

# Phase estimation implementation

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## I. SCALING THE HAMILTONIAN FOR QUANTUM PHASE ESTIMATION

Consider an eigensystem

$$H|u_j\rangle = u_j|u_j\rangle \quad (1)$$

We choose  $\tau > 0$  so that upon rescaling  $H' = -\tau H$ , the unitary describing evolution is

$$U = e^{-iH'} = e^{i\tau H}. \quad (2)$$

Then the phase imparted is determined by

$$U|u_j\rangle = e^{i2\pi\phi_j}|u_j\rangle, \quad \text{with } \phi_j = \tau \frac{u_j}{2\pi}. \quad (3)$$

Recall that  $e^{i2\pi(\phi_j+m)}$  has the same value for all integers  $m$ . The phase approximation algorithm provides an estimate  $\tilde{\phi}$  of  $\phi_j \bmod 1$ . We would like to choose  $\tau$  such that the phase satisfies  $0 \leq \phi_j < 1$ , which then guarantees a one-to-one correspondence between  $u_j$  and  $\phi_j$ .

### A. A single eigenstate and positive spectrum

Suppose the spectrum is positive

$$u_j \geq 0, \quad \text{for all } j. \quad (4)$$

The algorithm ideally measures the phase as  $\tilde{\phi} = \phi_j \bmod 1$ . So, we choose a bound  $u_b > u_{\max}$  where  $u_{\max} = \max_j u_j$  so that  $\tau = 2\pi/u_b$ , and  $\phi_j = u_j/u_b$  satisfies  $0 \leq \phi_j < 1$ . Then there is a one-to-one correspondence between values of  $\phi$  and  $u_j$ .

In summary, we supply to the algorithm an eigenstate  $|u_j\rangle$  and a unitary constructed<sup>1</sup> from

$$-\tau H = -\frac{2\pi}{u_b} H. \quad (5)$$

We read the output  $\tilde{\phi}$  and obtain our estimate of  $u_j$  as

$$\tilde{u}_j = u_b \tilde{\phi}. \quad (6)$$

In fact, the phase is read from a register with a finite number  $n$  of bits and so takes discrete values

$$\tilde{\phi} \in \{0, \epsilon, 2\epsilon, 3\epsilon, \dots, 1 - \epsilon\}, \quad \text{where } \epsilon = 2^{-n}. \quad (7)$$

The estimate  $\tilde{u}_j$  takes values

$$\tilde{u}_j \in \{0, \epsilon_u, 2\epsilon_u, 3\epsilon_u, \dots, u_b - \epsilon_u\}, \quad \text{where } \epsilon_u = u_b 2^{-n}. \quad (8)$$

In particular, if we choose  $u_b = u_{\max}$ , then  $u_{\max}$  is mapped to zero. This is why we required  $u_b > u_{\max}$  rather than  $u_b \geq u_{\max}$ .

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<sup>1</sup> On quantum hardware, we might construct  $-H$  and evolve for time  $\tau = 2\pi/u_b$ .

### 1. Example: Exact representation of minimum eigenvalue

When testing implementations, one may encounter problems such as the following. Still assuming  $u_j > 0$  for all  $j$ , we look for a scaling that allows at the same time

1. an exact representation of  $u_{\min}$  in the  $n$  bits of the phase register.
2.  $u_b > u_{\max}$ .

The second condition is required if we expect that a component  $|u_{\max}\rangle$  will be present in the input state. Referring to (8) we see that for the first condition we must have  $u_{\min} = m\epsilon_u$  or

$$u_b = \frac{2^n}{m} u_{\min}, \quad \text{for some } m \in 1, 2, \dots, n-1. \quad (9)$$

Note that we do not include  $m = 0$  as a possibility. We only scale the phase interval, but do not shift it. In particular, the phase  $\phi = 0$  corresponds only to  $u = 0$  (unless  $u_{\max} > u_b$ , which we want to avoid.) The second condition,  $u_b > u_{\max}$  may be written

$$u_{\max} < \frac{2^n}{m} u_{\min} \quad (10)$$

Clearly if (10) is satisfied for any  $m > 1$ , then it is satisfied for  $m = 1$ . That is  $m = 1$  gives the largest  $u_b$ . Thus, setting  $m = 1$ , we find the condition for the number of qubits in the phase register  $n$ .

$$n > \log_2 \left( \frac{u_{\max}}{u_{\min}} \right) \quad (11)$$

This is the number of qubits necessary to satisfy both conditions 1 and 2 above. On the other hand, to get the best resolution, we want to choose  $m$  as large as possible. From (10) we find that for fixed  $n$ , we can choose the largest  $m$  satisfying

$$m < 2^n \frac{u_{\max}}{u_{\min}}, \quad (12)$$

Explicitly,

$$m = \left\lfloor 2^n \frac{u_{\max}}{u_{\min}} \right\rfloor, \quad (13)$$

### B. Single eigenstate and positive and negative eigenvalues

Here we present a straightforward scaling that makes good use of the resolution in case the spectrum has both positive and negative values of the same magnitude. We map the positive eigenvalues to  $(0, \pi)$  and the negative eigenvalues to  $(-\pi, 0)$ . We choose  $u_b$  satisfying

$$u_b > \max \{|u_{\min}|, |u_{\max}|\}. \quad (14)$$

For a positive spectrum we chose  $\tau = 2\pi/u_b$ . Here, we choose  $\tau = \pi/u_b$ , so that  $\phi_j = u_j/(2u_b)$  satisfies

$$-\frac{1}{2} \leq \phi_j < \frac{1}{2}. \quad (15)$$

We obtain the unwrapped observed phase  $\tilde{\phi}'$  satisfying  $-(1/2) \leq \tilde{\phi}' < (1/2)$  via

$$\tilde{\phi}' = \begin{cases} \tilde{\phi} & \text{if } \tilde{\phi} < \frac{1}{2} \\ 1 - \tilde{\phi} & \text{if } \tilde{\phi} \geq \frac{1}{2} \end{cases}. \quad (16)$$

The sorted possible values of  $\tilde{\phi}'$  are given by

$$\tilde{\phi}' \in \left\{ -\frac{1}{2}, -\frac{1}{2} + \epsilon, -\frac{1}{2} + 2\epsilon, \dots, \frac{1}{2} - \epsilon \right\}, \quad \text{where } \epsilon = 2^{-n}. \quad (17)$$

The estimated eigenvalue, obtained via  $\tilde{u} = 2u_b\tilde{\phi}'$ , has value given by

$$\tilde{u} \in \{-u_b, -u_b + \epsilon_u, \dots, u_b - \epsilon_u\}, \quad \text{where } \epsilon_u = u_b 2^{-n+1}. \quad (18)$$

## II. FAST SIMULATION OF THE PHASE REGISTER PROBABILITIES

Here, we present a method to compute numerically the probabilities of the states of phase-estimation register in parallel QPE. The method is very straightforward. We simply compute intermediate steps classically rather than with quantum circuits. Recall that QPE works with a composite system with Hilbert space  $V_p \otimes V_U$  where  $V_p$  corresponds to an  $n$ -qubit phase-estimation register and  $V_U$  is the space of the eigenphase problem. Suppose for the moment that the input state  $|u\rangle \in V_U$  is an eigenvalue of  $U$ , that is  $U|u\rangle = e^{2\pi i \phi_u}|u\rangle$ . For our purposes, we break QPE into three steps.

1. Preparation of a state

$$\frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{2\pi i j \phi_u} |j\rangle |u\rangle, \quad (19)$$

where  $N = 2^n$  and the states  $|j\rangle$  are the computational basis vectors of the phase register.

2. Application of the inverse (quantum) Fourier transform of the prepared state, with the result

$$|\tilde{\phi}_u\rangle |u\rangle. \quad (20)$$

If  $\phi_u$  can be represented exactly in  $n$ -qubits, then  $\phi_u = k/N$  for some integer  $k$ . In this case we are performing the inverse Fourier transform of a Fourier transform with a single frequency component, given by  $k$ . In this case, the phase estimation register will be in the computational basis state  $|k\rangle$ .

3. Measurement of the state  $|\tilde{\phi}_u\rangle$  in the computational basis to obtain an estimate of  $\phi_u$

Our procedure for computing the amplitudes of  $|\tilde{\phi}_u\rangle$  takes as input the phase  $\phi_u$ , and the number of qubits  $n$ . In particular, we make no use of  $|u\rangle$  and  $U$ . We first prepare complex floating point vector  $x_0, \dots, x_{N-1}$  with values

$$x_j = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{2\pi i j \phi_u}. \quad (21)$$

We then compute the inverse Fourier transform, via the FFT, of the vector  $x_0, \dots, x_{N-1}$ . The result is a numerical approximation of amplitudes of  $|\tilde{\phi}_u\rangle$  in the computational basis, that is  $\langle j | \tilde{\phi}_u \rangle$  for  $j = 0, \dots, N-1$ . These are amplitudes of the phases in (7)

Suppose that instead of an eigenstate  $|u\rangle$  we have as input a generic pure state  $\sum_u c_u |u\rangle$ , where the sum runs over eigenvectors of  $U$ . In this case, the QPE algorithm leaves the phase register in the state

$$\sum_u c_u |\tilde{\phi}_u\rangle |u\rangle. \quad (22)$$

The state of the phase register alone is described by the reduced density matrix

$$\rho_{\text{phase}} = \sum_u |c_u|^2 |\tilde{\phi}_u\rangle \langle \tilde{\phi}_u|. \quad (23)$$

The probability of reading the computational basis state  $|j\rangle$  is then

$$p(j) = \text{tr}(|j\rangle \langle j| \rho_{\text{phase}}) = \sum_u |c_u|^2 |\langle j | \tilde{\phi}_u \rangle|^2. \quad (24)$$

Consider taking as input the number of qubits in the phase register  $n$  and pairs  $(\phi_u, c_u)$  representing the input state. We can compute  $p(j)$  numerically as follows. Initialize  $p(j)$  to zero for all  $j$ . Loop over  $u$ . For each iteration with fixed  $u$ , compute the vector of  $\langle j | \tilde{\phi}_u \rangle$  for  $j = 0, \dots, N-1$  as described above. For each  $j$  accumulate  $|c_u|^2 |\langle j | \tilde{\phi}_u \rangle|^2$  into  $p(j)$ . Continue to the next  $u$  until finished.