= \frac{\hat{p}^2}{2} + \frac{\hat{x}^2}{2} \\ &= \hat{n} + \frac{1}{2} \end{aligned} \tag{5}$$

   The form of the Hamiltonian that we will work with is the first, as it will be easiest to generalize the methods you develop here to other systems. Since quantum circuits (and quantum simulation) is nothing more than matrix multiplication, the first step is to convert this Hamiltonian into a matrix. In order to do this, we must choose a basis. For simplicity, let us work in the position basis.

   What is the form of the operators $\hat{x}$ and $\hat{p}$ in the position basis? As written, can this matrix be implemented on a (digital) finite computer, with a finite number of qubits?

   *I am putting a page break here as the next questions provide the answer to this question. I strongly encourage you to **NOT** read ahead until you have thought about this question*

2. In order to implement this system onto a quantum computer, the operators $\hat{x}$ and $\hat{p}$ must be discretized and truncated. This is somewhat analagous to how spacetime is discretized when writing a lattice gauge theory, but notice that we are already having to do this for a $0+1$ QFT (as quantum mechanics is simply $0+1$ QFT). Since we have decided to work in the position basis, it is easiest to discretize $\hat{x}$ first.

   What are the eigenvalues of a discretized and trunacted $\hat{x}$, assuming that you are working with n_q qubits? What is the matrix representation in the position basis of the operator $\hat{x}^2$? Your answer should only depend on $x_{\max}$ and n_q.

3. What are the eigenvalues of the operator $\hat{p}$. Are there different possibilities for the eigenvalues? How do you justify which set of eigenvalues you would like to choose? Regardless of your choice, your expression should only depend on $x_{\max}$ and n_q. Next, what is the form of the operator $\hat{p}^2$ in position space?

4. We are going to make use of a classical machine to check our choices and assumptions. You can use whatever computing program you are most comfortable with (ie Python, Mathematica, Matlab or anything else), as long as it can do numerically evaluate the eigenvalues of matrices.

   Combining your forms of $\hat{x}^2$ and $\hat{p}$, find the eigenvalues of the Hamiltonian for $n_q = 3$, for a choice of $x_{\max}$ (do not stress about choosing a good value at this point, just evaluate and see what happens). For your choice in $x_{\max}$, do your eigenvalues match the known results for a QHO? If not, carry out a scan over $x_{\max}$ and see if you can find an optimal value for x_{max}, defined as the value for $x_{\max}$ that gives you an eigenvalue closest to the (continuous) QHO:

$$E_n = n + \frac{1}{2} \tag{6}$$

5. Repeat this exercise for the other choice for the digitization and truncation of the momentum operator $\hat{p}$. Is there an optimal choice for $x_{\max}$ for this choice of the momentum operator?

   Note that the difference between these two choices is not the boundary conditions you choose, but whether the ratio of the eigenvalues is a polynomial or not. If this comment does not make sense, please come ask me - I am trying to not give away the answer.

6. Repeat this process with $n_q = 4$. You could also go to more qubits if you would like, but you should see a pattern emerging already and it is quite time-consuming to do $n_q = 5$.[1]

7. Next, we are going to implement this Hamiltonian onto a quantum computer and look at the time evolution of a state that is not an eigenstate of the system. If you would like, please feel free to check the form of $\hat{x}^2$ and $\hat{p}^2$ with me. We will begin with $\hat{x}^2$. Since we are working in the position basis, this operator is diagonal. To implement onto a quantum device, we are going to decompose this diagonal operator into a sum of Kronecker products of the Identity matrix and Z gates.[2]. Extend our definition of the Pauli matrices to have σ_0 be the identity matrix. To be more explicit, assuming three qubits, decompose the operator $\hat{x}^2$ into the basis

$$\begin{aligned}\hat{x}^2 = {} & c_0\,\sigma_0\otimes\sigma_0\otimes\sigma_0 + c_1\,\sigma_3\otimes\sigma_0\otimes\sigma_0 + c_2\,\sigma_3\otimes\sigma_3\otimes\sigma_0 + c_3\,\sigma_3\otimes\sigma_0\otimes\sigma_0 \\ & + c_4\,\sigma_0\otimes\sigma_3\otimes_3 + c_5\,\sigma_3\otimes\sigma_3\otimes\sigma_3 + c_6\,\sigma_3\otimes\sigma_0\otimes\sigma_3 + c_7\,\sigma_0\otimes\sigma_0\otimes\sigma_3\end{aligned} \tag{7}$$

   Calculate the value of the coefficients c_i using the fact that this basis is orthonormal and complete.

8. Do the same procedure for the $\hat{p}^2$ operator in the **momentum** basis ie the basis in which $\hat{p}^2$ is diagonal. Do you notice anything about how the operator $\hat{x}^2$ and $\hat{p}^2$ are decomposed in their own basis? If you do not see something striking, come check with me.

9. In order to carry out time evolution, we must exponentiate the Hamiltonian to create the time evolution operator. Since the position basis and the momentum basis are related by a Fourier transform and there exists an efficient implementation of this on quantum devices, called a Quantum Fourier Transform (QFT), we will separate the Hamiltonian into two components:

$$\hat{H} = \hat{H}_x + \hat{H}_p \tag{8}$$

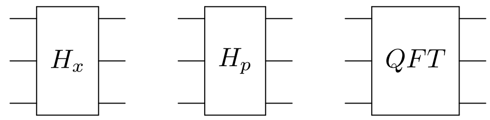
[1] There is a really lovely physics explanation for why the optimal value of $x_{\max}$ it is. If you are curious, take a look at the how the (continuous) ground state wavefunction in both (discretized) position and momentum space. Notice anything?

[2] Note that, for an arbitrary number of qubits, this basis forms a complete and orthonormal basis. This is related to Walsh-Hadamard matrices, but that goes beyond the scope of this exercise. I only mention it because it is just cool.

The exponentiation can then be realized via the **Lie Product formula**,

$$e^{A+B} = \lim_{n\to\infty} \left(e^{A/n} e^{B/n} \right)^n \, . \tag{9}$$

Using these two pieces of information, construct a quantum circuit schematically, using the components



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where H_x and H_p are defined in their own bases. The following questions will explicitly construct the circuit for H_x and H_p; QFT is built into Qiskit.

10. Convince yourself that all eight diagonal matrices, $\sigma_i \otimes \sigma_j \otimes \sigma_k$, with $i, j, k = 0, 3$ commute with each other. This implies that they can be independently exponentiated. Construct the quantum circuit for each $\sigma_i \otimes \sigma_j \otimes \sigma_k$ (again restricted to $i, j, k = 0, 3$). Limit yourself to the single qubit gate rotations $\{Rx, Ry, Rz\}$ and CNOT. Note that

$$Rz(\theta) = e^{-i\frac{\theta}{2}Z} \tag{11}$$

and that Qiskit has an implementation for Rx, Ry, Rz, so we are free to use them for circuit construction.

11. Combine the results above to create the circuit for H_x and H_p

12. We are going to simulate what happens when the system starts off in a state that is not an eigenstate. In particular, the state that we start off in is

$$|\psi\rangle = \frac{|0\rangle + |1\rangle}{2} \tag{12}$$

where here, the kets correspond to the eigenstate labels of the harmonic oscillator, not qubits in your system. What is the time-dependence of the probability density of this system if it starts off in this state?

13. Repeat this exercise on a quantum simulator, ie your laptop. You can write the initial state as a vector and H_x, H_p and QFT as a matrix. Matrix multiplication should be all that you need. Use the optimal value for $x_{\max}$ you found above.

14. Lastly, repeat this for a quantum computer. **Please note, this is actually quite a challenging question and my goal in asking it is not for you to actually find a solution, but for you to realize just how differently quantum computers work and how what might seem simple to do is actually quite challenging.**

    If you do want to attempt this, note that you are going to have to figure out how to initialize the quantum device with this initial state. This is somewhat non-trivial, but Qiskit documentation plus results from previous sections will be quite helpful. You are also going to have to figure out how to access the probability density on a quantum computer. This is actually quite non-trivial and one approach that i see involves a completely separate algorithm to try to access intermediate information needed for that calculation. There also may be another approach but I have not yet fully worked out the details. I would be happy to chat about this more if anyone is curious.

III. DENSITY MATRICES

Let us take a closer look at the Werner state and its density matrix. The purpose of doing so it to better understand pure versus mixed states, unentangled versus entangled states and separable versus not separable. As a reminder of definitions:

- **Pure:** ensemble contains only one state, ie

$$\rho = |\psi\rangle \langle\psi| \, . \tag{13}$$

It can be shown that the density matrices of pure states have $\rho = \rho.\rho$ and therefore

$$\mathrm{Tr}\rho = \mathrm{Tr}\rho.\rho = 1 \tag{14}$$

- **Mixed:** ensemble contains multiple states ie

$$\rho = \sum_i \rho_i \left|\psi_i\right\rangle \left\langle\psi_i\right| \ . \tag{15}$$

For these ensembles,

$$\mathrm{Tr}\rho = 1 \qquad \mathrm{Tr}\rho^2 < 1 \tag{16}$$

- **Entangled:** If the full system is the system AB, then the reduced density matrix for subsystem A and subsystem B,

$$\begin{aligned} \rho_A &= \mathrm{Tr}_B\rho \\ &= \sum_j \langle\psi_{jB}|\rho|\psi_{jB}\rangle \\ \rho_B &= \mathrm{Tr}_A\rho \\ &= \sum_j \langle\psi_{jA}|\rho|\psi_{jA}\rangle \end{aligned} \tag{17}$$

have the property that

$$\mathrm{Tr}\rho_A^2 < 1 \qquad \mathrm{Tr}\rho_B^2 < 1 \tag{18}$$

- **Unentangled:** The reduced density matrices have the property that

$$\mathrm{Tr}\rho_A^2 = \mathrm{Tr}\rho_B^2 = 1 \tag{19}$$

- **Separable:** If the state is a pure state, it can be written as

$$\left|\psi\right\rangle = \left|\phi\right\rangle_A \otimes \left|\phi\right\rangle_B \ . \tag{20}$$

If the state is a mixed state, it can be written as

$$\left|\psi\right\rangle = \sum_i \left|\phi_i\right\rangle_A \otimes \left|\phi_i\right\rangle_B \ . \tag{21}$$

- **Non-separable:** The state cannot be written as a tensor products

The Werner state is an ensemble in which there is a probability p that a given element in the ensemble is the Bell state

$$\left|\psi\right\rangle_{\mathrm{Bell}} = \frac{\left|00\right\rangle + \left|11\right\rangle}{\sqrt{2}} \tag{22}$$

and a probability $1 - p$ that a given element of the ensemble is a randomly aligned state.

1. Derive the density matrix ρ and prove that its trace is 1 and that it has positive eigenvalues.

2. Calculate $\mathrm{Tr}\rho^2$. Is there a range of p where the ensemble is a pure state? What about a mixed state?

3. Show that this density matrix can be written in terms of

$$\rho(\left|++\right\rangle_x), \rho(\left|--\right\rangle_x), \rho(\left|+-\right\rangle_y), \rho(\left|-+\right\rangle_y), \rho(\left|00\right\rangle), \rho(\left|01\right\rangle), \rho(\left|10\right\rangle), \rho(\left|11\right\rangle) \tag{23}$$

where

$$\rho(\left|\psi\right\rangle \equiv \left|\psi\right\rangle \left\langle\psi\right| \ . \tag{24}$$

Notice that all of these are tensor states and so if the density matrix of a Werner state can be written in terms of these tensor states, it is separable. Is this version of the density matrix always a valid density matrix? If not, what does this imply about the Werner state.

4. As an alternative to the brute force decomposition above, use the Peres–Horodecki criterion to determine whether the state is separable. For subsystems, each of dimension two, the condition is necessary and sufficient. The criterian states that if the density matrix ρ is seperable, the eigenvalues of the partial transpose density matrix are all non-negative. The partial transpose of the density matrix is defined to be

$$\rho^{T_B} = \sum_{ijkl} p_{lk}^{ij} |i\rangle \langle j| \otimes |k\rangle \langle l| \tag{25}$$

where the original density matrix was defined to be

$$\rho = \sum_{ijkl} p_{kl}^{ij} |i\rangle \langle j| \otimes |k\rangle \langle l| \tag{26}$$

For what range of p is this criterion satisfies? For which range is it not?

5. Summarize your results

IV. STABILIZER STATES

The definition of (linear) quantum magic is

$$\mathcal{M} \equiv 1 - 2^n \sum_P \chi_P^2 \qquad \chi_P \equiv \frac{c_P^2}{2^n} \qquad c_P = \mathrm{Tr}\left[\rho P\right] \tag{27}$$

where P is the tensor-product of the Pauli matrices (and the identity matrix) acting on all possible qubits.

A stabilizer state of n qubits is any state such that, out of the total of 4^n c_P coefficients, 2^n of them are ± 1 and the rest are zero.

1. Prove that

$$\sum_P \chi_P = 1 \tag{28}$$

2. Convince yourself that these states are stabilizer states:

$$|0\rangle\,, |1\rangle\,, \frac{|0\rangle \pm |1\rangle}{\sqrt{2}}\,, \frac{|0\rangle \pm i\,|1\rangle}{\sqrt{2}} \tag{29}$$

Are there any other stabilizer states for one qubit?

3. What is the lower bound on quantum magic for one qubit? What is the upper bound on quantum magic for one qubit? Repeat the exercise for two qubits (I highly recommend using Python or Mathematica to do the two qubit case)

V. NO CLONING THEOREM

The No-Cloning Theorem places fundamental restrictions on what one can and cannot do with states prepared on quantum devices. The goal of this problem is to answer the question whether it is possible to copy an arbitrary state.

The setup of the problem is a quantum machine with two slots, labeled A and B. The data slot A starts off in some arbitrary, but pure, state $|\psi\rangle$. This state is to be copied into the target slot B. Assume that the target slot starts off in some standard pure state $|s\rangle$.

1. What is the initial state of the copying machine, assuming Slot A and Slot B have no correlation between them.

2. Assume that some Unitary time evolution is able to copy the state from Slot A to Slot B. What is the final state of the copying machine?

3. Suppose that this copying procedure works for two particular pure states that slot A can generate, $|\psi\rangle$ and $|\phi\rangle$. If this copying procedure is possible, what does this imply about the states $|\psi\rangle$ and $|\phi\rangle$?

4. What does this result tell us about the ability to perfectly clone unknown quantum states using unitary evolutions. Are there any ways around this result that might still be useful for quantum computation?

VI. HOLEVO'S BOUND

Holevo's bound provides an incredibly useful upper bound on how much information is accessible when using quantum mechanics to store, transmit and access that information.

We will not prove the bound here, but merely quote it. The theorem goes as follows: Suppose that Alice prepares a state ρ_X where $X = 0, \ldots, n$ with probabilites $p_0, \ldots, p_X$. Bob performs measurements described by POVM[3] elements $\{E\}_y = \{E_0, \ldots E_m\}$ on that state, with measurement outcome Y. The Holevo bound is that for any such measurement Bob may do,

$$H(X:Y) \leq S(\rho) - \sum_x \rho_x S(\rho_x) \qquad \rho \equiv \sum_x p_x \rho_x \tag{30}$$

This problem will apply this bound to the question of how much information Alice can convey to Bob using a single qubit.

1. Alice prepares a single qubit in one of two quantum states. She decides which state, depending on a coin toss:

$$\begin{aligned} \text{Heads} &: |0\rangle \\ \text{Tails} &: \cos\theta\,|0\rangle + \sin\theta\,|1\rangle \end{aligned} \tag{31}$$

   What is the density matrix for this state?

2. What are the eigenvalues of this density operator?
3. What is the Holevo bound for this system, assuming θ is a free, real parameter.
4. What is the maximal amount of information that Alice can transmit to Bob. What is the minimum amount?
5. Use this bound to argue the maximum number of information that n_q qubits can transmit. Is this a surprising result?

VII. BIT FLIP CODE, PHASE FLIP CODE AND SHOR'S ALGORITHM

1. In lecture, we used CNOT gates to entangle the qubits with the ancilla. However, the stabilizer of the system are $Z_1 Z_2$ and $Z_1 Z_3$. Rewrite this circuit using only CZ gates (ie Control-Z gates). A useful operation is that a CNOT (also called a CX) gate is actually a projection gate,

$$\textbf{CNOT}: \frac{\mathbb{I} + \sigma_3}{2} \otimes \mathbb{I} + \frac{\mathbb{I} - \sigma_3}{2} \otimes \sigma_1 \tag{32}$$

2. Explicitly construct the circuit for error-correcting the phase-flip gate, including identifying the stabilizers for this system. For any two circuit gate, only use Control gates utilize the stabilizers (similar how above, the bit flip only uses CZ as its two-qubit gates). You will still need to use Toffoli gates in the recovery process.
3. For Shor's code, construct the eight stabilizer states. Can you argue that you should have expected eight of them? Can you now construct the circuit for the syndrome diagnosis? What about the recovery process?

[3] POVM are positive operator-valued measures. They are defined by having values that are positive semi-definite operators on a Hilbert space. POVMs are a generalization of projection-valued measures elements

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VIII. HINTS

- Problem One
  1. Recall the Bell State construction. While the CNOT gate is called an entangling gate, what is the role of the H gate in the circuit?
- Problem Two
  1. As written, is the position basis, $|x\rangle$ continuous or discrete? What is the size of the Hilbert space that a quantum computer with n_q qubits?
  2. Assume that your sampling of x is uniform and goes up to some eigenvalue $x_{\max}$.
  3. One possible choice is related to defining the momentum in terms of a finite-difference operator. Another choice is related to the undiscretized and undigitzed momentum operator. Recall also the commutation relation between $\hat{x}$ and $\hat{p}$ and what this implies about the relationship between the position and momentum basis.
  4. For the rest of this problem, it is hard to give hints (unfortunately). However, the solutions can be found in this paper: Digitization of Scalar Fields for Quantum Computing
- Problem Three
  1. For randomly aligned state, assume that the measurement always occurs in the $\hat{z}$ basis and so the experiment can only measure $|0\rangle, |1\rangle$.
- Problem Four
  1. We are only considering pure states when calculating quantum magic (at least here), so $\rho = \rho^2$.
- Problem Five
  1. Comparing various inner products will provide a fruitful path forward
- Problem Six
  1. How do the eigenvalues of the density matrix relate to the von Neumann entropy?
- Problem Seven
  1. Using the stabilizer formalism, the state of the total system is

$$|\psi\rangle_L |0\rangle_A \tag{33}$$

where $|\psi\rangle$ is the state that is to be encoded into the logical qubit and assuming that the ancilla qubit starts in the zero state. If a single qubit noise channel acts on this state, the total state of the system is

$$E|\psi\rangle_L |0\rangle_A \tag{34}$$

The question is how to design a unitary such that

$$E|\psi\rangle_L |0\rangle_A \to P_+ E|\psi\rangle_L |0\rangle_A + P_- E|\psi\rangle_L |0\rangle_A \tag{35}$$

where $P_\pm$ are projectors of some sort. The question is how that unitary is (and what those projectors are) based on the stabilizer states of the system.