

Preparing Eigenstate of a Hamiltonian

Problem :

Suppose we have a Hamiltonian 'H' fulfilling the following properties:

1. H has a dimension $2n - 1$ and $\|H\| = 1$
2. All it's eigenvalues are symmetric around 0 i.e., $\lambda_i = -\lambda_{2n-i}$ for $i \in \{1, 2, \dots, 2n - 1\}$, implying $\lambda_n = 0$.

Let, $|v_j\rangle$ be the eigenstates of the Hamiltonian H with eigenvalues λ_j . The 0-eigenvalue λ_n is separated from the rest by a gap Δ .

Starting from some initial state $|\psi_0\rangle = \sum_{l=1}^{2n-1} c_l |v_l\rangle$, prepare a state $|G\rangle$ such that $\| |G\rangle - |v_n\rangle \| \leq \varepsilon$.

Solution using QSP:

Suppose we have a $(\alpha, m, 0)$ block encoding U_H of the Hamiltonian H. Let P_{λ_n} be the projector into the λ_n -eigenspace of H, i.e. the null-space.

Now, we have to concoct such a projector. For this, suppose we have a polynomial P such that $P(0) = 1$ and $|P(x)| = 0$ for $x \in D_{\Delta/2\alpha}$, where $D_{1/\kappa} = [-1, -1/\kappa] \cup [1/\kappa, 1]$. Then

$$P((H - \lambda_n I)/2\alpha) \approx P_{\lambda_n}. \quad (1)$$

Now, for this problem we will use the following 2ℓ degree polynomial.

$$\mathbf{R}_\ell(x; \Delta) = \frac{\mathbf{T}_\ell\left(-1 + 2\frac{x^2 - \Delta^2}{1 - \Delta^2}\right)}{\mathbf{T}_\ell\left(-1 + 2\frac{-\Delta^2}{1 - \Delta^2}\right)} \quad (2)$$

Now, R is an even polynomial. Now we can apply the polynomial to $H - \lambda_n I$ using the techniques of Quantum Signal Processing and get rid of the unwanted components. Let's define

$$\tilde{H} = \frac{H - \lambda_n I}{\alpha + |\lambda_n|} \quad (3)$$

For our problem, $\lambda_n = 0$, so the operator becomes

$$\tilde{H} = \frac{H}{\alpha} \quad (4)$$

and we also define

$$\tilde{\Delta} = \frac{\Delta}{2\alpha} \quad (5)$$

Now, as we know

$$|R_\ell(x; \Delta)| \leq 2e^{-\sqrt{2}\ell\Delta} \quad (6)$$

for $x \in D_\Delta$.

Therefore, we have

$$\|R(\tilde{H}; \tilde{\Delta}) - P_{\lambda_n}\| \leq 2e^{-\sqrt{2}\ell\tilde{\Delta}} \quad (7)$$

Now we can create $(\alpha, m+1, \varepsilon)$ block encoding of $R(\tilde{H}; \tilde{\Delta})$ and let it be $U_{\tilde{H}}$. Now we can apply this block encoding to the given state $|\psi_0\rangle$ and the probability of getting all 0's while measuring the ancilla qubits is atleast c_n^2 . So we need to run the block encoding $O(1/c_n^2)$ times and can cut it down to $O(1/c_n)$ using amplitude amplification for the desired eigenstate, in our case $|v_n\rangle$.

Cost and Complexity Analysis of the Solution using QSP :

Number of qubits : If the Hamiltonian H works on n qubits and has a $(\alpha, m, 0)$ block encoding, then using the minmax polynomial of equation 2, we need only 1 more ancilla qubit for the Quantum Signal Processing method. So, the total number of qubits needed is $n + m + 1$. If we use amplitude amplification we will need one extra ancilla qubit pushing the qubit count to

$n + m + 2$.

Complexity of the algorithm : Suppose, the cost of implementing the unitary $U_{\tilde{H}}$ once is T . Assuming that we are using amplitude amplification, we need to run the block encoding $O(1/c_n)$ times. So, the cost is $O(T/c_n)$.

Now, if U_H is the $(\alpha, m, 0)$ block encoding of H , then we can obtain a $(1, m + 1, \epsilon)$ block encoding of $U_{\tilde{H}}$ using $O((\alpha/\Delta) \log(1/\epsilon))$ applications of controlled- U_H and it's conjugate and $O((m\alpha/\Delta) \log(1/\epsilon))$ other primitive gates.

Therefore, neglecting the cost of using other primitive gates, the overall complexity of filtering the desired state, given the block encoding U_H is $O((T\alpha/c_n\Delta) \log(1/\epsilon))$.

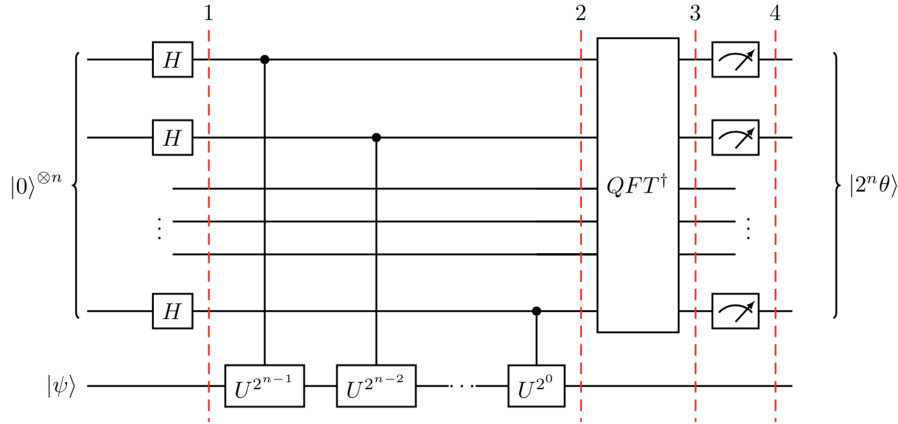
Solution using QPE:

We are given the state $|\psi_0\rangle$ that is a superposition in the eigenbasis of the Hamiltonian H . Now, suppose we have access to the controlled unitary U and

$$U = e^{-iH} \quad (8)$$

Now, if we want to find the eigenstate of H having eigenvalue 0 we need to look for the eigenstate of U , that has an eigenvalue of 1. So, we need to do Quantum Phase Estimation using U and look for the eigenvalue 1.

Below we have the circuit for Quantum Phase Estimation :



Now, as we don't have any particular eigenstate we will use the given superposition of eigenstates $|\psi_0\rangle$ as the target state and apply the operators U . As

$$|\psi_0\rangle = \sum_{l=1}^{2n-1} c_l |v_l\rangle \quad (9)$$

Therefore, after applying the QPE circuit, with a rough probability of $O(1/c_n^2)$, we will obtain an eigenstate close to 1, if all other parameters are properly taken into account. So, if we measure for the eigenvalue 1 in the control register, we will get the corresponding eigenstate $|v_n\rangle$ in the target register, which is our desired eigenstate.

Cost and Complexity Analysis of the Solution using QPE :

Number of qubits : For simplicity, let's assume we are given an eigenstate $|\psi\rangle$ of the operator U and it's corresponding eigenvalue is ω . Suppose after applying the QPE sub-routine we obtain an estimate $\tilde{\omega}$ of the eigenvalue ω . Assume we obtain $\tilde{\omega}$ with a probability at least $1 - \frac{1}{2^m}$ where the error term is $\frac{1}{2^m}$ and also $|\tilde{\omega} - \omega| \leq \frac{1}{2^r}$, i.e. the spectral gap measurable is bounded by $\frac{1}{2^r}$.

To meet the above conditions, it suffices to use a total of $m + r + 1$ control-qubits.

Now for our problem, we need to filter out the state $|v_n\rangle$ with an error upper-bounded by ϵ and spectral gap lower-bounded by Δ . Therefore, the number of control-qubits need is $t = \log(1/\Delta\epsilon) + 1$.

Therefore, assuming that U acts on n qubits, the total number of qubits need is $\log(1/\Delta\epsilon) + n + 1$.

Complexity of the algorithm : Let's assume, we can apply each unitary U in time $T(U)$. As we have t number of control-qubits, we need to apply U , $O(2^t)$ times. So, the complexity of applying the U 's is

$$O(2^t T(U)) = O(\widehat{T}) \quad (10)$$

Now, as we obtain our desired state with a probability $O(1/c_n^2)$, we need to run the QSP sub-routine $O(1/c_n^2)$ times to obtain our desired eigenstate

with a constant probability.

Therefore, the overall complexity of this algorithm to filter the desired state of the Hamiltonian H , neglecting the cost of applying the Hadamard and QFT gates, is $O\left(\hat{T}/c_n^2\right)$.