Quantum phase estimation is a good example of phase kickback and of the use of the quantum fourier transform. Suppose we have a unitary operator U with an eigenvector $|u\rangle$ and corresponding eigenvalue $e^{i\phi}$, where $0 \leq \phi < 2\pi$. We want to find the eigenvalue, which means finding phase ϕ, and we want to find this to a given level of precision. In particular, we want to find the best n-bit estimate of ϕ.

We can do this with a quantum circuit using

1. H gate,
2. controlled unitaries of the form c-U^{2^j}
3. an inverse QFT

We need two registers as input. The first register contains n qubits and will contain the n-bit estimate of ϕ on output. The second register describes the state $|u\rangle$ and so must contain some m qubits, but this value is irrelevant for our purposes as long as it is large enough to give ϕ to at least the required accuracy. Note that $U^{2^j}|u\rangle = e^{i2^j\phi}|u\rangle = \left(e^{i\phi}\right)^{2^j}|u\rangle$.

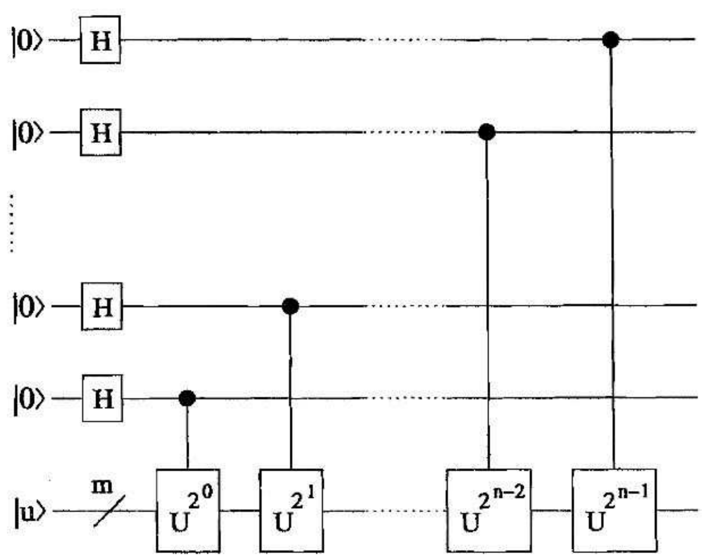

Figure 1: Quantum circuit for first part of phase estimation algorithm (steps i) and ii)). Following this circuit by an inverse QFT circuit will produce the best $n-$bit estimate of the phase ϕ.

Figure 1 shows steps i) and ii) of the quantum circuit. Step i) consists of making the uniform superposition state. Step ii) is the sequential action of the controlled unitary gates c-U^{2^j} on the second register, with each of the qubits in the first register acting as control qubit in turn. The action of any one of these gates on a state $\frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)|u\rangle$ is

$$\begin{aligned}\frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)|u\rangle &\overset{c-U^{2^j}}{\rightarrow} \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)U^{2^j}|u\rangle \\ &= \frac{1}{\sqrt{2}}\left(|0\rangle|u\rangle + |1\rangle e^{i2^j\phi}|u\rangle\right) \\ &= \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i2^j\phi}|1\rangle\right)|u\rangle\end{aligned}$$

where we have used the 2^j th repeated action of c-U.

Applying these gates with j increasing from 0 (with qubit n of register 1 as control) to $n-1$ (with qubit 1 of register 1 as control) as shown in Figure 1 yields the state

$$\frac{1}{\sqrt{2^n}}\left(|0\rangle + e^{i2^{n-1}\phi}|1\rangle\right)\ldots\left(|0\rangle + e^{i2\phi}|1\rangle\right)\left(|0\rangle + e^{i\phi}|1\rangle\right)|u\rangle$$
$$= \frac{1}{\sqrt{2^n}}\sum_{y=0}^{2^n-1} e^{i\phi y}|y\rangle|u\rangle.$$

We see that the phase factors $e^{i\phi y}$ have been propagated back from the second, eigenstate register, to the first, control register. This is another example of phase kick-back.

Recalling that the Quantum Fourier Transform of an n-qubit state $|a\rangle$ is

$$\mathrm{QFT}|a\rangle = \frac{1}{\sqrt{2^n}}\sum_{k=0}^{2^n-1} e^{i(2\pi a/2^k)k}|k\rangle,$$

we then write

$$\phi = 2\pi\left(\frac{a}{2^n} + \delta\right)$$

where $a = a_{n-1}a_{n-2}\ldots a_0$ in binary notation. Then $2\pi a/2^n$ is the best n-bit binary approximation of ϕ and the value of $0 \le |\delta| \le 1/2^{n+1}$ is the associated error.

Performing an inverse Quantum Fourier Transform on the control register will now bring the n-qubit estimate of the phase ϕ down into the qubit states where it can then be measured. The inverse transform is realised by running the QFT circuit from last lecture backwards, i.e., replacing each gate with its inverse ($R_k \to R_k^{-1}$) and run the circuit in reverse order:

$$\mathrm{QFT}^{-1}|y\rangle = \frac{1}{\sqrt{2^n}}\sum_{x=0}^{2^n-1} e^{-2\pi ixy/2^n}|x\rangle.$$

Writing ϕ in terms of a and then applying QFT^{-1} to the sum over states reached after steps i) and ii) yields

$$\frac{1}{2^n}\sum_{x=0}^{2^n-1}\sum_{y=0}^{2^n-1} e^{2\pi i(a-x)y/2^n} e^{2\pi i\delta y}|x\rangle|u\rangle.$$

Note that we have applied QFT^{-1} only to the control register. In fact everything from now on is happening only to the control register. We are keeping the eigenstate register in the equations for correctness, to remind you that it is still there.

Now we perform a measurement of the qubits in the first register, in the computational basis. There are two possible types of outcomes:

1. If $\delta = 0$, then the wave function of the first register reduces to the single term $x = a$. This can be seen by noting that when $x = a$ the phase term is unity for all y and hence the sum over y gives $\frac{1}{2^n}\sum_y 1|a\rangle = |a\rangle$, i.e., the term $x = a$ exhausts the unitarity of the sum. So all other terms must cancel by destructive interference. In this case, measuring the first register gives all n bits of a with certainty and the phase ϕ is exactly determined as $\phi = 2\pi a/2^n$.

2. If $\delta \neq 0$, the result of measuring the first register and getting the state $|x\rangle = |a\rangle$ is the best n-bit estimate of ϕ and is obtained with probability $p_a = |c_a|^2$, where

$$c_a = \frac{1}{2^n}\sum_{y=0}^{2^n-1}\left(e^{2\pi i\delta}\right)^y.$$

   This is a geometric series in δ, which can be summed and bounded by means of some trigonometric manipulations (Benenti, p. 157), to show that

$$|c_a|^2 \geq \frac{4}{\pi^2} \simeq 0.405.$$

   So the best n-bit estimate of the phase ϕ is obtained with a high probability. Note that the probabilistic nature of the measurement means that we need to repeat the calculation multiple times.

Increasing the number of qubits n will improve the precision of the phase estimation. What is not so obvious but is also true, is that increasing n will also increase the probability of success (Cleve et al., Proc. Roy. Soc. Lond. A 454, p.339 (1998).) Sub

If it can be guaranteed that the unitary operator U can be efficiently decomposed into elementary gates (i.e., this decomposition scales polynomially with the number of qubits m needed for $|u\rangle$), then this algorithm will perform exponentially faster than any known classical algorithm solving the phase estimation problem since a classical algorithm will require at least 2^m operations (note that $|u\rangle$ is a superposition over 2^m states).

However, the scaling with bits of precision required, n, is not so good. While for some U one can perform U^{2^j} in $O(j)$ steps, in general, simulating U^{2^j} requires $O(2^j)$ gates, so that the cost of the algorithm grows exponentially with the number of bits of precision n desired for the phase. See the third paper listed above, Brown et al., Phys. Rev. Lett. **97**, 050504 (2006).

1 Finding eigenvalues

The phase estimation method may be immediately applied to the problem of finding eigenvalues of a quantum Hamiltonian. Here

$$U(t) = e^{-iHt/\hbar}$$

with eigenvalues $e^{-iE_j/\hbar t}$, where $H|\phi_j\rangle = E_j|\phi_j\rangle$. We define $\omega_j = E_j/\hbar$.

Assume that we can efficiently generate some guess for an eigenstate

$$|\psi_0\rangle = \sum_j^{2^j-1} a_j|j\rangle.$$

Now all we need is some efficient way to realize the time evolution operator, i.e., gates $U(t)$. This can be done in a variety of ways provided that the time t is short, i.e., we really have $U(t_2 - t_2) = U(\Delta t)$. The guess $|\psi_0\rangle$ for the eigenstate is stored in the second register (m qubits). The first, control register with n qubits is prepared in the uniform superposition state $\sum_y |y\rangle/\sqrt{2^n}$, according to step i) of the quantum circuit above. Acting on the second register then with $U(\Delta t)$, we can construct the controlled unitaries c-U^{2^y} where $U^{2^y} \equiv U(2^y \Delta t)$. After step ii) we then have the state

$$\begin{aligned}
\Psi &= \frac{1}{\sqrt{2^n}} \sum_{y=0}^{2^n-1} |y\rangle U^y |\psi_0\rangle \\
&= \frac{1}{\sqrt{2^n}} \sum_{y=0}^{2^n-1} |y\rangle \sum_{j}^{2^n-1} a_j e^{-i\omega_j y t} |\psi_j\rangle
\end{aligned}$$

where we have used the eigenstate expansion of $U|\psi_0\rangle$. The inverse Fourier transform of this state contains a number of frequencies ω_j. Thus if ψ_0 is a good approximation to an eigenstate, there will be primarily one such frequency ω_0. Measurement of the first register will then yield this frequency with high probability, as in phase estimation, yielding the best n-bit estimation of energy ω_j. If there are many terms in the expansion of ψ_0, then the algorithm has to be repeated many times in order to build up the frequency spectrum of ω_j. As long as the desired energies are still obtained after a polynomial number of repeats, the algorithm is still exponentially more efficient than the classical analog.

Applications of this to quantum chemical calculations of electronic energies of atoms and molecules are described in the first two literature papers referenced below. The second paper (Aspuru-Guzik et al.) describes a recursive modification to the quantum phase estimation that allows the energy to be put into the first register 4 qubits at a time, thereby reducing the size of this from about 20 to 4 qubits for calculation of ground state energies of a small molecule. The third paper (Brown et al.) discusses the exponential growth of gates with desired precision.

2 Readings

Benenti et al., Ch. 3.12 - 3.13

Kaye et al., Ch. 7.1 - 7.2

Nielsen and Chuang, Ch. 5.2

Literature: Abrams and Lloyd, Phys. Rev. Lett. **83**, 5162 (1999); Aspuru-Guzik et al., Science **309**, 1704 (2005); Brown et al., Phys. Rev. Lett. **97**, 050504 (2006).