# 1 Readings

Benenti et al., Ch. 3.12 - 3.13

Stolze and Suter, Quantum Computing, Ch. 8.4.5

Nielsen and Chuang, Quantum Computation and Quantum Information, Ch. 5.2

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

# 2 Quantum phase estimation

This is a good example 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 $\phi$, and we want to find this to a given level of precision. In particular, we want to find the best $n$-bit estimate of $\phi$.

We can do this with a quantum circuit using i) H gate, ii) controlled unitaries of the form c-$U^{2^j}$, and iii) an inverse QFT. We need two registers as input. The first register contains $n$ qubits and will contain the $n$-bit estimate of $\phi$ 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 $\phi$ to at least the required accuracy.

Figure 1 below 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

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

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

Applying these gates with $j$ increasing from 0 (with qubit 1 of register 1 as control) to $n = 1$ (with qubit $n$

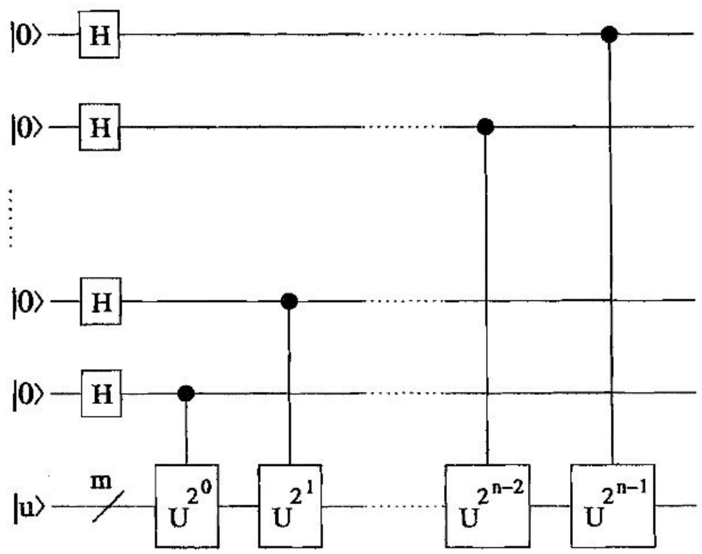


Figure 1: Quantum circuit for first part of phase estimation algorithm (steps i) and ii)). Following this circuit by an inverse QFT circuit will produce the best $n-$bit estimate of the phase $\phi$.

of register 1 as control) as shown in Figure 1 yields the state

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

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

Writing

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

where $a = a_{n-1}a_{n-2}\ldots a_0$, and $0 \le |\delta| \le 1/2^{n+1}$, defines $2\pi a/2^n$ as the best $n$-bit binary approximation of $\phi$. (Alternatively one could work with

$$\begin{aligned}\phi &= 2\pi\tilde{\phi}\\ \tilde{\phi} &= 0.\phi_{n-1}\phi_{n-2}\ldots\phi_0\end{aligned}$$

where the binary fraction $\tilde{\phi}$ provides an $n$-bit representation of the phase mod $2\pi$.)

Making this substitution for $\phi$ in terms of $a$ and then applying the inverse Fourier transform $F^{-1}$ of the state $|y\rangle$,

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

to the sum over states reached after steps i) and ii) yields

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

Note that we have applied the inverse QFT 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 there and should not be 'cancelled' out!

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, e.g., as in previous lectures, by noting that when $x = a$ the phase term is unity for all $y$ and hence the sum over $y$ gives $\frac{1}{2^n}\sum_y 1\left|a\right\rangle = \left|a\right\rangle$, 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 $\phi$ is exactly determined.

2. If $\delta \neq 0$, the result of measuring the first register is the best $n$-bit estimate of $\phi$ 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, 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 $\phi$ is obtained with a high probability.

Clearly increasing the number of qubits $n$ will improve the accuracy 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).)

# 3 Finding eigenvalues

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

$$U\left|\psi\right\rangle = \sum_j e^{-i\omega_j t}\left|\phi_j\right\rangle$$

or in position representation,

$$\psi(x,t) = \sum_j a_j e^{-i\omega_j t}\phi_j(x)$$

is a superposition of eigenstates $\phi_j$ of $H(x)$ and equivalently, also of $U(t) = e^{-iHt/\hbar}$, where $\omega_j = E_j\hbar$ and $E_j$ is the eigenvalue of $H(x)$ corresponding to $\phi_j$. The eigenvalues of $U$ are $e^{-i\omega_j t}$, so we may work with the phase estimation algorithm and a eigenstate register containing $\phi_j$ to determine the eigenvalues $E_j$.

Assume that we can efficiently generate some guess for an eigenstate

$$\left|\psi_0\right\rangle = \sum_{i}^{2^i-1} \psi_0(k)\left|k\right\rangle.$$

The basis $k$ could be a position dependent basis. 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 $U(t_2 - t_2) = U(\Delta t)$. This guess 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 $\sum_y \left|y\right\rangle/\sqrt{2^n}$, 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

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

where we have used the eigenstate expansion of $U\left|\psi_0\right\rangle$. The inverse Fourier transform of this state contains a number of frequencies $\omega_j$. Thus if $\psi_0$ is a good approximation to an eigenstate, there will be primarily one such frequency $\omega_0$ and to a high probability this will result, giving the energy $E_j$. If there are many terms in the expansion of $\psi_0$, then the algorithm has to be repeated many times in order to build up the frequency spectrum of $\omega_j$. 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 two literature papers referenced in Section 1. 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.