- Each student should provide and come up with their solutions independently.
- You are allowed to use any literature/source you want, but don't forget to add references when required.
- There are 5 problems in total.

Problem 1. (Mathematical background).

Consider the following Hermitian matrix

$$H = \begin{pmatrix} -\frac{1}{2} & 1\\ 1 & -\frac{1}{2} \end{pmatrix}.$$

Note that $|+\rangle$ and $|-\rangle$ are the eigenvectors of H.

- (a) Write down the spectral decomposition of H.
- (b) What are the eigenvalues of the unitary $U = e^{2\pi i H} = \sum_{k=0}^{\infty} \frac{(2\pi i H)^k}{k!}$?

Remark.

- Use the knowledge that the eigenvectors of H are also the eigenvectors of U.
- You may use that for any vector $|v\rangle \in \mathbb{C}^2$ the following holds:

$$\left(\sum_{k=0}^{\infty} \frac{\left(2\pi i H\right)^k}{k!}\right) \cdot \left|v\right\rangle = \sum_{k=0}^{\infty} \frac{\left(2\pi i H\right)^k \left|v\right\rangle}{k!}.$$

- You do not have to derive eigenvalues using the characteristic polynomial, just give them and show why they are correct.
- (c) Compute the matrix of U using its spectral decomposition.
- (d) Show that U is unitary.

Problem 2. (Circuit logic 1 [Controlled application of labeled gates]).

Consider a collection of *n*-qubit unitaries $\{V_1, \ldots, V_k\}$ and let $m = \log_2(k)$ (you may assume k is a power of two). Suppose you are given access to the controlled- V_i gates, i.e., for $j \in \{0, 1\}$ and $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$ mapping

(controlled-
$$V_i$$
) $|j\rangle |\psi\rangle = \begin{cases} |j\rangle V_i |\psi\rangle & \text{if } j = 1, \\ |j\rangle |\psi\rangle & \text{otherwise.} \end{cases}$

(a) Show that having access to (any of the) controlled- V_i gates suffices to construct m-qubit controlled- V_i gates, i.e., for $\vec{j} \in \{0,1\}^m$ and $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$ mapping

(m-controlled-
$$V_i$$
) $|\vec{j}\rangle |\psi\rangle = \begin{cases} |\vec{j}\rangle V_i |\psi\rangle & \text{if } \vec{j} = 1^m = 11...1, \\ |\vec{j}\rangle |\psi\rangle & \text{otherwise.} \end{cases}$

Note, you may need to use ancillas for this, and don't forget to "collect your garbage". Of course you are allowed to use other V_i -independent gates (controlled and otherwise).

(b) Let $\vec{j}^* \in \{0, 1\}^m$ be some fixed (known) *m*-bit string. Give a circuit that implements the following unitary transformation, for a given *i*:

$$|\vec{j}\rangle |\psi\rangle \mapsto \begin{cases} |\vec{j}\rangle V_i |\psi\rangle & \text{if } \vec{j} = \vec{j}^*, \\ |\vec{j}\rangle |\psi\rangle & \text{otherwise.} \end{cases} \quad \forall \vec{j} \in \{0,1\}^m \text{ and } \forall |\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$$

(c) Give a circuit that implements the following unitary transformation:

$$|\vec{j}\rangle |\psi\rangle \mapsto |\vec{j}\rangle V_j |\psi\rangle, \forall \vec{j} \in \{0,1\}^m \text{ and } \forall |\psi\rangle \in (\mathbb{C}^2)^{\otimes n}.$$

Remark. You may use the circuits of questions (a) as a (primitive) gate in the new circuits. Note the final circuit in question (a) activates the gate V_i if and only only if the controlling bitstring is "all ones". The final circuit in question (b) activates the gate V_i if and only only if the controlling bitstring is \vec{j}^* . The circuit in question (c) activates V_j if the control wires are in the state $|\vec{j}\rangle$, where \vec{j} is the binary representation of j. Note the last circuit can activate all the gates V_i .

Problem 3. (Circuit logic 2 [3SAT formula evaluation]).

Consider an *n*-variable 3SAT formula $C(x_1, \ldots, x_n) = \bigwedge_{i=1}^k C_i(x_1, \ldots, x_n)$, where each clause C_i is a disjunction of 3 variables. For example, $C_i(x) = (x_{i_1} \vee \neg x_{i_2} \vee x_{i_3})$, where the symbol \neg denotes the *negation*, i.e., $\neg 1 = 0$ and $\neg 0 = 1$.

(a) Give a circuit that implements the following unitary transformation:

$$|x_1, x_2, x_3\rangle |b\rangle \mapsto |x_1, x_2, x_3\rangle |b \oplus (x_1 \lor x_2 \lor x_3)\rangle, \forall x_1, x_2, x_3, b \in \{0, 1\}.$$

Remark.

- Throughout this problem you are allowed to use arbitrary multi-controlled NOT gates.
- It might be useful to recall De Morgan's laws for boolean logic.

(b) Using the circuit from question (a) it is easy to construct a circuit that implements the following unitary transformation:

 $U_{C_i}: |x_1, \dots, x_n\rangle |b\rangle \mapsto |x_1, \dots, x_n\rangle |b \oplus C_i(x_1, \dots, x_n)\rangle, \, \forall x_i, b \in \{0, 1\}.$ (1)

for say $C_i(x) = (x_1 \vee \neg x_2 \vee x_4)$. Provide this construction.

Remark. Note there are more wires in the input than variables in the clause. Take care how to incorporate negated literals, and do not forget to "clean up" after your gates (the first register containing all the variables is not perturbed in the end).

(c) Finally we evaluate the entire formula, where all the clauses must be satisfied: give a circuit that implements the following unitary transformation:

$$|x_1,\ldots,x_n\rangle |0^k\rangle |b\rangle \mapsto |x_1,\ldots,x_n\rangle |0^k\rangle |b \oplus C(x_1,\ldots,x_n)\rangle, \forall x_i, b \in \{0,1\}.$$

Remark.

- You are allowed to use the U_{Ci} gates as defined in Equation 1 as "primitive gates" for question (c).
- **Bonus:** implement the required unitary using only $\mathcal{O}(\log(k))$ ancillary qubits instead of k. For this you are allowed to use a (controlled) version of the *l*-qubit "incrementer" unitary: $U_{inc}|k\rangle = |k+1 \mod 2^l\rangle$.

Problem 4. (*Circuit logic 3 [Controlled rotation]*).

Let $\tilde{\theta} \in \{0, 1\}^d$ represent a *d*-bit number in [0, 1), that is, $\tilde{\theta} = \sum_{i=1}^d \tilde{\theta}_i 2^{-i}$. Consider the *controlled-rotation* unitary U_{θ} that acts as

$$U_{\theta} : |\tilde{\theta}\rangle |0\rangle \mapsto |\tilde{\theta}\rangle \left(\cos(2\pi\tilde{\theta}) |0\rangle + \sin(2\pi\tilde{\theta}) |1\rangle\right).$$
(2)

In this problem you will construct a circuit that implements the unitary U_{θ} using controlled- U_i gates, where U_i is defined as

$$U_i = \begin{pmatrix} \cos(2\pi \cdot 2^{-i}) & -\sin(2\pi \cdot 2^{-i}) \\ \sin(2\pi \cdot 2^{-i}) & \cos(2\pi \cdot 2^{-i}) \end{pmatrix}, \text{ for } i = 1, \dots, d.$$

(a) Consider the following circuit:



Compute the output state of the circuit (the state $|\varphi_a\rangle$ suffices).

(b) Consider the following circuit:



Compute the output state of the circuit, (the state $|\varphi_b\rangle$ suffices).

(c) Give a circuit that implements the unitary U_{θ} , as defined in Equation 2.

Remark. You may assume you are given access to controlled- U_i gates.

Problem 5. (Quantum algorithms [Preparing ground states of Hamiltonians]). Let $H \in \mathbb{C}^{N \times N}$ be a Hermitian matrix with eigenvalues $0 = \lambda_0 < \lambda_1 < \cdots < \lambda_{N-1} < 1$ and corresponding (normalized) eigenvectors $|\psi_0\rangle, \ldots, |\psi_{N-1}\rangle$.

In this problem we will prepare the so-called ground state of H, i.e., the state $|\psi_0\rangle$, using Hamiltonian simulation and quantum phase estimation. Preparing ground states of Hamiltonians is a central problem in quantum simulation and quantum chemistry.

Remark. Throughout this problem you may use that the eigenvectors of H, i.e., the vectors $|\psi_1\rangle, \ldots, |\psi_{N-1}\rangle$, are also the eigenvectors of the unitary $U = e^{2\pi i H}$.

(a) What is the relationship between the eigenphases $e^{2\pi i\phi_j}$ (with $0 \le \phi_j < 1$) of the unitary $U = e^{2\pi i H}$ and the eigenvalues λ_j of the Hermitian matrix H?

Remark. You may use results from the tutorials here (you don't have to prove anything).

Suppose we can efficiently implement the unitary $U = e^{2\pi i H}$ using Hamiltonian simulation. Using this, consider the following circuit:



Suppose the measurement of the eigenvalue register after the quantum phase estimation yields $\overline{\lambda_j}$, that is, the best *t*-bit approximation (actually, the best *t*-bit approximation that is smaller than the actual angle) of the eigenvalue λ_j (as depicted in the above circuit), then the postulates of quantum mechanics tell us that the eigenvector register must be in the corresponding eigenstate $|\psi_j\rangle$ after this measurement. Note QPE does not actually achieve exactly this (for t bit precision, something like t+2 are required, see remark), but it illustrates our point.

- (b) Argue why at least $t = \log_2(1/\lambda_1)$ bits are required to guarantee that the eigenvector register is in the state $|\psi_0\rangle$ when the measurement outcome is $\overline{\lambda_j} = 0^t$.
- (c) Suppose $|\varphi\rangle = \sum_{j=0}^{N-1} \alpha_j |\psi_j\rangle$. What is the probability that the above circuit produces the state $|\psi_0\rangle$ in the eigenvector register when $t \ge \log_2(1/\lambda_1)$?

Remark. In reality, QPE on its own is not guaranteed to output the best t-bit approximation of the eigenvalue as in general the output is probabilistic. One can achieve arbitrarily high probability $> 1 - \epsilon$ of outputting the best approximation that is smaller than the angle by using $t + \lceil \log(2 + 1/(2\epsilon)) \rceil$ ancillary qubits in QPE. See N&C, p.g. 223 for more on this. For simplicity, we assume this output is actually guaranteed. In the problems above, it will be convenient to consider the scenarios where all the eigenvalues can be exactly represented using binary fractions.