Notes 8.370/18.435 Fall 2022

Lecture 26 Prof. Peter Shor

In this lecture, we discuss an algorithm for simulating quantum dynamics. Before we can discuss the algorithm, we need to explain how continuous quamtum systems evolve.

There are two main differences between continuous quantum mechanics and the quantum mechanics of the circuit model.

1. Time is continuous (at least, most physicists believe it is up to the Planck scale, which is around 10^{-44} seconds).

2. Everything evolves at once, unlike the circuit model, where the gates operate on various qubits one at a time.

In the circuit model, we had discrete time. So $\psi_{t+1} = U_t\psi_t$. In actual quantum mechanics, we have the Schrödinger equation, which is the differential equation

$$\frac{d}{dt}\,|\,\psi(t)\rangle = \frac{-i}{\hbar} H\,|\,\psi(t)\rangle\,.$$

Here, H is the Hamiltonian, which gives the energy of the system. In the rest of this lecture, we will choose are units so that $\hbar = 1$, so we don't have all these $\hbar$s floating around.

Let's look at the equation more closely. The left side, $\frac{d}{dt}\,|\,\psi(t)\rangle$, has units of sec^{-1}, or Hertz. The right side, $H\,|\,\psi(t)\rangle$ has units of energy. We thus need a constant to relate them. This contant turns out to be $\hbar \approx 1.05 \times 10^{-34}$ Joule-sec. The reason that we do not generally observe macroscopic quantum effects is that this constant is so small.

How can we derive the Schrödinger equation? We know quantum mechanics is linear, so let's assume that the dynamics is given by a linear first-order differential equation. We then get

$$\frac{d}{dt}\,|\,\psi(t)\rangle = A\,|\,\psi(t)\rangle\,. \tag{1}$$

Now, let's differentiate $\langle\psi(t)|\psi(t)\rangle$. We then have

$$\begin{aligned}\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle &= \left(\frac{d}{dt}\,\langle\psi(t)\,|\right)\,|\,\psi(t)\rangle + \langle\psi(t)\,|\left(\frac{d}{dt}\,|\,\psi(t)\rangle\right)\\ &= \langle\psi(t)\,|\,A^\dagger\,|\,\psi(t)\rangle + \langle\psi(t)\,|\,A\,|\,\psi(t)\rangle = \langle\psi(t)\,|\,(A^\dagger + A)\,|\,\psi t\rangle\ ,\end{aligned}$$

where the first equality comes from the product formula for differentiation, and the second from plugging in Eq. 1.

However, we know that $\langle\psi(t)|\psi(t)\rangle = 1$, and thus its derivative must be 0, so the expression above must be 0, no matter what $|\,\psi(t)\rangle$ is. The only way this could happen is for $A^\dagger + A = 0$. Thus, $A^\dagger = -A$. If we let $H = iA$, this makes H real and gives the differential equation

$$\frac{d}{dt}\,|\,\psi(t)\rangle = -iH\,|\,\psi(t)\rangle\,,$$

which is the Schrödinger equation with $\hbar = 1$. Solving this equation gives

$$|\,\psi(t)\rangle = e^{-iHt}\,|\,\psi(0)\rangle\,.$$

To simulate quantum dynamics, we have to simulate the real world, which behaves quite differently than our gate model, because we have continuous time and because everything evolves simultaneously. There are some other differences. (For example the real world evolves according to quantum field theory, where there is no non-local action. Two electrons repel each other not because there is action at a distance, but because they are coninually exchanging photons.) However, in this course we will stick with quantum mechanics, which is much less complicated.

Let's now discuss the Schrödinger equation some more, and give some examples. The equation (setting $\hbar = 1$) was

$$\frac{d}{dt}\,|\,\psi(t)\rangle = -iH\,|\,\psi(t)\rangle\,.$$

Recall that H is a Hermitian operator that gives the energy of the system $|\,\psi\rangle$. The solution of the Schrödinger equation is

$$|\,\psi(t)\rangle = e^{-iHt}\,|\,\psi(0)\rangle$$

We can expand this equation in a Taylor series which is reasonably accurate for small t:

$$e^{-iHt} = I - iHt - \frac{1}{2}H^2t^2 + \ldots$$

There is another way of looking at the solutions of the Schrödinger equation.

For our first example, let's look at a qubit. Any 2×2 complex matrix can be expressed as

$$v_x\sigma_x + v_y\sigma_y + v_z\sigma_z + v_I\sigma_I$$

However, we can disregard the last term. Consider what happens if we have a Hamiltonian of vI. The energy of a state $|\,\psi\rangle$ is $\langle\psi\,|\,vI\,|\,\psi\rangle = v$, and the evolution is

$$|\,\psi(t)\rangle = e^{-vt}\,|\,\psi_0\rangle\,.$$

Because a global phase doesn't affect the state, this state is essentially $|\,\phi_0\rangle$. I won't work out the details here, but similarly adding a term proportional to I just adds a global phase, which can be ignored. So the absolute energy of a system is not important for quantum evolution; the only thing that mastters is the relative energy of the states of the system. Thus, we can assume that this Hamiltonian is $\vec{v}\cdot\vec{\sigma}$, where $\vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$

Now, let's look at how we might simulate the dynamics of a qubit evolving under a Hamiltonian. Consider two times, t and $t + \Delta t$. We have that

$$\begin{aligned}
|\,\psi(t+\Delta t)\rangle &= e^{iH\Delta t}\,|\,\psi(t)\rangle \\
&\approx (I + iH\Delta t)\,|\,\psi(t)\rangle \\
&= |\,\psi(t)\rangle + i\Delta t H\,|\,\psi(t)\rangle
\end{aligned}$$

This equation is quite easy to simulate, and for small t, it should work fairly well.

Another thing we can do is write $|\psi_0\rangle$ in the basis of eigenstates of H. Let $|v_E\rangle$ be the eigenstate of energy E, and let

$$|\psi_0\rangle = \sum_E c_E |v_E\rangle .$$

Then

$$|\psi_t\rangle = \sum_E c_E e^{-iEt} |v_E\rangle$$

Exercise: using these ideas, show that when we have the Hamiltonian $\vec{v}\cdot\vec{\sigma}$, the state $|\psi\rangle$ rotates around the vector $\vec{v}$.

Now, let's look at another Hamiltonian; specifically, one called the transverse Ising model. This is a Hamiltonian on a *spin chain* — we have qubits at sites $0, 1, \ldots, N$, and the Hamiltonian is

$$\sum_{j=0}^{N-1} \sigma_z^j \sigma_z^{j+1} - g \sum_{j=0}^{N} \sigma_x^j,$$

where σ_x^j is a Pauli matrix acting on site j.

This is a *local Hamiltonian*; this means that the Hamiltonian is a sum of terms, each of which acts only on a small (in this case, two) number of qubits. Here, the Hamiltonian can be expressed as $H = A + B$, where the local terms in A all commute (they are all composed of σ_z's, which all commute) and the local terms in B (composed of σ_x's) all commute. We will give the Trotter-Suzuki method, which can be used to simulate such Hamiltoniaans.

The first thing to realize is that if all the local terms H_j of the Hamiltonian commuted, there would be no problem—we could simulate them all sequentially; because they commute, applying the unitaries e^{-iH_j} in any order would give the right answer.

We will show that by alternately applying the A Hamiltonian and the B Hamiltonian, we can achieve a good approximation of the $A + B$ Hamiltonian.

First, let's compare applying the $A+B$ Hamiltonian for time t with applying the A Hamiltonian and then the B Hamiltonian for time t. Using the Taylor approximation, we get

$$\begin{aligned} e^{-i(A+B)t} &\approx I - i(A+B)t - (A+B)^2 t^2 + O(t^3) \\ &= I - i(A+B)t - \frac{1}{2}(A^2 + B^2 + AB + BA)t^2 + O(t^3) \end{aligned}$$

and

$$\begin{aligned} e^{-iAt}e^{-iBt} &\approx \big(I - iAt - \frac{1}{2}A^2t^2 + O(t^3)\big)\big(I - iBt - \frac{1}{2}B^2t^2 + O(t^3)\big) \\ &= I - i(A+B)t - \frac{1}{2}(A^2 + B^2 + 2AB)t^2 + O(t^3) \end{aligned}$$

We can then see that the commutator

$$[e^{-(A+B)t}, e^{-iAt}e^{-iBt}] = -\frac{1}{2}[A,B]t^2 + O(t^3).$$

For small t, this is small.

What we will do is compute the evolution

$$\left(e^{-iA\frac{t}{L}}e^{-iB\frac{t}{L}}\right)^L \approx \left(e^{-i(A+B)\frac{t}{L}}\right)^L$$

Intuitively, each of the L terms of this product differs from the correct evolution by order $\left(\frac{t}{L}\right)^2$. When we multiply all L terms together, this increases the difference by a factor of L, so the approximation is good to $O\left(\frac{t^2}{L}\right)$. To make this rigorous, we first need to decide hwo we will measure the difference, and then show that our intuition above holds.

What we use to measure the difference is the operator norm. This norm is

$$\|R\| = \max_{|\,\psi\rangle}\{|R\,|\,\psi\rangle\,| : |\,|\,\psi\rangle\,| = 1\}$$

If we want to approximate R by S, we measure how good our approximation is by the matrix $\|R - S\|$.

We will need several properties of the operator norm. These are

$$\|R + S\| \leq \|R\| + \|S\|;$$

For U unitary,

$$\|UR\| = \|AR\| = \|A\|;$$

and

$$\|R_1R_2\ldots R_m - S_1S_2\ldots S_m\| \leq \sum_{j=1}^{M}\|R_j - S_j\|$$

The last of these properties shows that

$$\|e^{-i(A+B)t} - e^{-At}e^{-Bt}\| \leq L\left\|\left(e^{-i(A+B)\frac{t}{L}} - e^{-A\frac{t}{L}}e^{-B\frac{t}{L}}\right)\right\|$$

Thus, if we divide the time t into L subintervals of length $\frac{t}{L}$, we can make the error of order $\frac{t^2}{L}$. By making L large enough, we can make the approximation as accurate as desired. We thus have that to get the error down to ϵ, we need to set $\epsilon = O\left(\frac{t^2}{L}\right)$, or $L = O\left(\frac{t^2}{\epsilon}\right)$.

There are also better Trotter-Suzuki formulas which work with higher order. I am only going to give the second-order one in this lecture (they get quite a bit more complicated as the orders get higher. Here, instead of repeating the evolution $e^{iAt}e^{iBt}$, we repeat the evolution

$$e^{-\frac{1}{2}iAt}e^{-iBt}e^{-\frac{1}{2}iAt}$$

Expanding the exponentials in Taylor series, we have

$$e^{-\frac{1}{2}iAt}e^{-iBt}e^{-\frac{1}{2}iAt} = (I - \frac{1}{2}iA - \frac{1}{8}A^2\ldots)(I - iB - \frac{1}{2}B^2\ldots)(I - \frac{1}{2}iA - \frac{1}{8}A^2\ldots)$$

Expanding and collecting terms, we find that

$$e^{\frac{1}{2}iAt}e^{iBt}e^{\frac{1}{2}iAt} = I - \frac{1}{2}i(A+B) - \frac{1}{2}(A^2 + AB + BA + B^2)t^2 + O(t^3),$$

which agrees with $e^{-i(A+B)}$ up to an error of $O(t^3)$.

Now, if we divide the time up into L intervals of size $\frac{t}{L}$, we see that

$$e^{-\frac{1}{2}iA\frac{t}{L}}e^{-iB\frac{t}{L}}e^{-\frac{1}{2}iA\frac{t}{L}}$$

is accurate to order $L\left(\frac{t}{L}\right)^3$. So to get accuracy of ϵ, we need to set $\epsilon = O\left(\frac{t^3}{L^2}\right)$, i.e., make L of order $\frac{t^{3/2}}{\epsilon^{1/2}}$.