# Hamiltonian Time Evolution <br> Quantum Computing Internship for Physics Undergraduates 2021 Fermilab 

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These notes are based on two lectures given at the summer school QCIPU 2021 (Quantum Computing Internship for Physics Undergraduates) held virtually at Fermilab during July 6-23 2021.

The goal of these lectures was to introduce the idea of Hamiltonian time evolution in quantum mechanics, and to understand how we might simulate many-body quantum systems on digital quantum computers.

If you find any errors or have any other comments, please feel free to let me know.

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## 1 Time evolution of quantum systems

So far in this school, you have developed an understanding of quantum bits and how you can act on them to perform computations. We might call that a computational perspective. In these lectures, we will take a more physical perspective. That is, we will think of the qubits as an interacting physical system.

### 1.1 Schrodinger equation

Imagine a pendulum with a rigid massless rod attached to a bob. There are two kinds of questions that you can ask about this. One is: what are the states of equilibrium for this system? In other words, what are the initial states which do not change with the passage of time? To find the equilibrium configurations of the pendulum, you know what to do. You set the net force acting on the bob to be zero: $\vec{F}_{\text {total }}=0$.

Another kind of question you can ask is, what happens when you start with a non-equilibrium state? For this pendulum, imagine releasing the pendulum at some angle $\theta$ from the vertical at time $t=0$. What is the angle $\theta(t)$ at some time $t>0$ ? This is a question about non-equilibrium phenomenon. In particular, we would like to know how the system evolves under time, given any arbitrary initial state. We also know how to do this. Provided we know all the forces acting on the system, we use Newton's second law

$$
\begin{equation*}
\vec{F}_{\text {total }}=m \frac{\mathrm{~d}^{2} \vec{x}}{\mathrm{~d} t^{2}} \tag{1}
\end{equation*}
$$

This is a second-order differential equation in $\vec{x}$ which can be solved to find the time evolution of the system, described by the function $\vec{x}(t)$.

In quantum mechanics, we can similarly ask these two kinds of questions: (i) What are the stationary states of the system?, and (ii) How does the system evolve if you start away from a stationary state? Recall that in classical mechanics, you need a description of all the forces acting on the system to answer these questions, and then you can proceed to use Newton's second law. What is the analog in quantum mechanics?

In quantum mechanics, the equation which describes how a quantum state $|\psi\rangle$ evolves with time is the Schrodinger equation,

$$
\begin{equation*}
i \frac{\partial|\psi\rangle}{\partial t}=H|\psi\rangle \tag{2}
\end{equation*}
$$

where $H$ is a Hermitian operator called the Hamiltonian. Specifying the Hamiltonian operator for a quantum system is akin to specifying the forces on a classical system, and the Schrodinger equation is analogous to Newton's second law.

Let's see what the Schrodinger equation says about stationary states. Let us say that the state is $\left|\psi_{0}\right\rangle$ at $t=0$. We might be tempted to say that a stationary state is one that does not depend on time at all, such that if $|\psi(t)\rangle=\left|\psi_{0}\right\rangle$ for all $t \geq 0$. But we know that in quantum mechanics, an overall phase does not change any measurements. So, a better definition would be to allow for a phase:

$$
\begin{equation*}
|\psi(t)\rangle=e^{-i \lambda(t)}\left|\psi_{0}\right\rangle \tag{3}
\end{equation*}
$$

where have allowed for the phase $\lambda(t)$ to depend on time. Plugging this in the Schrodinger equation (2) gives

$$
\begin{equation*}
\lambda^{\prime}(t)\left(e^{i \lambda(t)}\left|\psi_{0}\right\rangle\right)=H\left(e^{i \lambda(t)}\left|\psi_{0}\right\rangle\right) \tag{4}
\end{equation*}
$$

Let us further assume that the Hamiltonian $H$ itself does not depend on time. Canceling the phase on both sides, we get

$$
\begin{equation*}
\lambda^{\prime}(t)\left|\psi_{0}\right\rangle=H\left|\psi_{0}\right\rangle \tag{5}
\end{equation*}
$$

Here, notice that the right-hand side is independent of time, therefore the function $\lambda^{\prime}(t)=\lambda$ must be time-independent as well, which gives $\lambda(t)=\lambda t$ (plus an irrelevant constant which can be absorbed in the definition of the initial state). For stationary states, the Schrodinger equation (2) therefore simplifies to

$$
\begin{equation*}
\lambda\left|\psi_{0}\right\rangle=H\left|\psi_{0}\right\rangle \tag{6}
\end{equation*}
$$

This equation sometimes goes by the name of time-independent Schrodinger equation. What it is, is just an eigenvalue equation for the operator $H$. It says that any eigenstate $\left|\psi_{0}\right\rangle$ of the operator $H$ with eigenvalue $\lambda$ is a stationary states, with the time-evolution given by

$$
\begin{equation*}
|\psi(t)\rangle=e^{-i \lambda t}\left|\psi_{0}\right\rangle \tag{7}
\end{equation*}
$$

To find the set of all stationary states of a quantum system, you must find all the eigenstates of the Hamiltonian, also called energy eigenstates. The set of all eigenvalues $\lambda$ of the Hamiltonian operator is also called the spectrum of the system.

Now, let's move on the second question: what if the initial state of a system $|\psi(0)\rangle$ is not a stationary state?

$$
\begin{equation*}
|\psi(0)\rangle=\left|\psi_{0}\right\rangle \xrightarrow{\text { time evolution }}|\psi(t)\rangle=? \tag{8}
\end{equation*}
$$

Well, now we really need to look at the time-dependent Schrodinger equation. Note that it is clearly a linear differential equation. (This means that if you have two solutions $|\alpha(t)\rangle$ and $|\beta(t)\rangle$, then any linear combination $a|\alpha(t)\rangle+b|\beta(t)\rangle$ is also a solution.) So we should look for a linear operator $U(t)$, such that

$$
\begin{equation*}
\left|\psi_{0}\right\rangle \xrightarrow{\text { time evolution }}|\psi(t)\rangle=U(t)\left|\psi_{0}\right\rangle . \tag{9}
\end{equation*}
$$

What can we say about $U(t)$ ? Something we would like in quantum mechanics is for timeevolution to preserve the norm of a state. Requiring $\langle\psi(t) \mid \psi(t)\rangle=1$ gives us

$$
\begin{align*}
\left\langle\psi_{0} \mid \psi_{0}\right\rangle=1 & =\langle\psi(t) \mid \psi(t)\rangle \\
& =\left\langle\psi_{0}\right| U(t)^{\dagger} U(t)\left|\psi_{0}\right\rangle \tag{10}
\end{align*}
$$

If this must be true for any initial state $\left|\psi_{0}\right\rangle$, we must have $U(t)^{\dagger} U(t)=1$. Therefore the operator $U(t)$ must be a unitary operator. Further, if $|\psi(t)\rangle=U(t)\left|\psi_{0}\right\rangle$ describes the time-evolution, it must solve the Schrodinger equation. So let's plug this into the Schrodinger equation:

$$
\begin{equation*}
i U^{\prime}(t)\left|\psi_{0}\right\rangle=H U(t)\left|\psi_{0}\right\rangle \tag{11}
\end{equation*}
$$

Since this must be true for any initial state $\left|\psi_{0}\right\rangle$, we can get rid of the state and write this a first-order linear differential equation for the operator $U(t)$ itself:

$$
\begin{equation*}
i U^{\prime}(t)=H U(t) \tag{12}
\end{equation*}
$$

So we need to solve this equation (12). If $U(t)$ and $H$ were just scalars, then you know that this equation would be solved by $U(t)=e^{-i H t}$. But what should we do if have operators? Well, it turns out that this solution also works for operators! You can easily check this by just plugging this solution into Eq. (12). So we can write the solution to the Schrodinger equation

$$
\begin{equation*}
U(t)=e^{-i H t} \tag{13}
\end{equation*}
$$

Recall that we need $U(t)$ to be unitary. Is it?
Exponential of a matrix? You might be a bit puzzled about the exponential of a matrix suddenly making an appearance. How should we define this object? We know that that the exponential of a number $x$ can be expanded as a power series

$$
\begin{equation*}
e^{x}=\sum_{n} \frac{x^{n}}{n!} \tag{14}
\end{equation*}
$$

We can generalize this definition for matrices too:

$$
\begin{equation*}
e^{A}=\sum_{n} \frac{A^{n}}{n!} . \tag{15}
\end{equation*}
$$

where now $A$ is a matrix. Since we know how to compute powers $A^{n}$ of the matrix $A$, we can use the above power series to define the matrix exponential $e^{A}$. The only remaining question here would be to show that the power series in Eq. (15) actually converges. Turns out this is true and the matrix exponential is well-defined, but we will not worry about the proof here. (As you will find out in your future studies, not worrying about convergence issues (until you really have to) is somewhat of a recurring theme in physics.)

Using the power series, you can also show that the identity $\frac{\mathrm{d} e^{\lambda A}}{\mathrm{~d} \lambda}=\lambda e^{\lambda A}$ holds, which is something we used above.

### 1.2 A single qubit

As we already know, a cool way to visualize the state of a single qubit is to use the Bloch sphere. We can parametrize the state $|\psi\rangle$ by two angles $\theta, \phi$ as

$$
\begin{equation*}
|\Psi\rangle=\cos (\theta / 2)|\uparrow\rangle+e^{i \phi} \sin (\theta / 2)|\downarrow\rangle . \tag{16}
\end{equation*}
$$

This state can be represented as a vector on the Bloch sphere, as shown in Fig. 1.
Now, let's write down the simplest Hamiltonian we can. What could that be? Remember that Hamiltonian needs to be a Hermitian operator. It needs to act on a 2-dimensional Hilbert space. So, we're looking for $2 \times 2$ Hermitian matrices. Any such matrix would be a legitimate Hamiltonian. But any such matrix can be written as a linear combination of the Pauli sigma matrices and the identity matrix. (Make sure that this works by counting the number of free parameters.) So the most general Hamiltonian would be

$$
\begin{equation*}
H=h_{x} X+h_{y} Y+h_{z} Z+c I \tag{17}
\end{equation*}
$$

where $h_{x}, h_{y}, h_{z}, c$ are real parameters. We can simplify the notation by introducing the vector $\vec{h}=\left(h_{x}, h_{y}, h_{z}\right)$ and write $\vec{h}=h \hat{n}$, where $h=|\vec{h}|$ and $\hat{n}$ is a unit vector in the direction of


Figure 1: The state of a single qubit represented on the Bloch sphere.
$\vec{h}$. If we write the Pauli matrices as a vector $\vec{\sigma}=(X, Y, Z)$, then we can compactly write the Hamiltonian $H$ as

$$
\begin{equation*}
H=\vec{h} \cdot \vec{\sigma}+c I . \tag{18}
\end{equation*}
$$

OK, so what does a qubit do we apply the time-evolution operator to it? Let's start with the simplest case and set $h_{x}=h_{y}=c=0$, leaving us with

$$
\begin{equation*}
H=h Z . \tag{19}
\end{equation*}
$$

To find the time evolution of this, we must compute the exponential $e^{-i H t}$. We can directly compute

$$
e^{-i H}=e^{-i h t Z}=\left(\begin{array}{cc}
e^{-i h t} & 0  \tag{20}\\
0 & e^{i h t}
\end{array}\right)
$$

Therefore, we can compute the action on the inital state given by Eq. (22)

$$
\begin{align*}
|\Psi(t)\rangle & =\left(\begin{array}{cc}
e^{-i h t} & 0 \\
0 & e^{i h t}
\end{array}\right)\binom{\cos (\theta / 2)}{e^{i \phi} \sin (\theta / 2)}  \tag{21}\\
& =e^{-i h t}\left(\cos (\theta / 2)|\uparrow\rangle+e^{i(\phi+2 h t)} \sin (\theta / 2)|\downarrow\rangle\right) \tag{22}
\end{align*}
$$

Since the overall phase does not matter on the block sphere, we see that time evolution under this Hamiltonian makes

$$
\begin{equation*}
(\theta, \phi) \xrightarrow{e^{i \hat{H} t}}(\theta, \phi+2 h t) \tag{23}
\end{equation*}
$$

This is just a rotation about the $z$-axis! So that's what this Hamiltonian does. It rotates the qubit about the $Z$-axis. Actually, this is not a coincidence. A slightly less trivial check would be to repeat this exercise for

$$
\begin{equation*}
H=h \hat{X} \tag{24}
\end{equation*}
$$

and show that in fact this is a rotation about the $X$ axis,

$$
\begin{equation*}
(\theta, \phi) \xrightarrow{e^{i \hat{H} t}}(\theta-2 h t, \phi) . \tag{25}
\end{equation*}
$$

More generally, $\vec{n} \cdot \hat{\vec{\sigma}}$ is a rotation about the axis given by the vector $\hat{n}$. For the most general single-qubit Hamiltonian given in Eq. (17),

$$
\begin{equation*}
\hat{H}=h \sum_{i} n_{i} \sigma_{i}+c I \tag{26}
\end{equation*}
$$

the time-evolution is just

$$
\begin{equation*}
e^{-i \hat{H} t}=\underbrace{e^{-i h t \vec{n} \cdot \vec{\sigma}}}_{\substack{\text { rotation } \\ \text { about } \vec{n}}} \underbrace{e^{-i c}}_{\text {overall phase }} \tag{27}
\end{equation*}
$$

Let us remark that, in the language of quantum circuits that you already familiar with, the time-evolution is just given by the single-qubit rotations. For example, the Hamiltonian above can be implemented on a quantum circuit using a $Z$-rotation:

$$
\begin{align*}
H=-h Z & \Longrightarrow e^{-i t H}=R_{Z}(2 j t)  \tag{28}\\
|\psi\rangle & =R_{Z}(2 j t) \\
& e^{-i H t}|\psi\rangle
\end{align*}
$$

Similarly, $H=-h X$ or $H=-h Y$ can be simulated using single-qubit $X$ or $Y$ rotations.

### 1.3 Summary

- To summarize, I would like to emphasize that we have two equivalent ways of writing the time-dependent Schrodinger equation

$$
\begin{equation*}
i \frac{d}{d t}|\psi\rangle=H|\psi\rangle \Longleftrightarrow|\psi(t)\rangle=e^{-i H t}|\psi(0)\rangle \tag{29}
\end{equation*}
$$

provided that the Hamiltonian $H$ itself does not depend on time. The Schrodinger equation, along with the knowledge of the Hamiltonian $H$, tells you how a state $|\psi(t)\rangle$ evolves as a function of time.

- Further, if we take the state $|\psi(0)\rangle$ to be some eigenstate $|\lambda\rangle$ of the Hamiltonian with eigenvalue $\lambda$ such that

$$
\begin{equation*}
H|\lambda\rangle=\lambda|\lambda\rangle \tag{30}
\end{equation*}
$$

then the time-dependent Schrodinger equation immediately tells us that these are "stationary states," meaning that they don't evolve with time (except for an overall phase)

$$
\begin{equation*}
|\psi(t)\rangle=e^{-i \lambda t}|\lambda\rangle \tag{31}
\end{equation*}
$$

- For a single qubit, the most general Hamiltonian is $H=\vec{h} \cdot \vec{\sigma}+c I$. Time evolution under this Hamilonian can be visualized on the Bloch sphere as rotation of the qubit state about about the axis given by $\vec{h}$ with constant angular velocity determined by $|\vec{h}|$.


## 2 Quantum simulation on digital quantum computers

### 2.1 Two interacting qubits

Now let's look a slightly more complicated system: two interacting spins. The Hilbert space $\mathcal{H}$ is given by the tensor product of the Hilbert spaces of each individual spin $\mathbb{C}^{2}$, so that the

$$
\begin{equation*}
\mathcal{H}=\mathbb{C}^{2} \otimes \mathbb{C}^{2} \cong \mathbb{C}^{4} \tag{32}
\end{equation*}
$$

What is the most general Hamiltonian which could act on such a system? We need a $4 \times 4$ dimensional Hermitian matrix, which has 16 real parameters. We already know that the operators $I, X, Y, Z$ form a basis for the Hermitian operators on a single qubit. We can try to form all possible combinations of these operators on the two-qubit space. This gives us:

$$
\begin{equation*}
H=\sum_{i} h_{i}^{(1)} \sigma_{i}^{(1)} \otimes I^{(2)}+\sum_{i} h_{i}^{(2)} I^{(1)} \otimes \sigma^{(2)}+\sum_{i j} J_{i j} \sigma_{i}^{(1)} \otimes \sigma_{j}^{(2)}+c I^{(1)} \otimes I^{(2)} \tag{33}
\end{equation*}
$$

If you count the number of parameters, you see that these are exactly 16 real parameters ( 3 from $h_{i}^{(1)}, 3$ from $h_{i}^{(2)}, 9$ from $J_{i j}$, and 1 from $\left.c\right)$.

Let us simplify the most general two-qubit Hamiltonian to understand the physics in a specific case. First, we get rid of the single-spin operators, and the irrelevant constant term. This leaves us with a genuine two-qubit interaction term

$$
\begin{equation*}
H=\sum_{i j} J_{i j} \sigma_{i}^{(1)} \otimes \sigma_{j}^{(2)} . \tag{34}
\end{equation*}
$$

Let's simplify this even further. We set all the $J_{i j}=0$ except $J_{33}=-J$. We get

$$
\begin{equation*}
H=-J Z^{(1)} \otimes Z^{(2)} . \tag{35}
\end{equation*}
$$

Now, what's happening here? This Hamiltonian is already diagonal, so we can easily write down the energy eigenstates and eigenvalues. The full spectrum is given by the following states and energies:

$$
\begin{array}{ll}
|\uparrow \uparrow\rangle & E=-J \\
|\downarrow \downarrow\rangle & E=-J \\
|\uparrow \downarrow\rangle & E=J \\
|\downarrow \uparrow\rangle & E=J . \tag{39}
\end{array}
$$

Which states have the lowest energy depends on the sign of $J$. For $J>0$, we see that the spins like to be aligned with each other. That is, the lowest energy states are the ones where both the
spins are either up, or both of them are down. Such a system is called ferromagnetic. On the other hand if $J<0$, the spins like to be anti-aligned, and such a system is called antiferromagnetic.

We would like to study the time-evolution of the two-qubit system under this Hamiltonian. Since this is still diagonal, we can of course trivially exponentiate it. But let's imagine that we do not know how to exponentiate it, but we do have a digital quantum computer. Can we construct a circuit to perform time evolution on this two-spin system? We need to implement the operator $e^{i \theta Z_{1} Z_{2}}$. It turns out there is a nice trick to implement this operator. Here, we use the notation $x \oplus y$ to denote the parity of the bits: $x \oplus y=0$ if the sum $x+y$ is even; and $x \oplus y=1$ if the sum is odd. Now, if you start in a state $|x\rangle|y\rangle$ in the computational basis, then this operator just applies a phase depending on the parity $x \oplus y$,

$$
\begin{array}{ll}
|x y\rangle \rightarrow e^{i \theta}|x y\rangle & \text { if } \quad x \oplus y \equiv 0, \\
|x y\rangle \rightarrow e^{-i \theta}|x y\rangle & \text { if } \quad x \oplus y \equiv 1 . \tag{41}
\end{array}
$$

This tells us how to implement the operator $e^{i \theta Z_{1} Z_{2}}$. We just need to measure the parity of the state $|x y\rangle$, and apply the phase $e^{i \theta}$ or $e^{-i \theta}$ depending on the parity. This can be done easily using CNOT gates and an auxiliary qubit, as shown in Fig. 2.


Figure 2: Quantum circuit to implement the operator $e^{i \theta Z_{1} Z_{2}}$. The first two CNOT gates compute the parity of the first two qubits and store it in the auxiliary qubit $|x y\rangle|0\rangle \rightarrow|x y\rangle|x \oplus y\rangle$. The operator $e^{i \theta Z}$ then applies an overall phase depending on the state of the third qubit: $|x y\rangle|x \oplus y\rangle \rightarrow e^{i \theta f(x \oplus y)}|x y\rangle|x \oplus y\rangle$. Finally, we undo the CNOT gates, so that the final state becomes $e^{i \theta f(x \oplus y)}|x y\rangle|x \oplus y\rangle \rightarrow e^{i \theta(x \oplus y)}|x y\rangle|0\rangle$, which is what we need.

But what if you instead had the Hamiltonian $H=-J X_{1} X_{2}$ ? In that case, you could wrap the time-evolution operator with Hadamard gates on each qubit to turn the $X$ operators into $Z$, and then just use the circuit described above, as shown in Fig. 3,

$$
\begin{equation*}
e^{i \theta X_{1} X_{2}}=H_{1} H_{2} e^{i \theta Z_{1} Z_{2}} H_{1} H_{2} . \tag{42}
\end{equation*}
$$

How would you simulate the Hamiltonian $H=-J Y_{1} Y_{2}$ ?

### 2.2 More interacting qubits and the Suzuki-Trotter formula

In the previous sections, we completely solved the time evolution of a single qubit and even made some progress for two interacting qubits. You could already see that the most general Hamilonian for the two-qubit (which had 16 parameters) looked harder than the single-qubit case (which only


Figure 3: Quantum circuit to implement the operator $e^{i \theta X_{1} X_{2}}$. We use Hadamard gates to convert the $X$ operators to the $Z$ operators and then use the circuit shown in Fig. 2.
had 4 parameters). As we start considering systems with larger and larger number of interacting qubits $N$, you can see that this might quickly become very hard. (Merely the description of such a Hamiltonian would require $4^{N}$ parameters, which grows exponentially in $N$.)

Further, simulating such a generic Hamiltonian will require us to construct the operator $e^{i H t}$. We saw how construct this operator for the cases $N=1$ and $N=2$. What if $N \gg 2$ ? Systems with larger $N$ are not merely a curiosity. In fact, it is usually the limit of $N \rightarrow \infty$ that is of most interest in high-energy physics (where we encounter quantum fields) and condensed matter physics (where we deal with a very large number of atoms in a material, for example).

So we need a way to simplify the problem of a large number of interacting qubits. Can we perhaps restrict the class of Hamiltonians that we work with? Indeed, it turns out that the Hamiltonians that appear in nature often have an additional property called locality. Intuitively, locality is the idea that a qubit should not interact with a qubit which is far away.

For concreteness, imagine a solid material with $N$ qubits arranged on a $d$-dimensional lattice. Locality implies that the force exerted by one qubit only affects the qubits in its vicinity. For example, we might have that each qubit in our lattice only interacts with its immediate neighbor on the lattice. What should be the precise form of the interaction between a qubit and its neighbor? In the last section, we already wrote down the most general two-qubit Hamiltonian, and then considered the physics in a simpler case with the Hamiltonian $H=-J Z_{1} Z_{2}$. We can imagine that the interaction energy of each neighboring pair $(i, j)$ is just given by the two-qubit Hamiltonian $H_{i j}=-J Z_{i} Z_{j}$. The total energy of the system would then be just the sum of all the interaction energies

$$
\begin{equation*}
H=-J \sum_{[i, j]} Z_{i} Z_{j} \tag{43}
\end{equation*}
$$

where the notation $[i, j]$ just means that the sum is over all neighboring pairs of qubits $(i, j)$. As we briefly mentioned with two qubits, for $J>0$, this Hamiltonian favors aligned in the $z$ direction. As you can imagine, with larger number of qubits, each qubit would like to get aligned with its neighbors, which get aligned with their neighbors, and so on. Tiny local interactions can therefore cause all the qubits to get aligned, and cause big changes on a large scale. Let's also add a single-qubit term to finally obtain

$$
\begin{equation*}
H=-J \sum_{[i, j]} Z_{i} Z_{j}-h \sum_{i} X_{i} \tag{44}
\end{equation*}
$$

This particular Hamiltonian on $N$ qubits is perhaps one of the most famous systems in physics. It is called the Ising model, and it was originally introduced as a model of ferromagnetism. Unfortunately, we do not have the time to study the physics of this model today, but I am sure you will see much more of this as you go further in your studies.

What we would like to today ask is: how can we study the time-evolution of such a local Hamiltonian on a large number of qubits $N$ ? We need to find a way to apply the operator $e^{-i H t}$ to a state $|\psi\rangle$. This is of course a very large dimensional unitary matrix. However, each of the terms in the Hamilonian (44) only consists of two-qubit and single-qubit terms. How can we exploit this property?

We have an exponential of a sum of matrices. It is tempting write this as a product of exponentials by using an identity of the sort

$$
\begin{equation*}
e^{-i t(A+B)} \stackrel{?}{=} e^{-i t A} e^{-i t B} \tag{45}
\end{equation*}
$$

If we could do something like this, we would be able to simply our job drastically, since we would have converted the large $N \times N$ unitary matrix as a product of unitaries that act only on at most two qubits at a time:

$$
\begin{align*}
e^{-i H T} & =e^{i T J \sum_{[i, j]} Z_{i} Z_{j}+i T h \sum_{i} X_{i}}  \tag{46}\\
& \stackrel{?}{=} \prod_{[i, j]} e^{i T J Z_{i} Z_{j}} \prod_{i} e^{i T h X_{i}} \tag{47}
\end{align*}
$$

But, unfortunately, this is false in general if $A$ and $B$ are matrices!

$$
\begin{equation*}
e^{-i t(A+B)} \neq e^{-i t A} e^{-i t B} \tag{48}
\end{equation*}
$$

Let's try to explore what goes wrong in this formula. We can expand both sides and keep terms up to order $t^{2}$,

$$
\begin{align*}
e^{-i t(A+B)} & =1-i t(A+B)-\frac{1}{2} t^{2}\left(A^{2}+B^{2}+A B+B A\right)+O\left(t^{3}\right)  \tag{49}\\
e^{-i t(A)} e^{-i t B} & =\left(1-i t A-\frac{1}{2} t^{2} A+O\left(t^{3}\right)\right)\left(1-i t B-\frac{1}{2} t^{2} B+O\left(t^{3}\right)\right)  \tag{50}\\
& =1-i t(A+B)-\frac{1}{2} t^{2}\left(A^{2}+B^{2}+2 A B\right)+O\left(t^{3}\right) \tag{51}
\end{align*}
$$

To study what's going on, we can look at the difference

$$
\begin{equation*}
e^{-i t(A+B)}-e^{-i t A} e^{-i t B}=\frac{1}{2} t^{2}[A, B]+O\left(t^{3}\right) \tag{52}
\end{equation*}
$$

There are two interesting aspects to note here. The first one is that the "error" is proportional to the commutator $[A, B]$. This is expected since we know that this formula should work when $A$ and $B$ commute! The second aspect is that the error term goes is in fact $O\left(t^{2}\right)$. This suggests that if we were looking at very small $t$, then the error would be very small and we could get away
with it. Here's the final trick. We can always take up a large time $t$ and divide it up into much $n$ smaller chunks, each of size $\varepsilon$, such that $n \varepsilon=t$. This lets us write

$$
\begin{equation*}
e^{-i t(A+B)}=e^{-i \varepsilon(A+B)} e^{-i \varepsilon(A+B)} \cdots e^{-i \varepsilon(A+B)} \tag{53}
\end{equation*}
$$

But, for each of the pieces, we could just write $e^{-i \varepsilon(A+B)}=e^{-i \varepsilon A} e^{-i \varepsilon B}$. Finally, we get

$$
\begin{equation*}
e^{-i t(A+B)}=\lim _{n \rightarrow \infty}\left[e^{-i t A / n} e^{-i t B / n}\right]^{n} \tag{54}
\end{equation*}
$$

This kind of decomposition goes by the name of Suzuki-Trotter formulas.

### 2.3 Putting it all together

Now, we can put together everything we have learned to construct a simple quantum circuit to do time-evolution of the Ising model. It is enough to do this for a single time step. Secondly, we already know how to implement the single qubit rotation $e^{i t h X_{i}}$ for qubit $i$, as well as the two-qubit gates $e^{i t J Z_{j} Z_{k}}$ for qubits $j, k$. So we have decomposed the circuit as:
where each of the time steps $e^{i H \varepsilon}$ is just composed of single-qubit and two-qubit gates.

### 2.4 Summary

- As the number of qubits $N$ becomes larger, it quickly becomes very difficult to compute the time evolution of a state $e^{-i H t}|\psi\rangle$.
- The paradigmatic example of a system of large number of interacting qubits is the Ising model given by the Hamiltonian $H=-J \sum_{\langle i j\rangle} Z_{i} Z_{j}+h \sum_{i} X_{i}$.
- Such Hamiltonians that appear in nature have the property of locality, where a given qubit only interacts with a few qubits around it. We can exploit this property to construct a quantum algorithm to perform the time evolution of this system starting from an arbitrary initial state.
- For a Hamilonian $H$ which is a sum of non-commuting operators, $H=A+B$, the Suzuki-Trotter formula states that we may divide the total time $T$ into $n$ timesteps, and repeatedly apply $e^{-i \varepsilon H} \approx e^{-i \varepsilon A} e^{-i \varepsilon B}$

$$
\begin{equation*}
e^{-i t(A+B)}=\lim _{n \rightarrow \infty}\left[e^{-i t A / n} e^{-i t B / n}\right]^{n} \tag{56}
\end{equation*}
$$

