ITIS 6260/8260 Quantum Computing

Lecture 3: Quantum simulation/Adiabatic Quantum Computing

Yongge Wang

UNC Charlotte, USA

January 7, 2019

Outline

Classical mechanics

- A particle of mass m moves along the x-axis subject to some external force $F(x,t)$, the initial condition:

the velocity	$v = dx/dt$
the momentum	$p = mv$
the kinetic energy	$T = mv^2/2$

- Newton's second law: the rate of momentum change is directly proportional to the force applied

$$\mathbf{F} = \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = \frac{\mathrm{d}(m\mathbf{v})}{\mathrm{d}t} = m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = m\mathbf{a}$$

  where $a = d^2x/dt^2$ is the acceleration
- This law can be used to determine the particle position $x(t)$ at time t given the initial conditions (e.g., the position and velocity at $t = 0$)

Classical mechanics

- A particle of mass m moves along the x-axis subject to some external force $F(x,t)$, the initial condition:

the velocity	$v = dx/dt$
the momentum	$p = mv$
the kinetic energy	$T = mv^2/2$

- Newton's second law: the rate of momentum change is directly proportional to the force applied

$$\mathbf{F} = \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = \frac{\mathrm{d}(m\mathbf{v})}{\mathrm{d}t} = m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = m\mathbf{a}$$

  where $a = d^2x/dt^2$ is the acceleration

- This law can be used to determine the particle position $x(t)$ at time t given the initial conditions (e.g., the position and velocity at $t = 0$)

Classical mechanics

- A particle of mass m moves along the x-axis subject to some external force $F(x,t)$, the initial condition:

the velocity	$v = dx/dt$
the momentum	$p = mv$
the kinetic energy	$T = mv^2/2$

- Newton's second law: the rate of momentum change is directly proportional to the force applied

$$\mathbf{F} = \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = \frac{\mathrm{d}(m\mathbf{v})}{\mathrm{d}t} = m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = m\mathbf{a}$$

  where $a = d^2x/dt^2$ is the acceleration
- This law can be used to determine the particle position $x(t)$ at time t given the initial conditions (e.g., the position and velocity at $t = 0$)

Quantum mechanics – Schrödinger's equation

- In quantum mechanics, the analogue of Newton's law is Schrödinger's equation with the wave function $\Psi(x,t)$.
- The time-dependent Schrödinger equation (general)

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

where $i = \sqrt{-1}$, $\hbar = 1.054573 \times 10^{-34}$J is the Planck's constant, and $\hat{H}$ is the Hamiltonian operator (the total energy of the system)

Quantum mechanics – Schrödinger's equation

- In quantum mechanics, the analogue of Newton's law is Schrödinger's equation with the wave function $\Psi(x,t)$.
- The time-dependent Schrödinger equation (general)

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

where $i = \sqrt{-1}$, $\hbar = 1.054573 \times 10^{-34}$J is the Planck's constant, and $\hat{H}$ is the Hamiltonian operator (the total energy of the system)

Hamiltonian operator

- By analogy with classical mechanics, the Hamiltonian is expressed as the sum of operators corresponding to the kinetic and potential energies of a system in the form

$$\hat{H} = \hat{T} + \hat{V},$$

where

$$\hat{V} = V = V(\mathbf{r}, t),$$

is the potential energy operator and

$$\hat{T} = \frac{\hat{p} \cdot \hat{p}}{2m} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial t^2},$$

is the kinetic energy operator and

$$\hat{p} = -i\hbar\frac{\partial}{\partial t},$$

is the momentum operator

Schrödinger's equation in position basis

- Time-dependent Schrödinger equation in position basis

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) = \left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial t^2} + V(\mathbf{x},t)\right]\Psi(\mathbf{x},t)$$

where V is its potential energy. In plain language, it means "total energy equals kinetic energy plus potential energy".

The statistical interpretation

- A particle is localized at a point and a wave funcftion is spread out in space (a function of x for time time t)
- Born's statistical interpretation of the wave function: $|\Psi(x,t)|^2$ gives the probability of finding the particle at point x at time t. Precisely:

$$|\Psi(x,t)|^2 dx = \left\{ \begin{array}{l} \text{probability of finding the particle} \\ \text{in the interval } [x, x+dx] \text{ at time } t \end{array} \right.$$

The statistical interpretation

- A particle is localized at a point and a wave funcftion is spread out in space (a function of x for time time t)
- Born's statistical interpretation of the wave function: $|\Psi(x,t)|^2$ gives the probability of finding the particle at point x at time t. Precisely:

$$|\Psi(x,t)|^2 dx = \left\{ \begin{array}{l} \text{probability of finding the particle} \\ \text{in the interval } [x, x+dx] \text{ at time } t \end{array} \right.$$

Simulating a time independent Hamiltonian

- A system staring in state $|\psi(0)\rangle$ with energy operator (Hamiltonian) $\hat{H}$ over a period of time t will evolve into (obtained by solving the Schrödinger's equation and renormalized to get rid of $\hbar$)

$$|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle$$

Raise e to the power of a matrix?

- The "definition" is from the Taylor series e^x

$$e^A = \sum_{k=0}^{\infty} \frac{A^k}{k!}$$

- E.g.,

$$e^{\begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}} = \begin{pmatrix} e^{\lambda_1} & & \\ & \ddots & \\ & & e^{\lambda_n} \end{pmatrix}$$

Raise e to the power of a matrix?

- The "definition" is from the Taylor series e^x

$$e^A = \sum_{k=0}^{\infty} \frac{A^k}{k!}$$

- E.g.,

$$e^{\begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}} = \begin{pmatrix} e^{\lambda_1} & & \\ & \ddots & \\ & & e^{\lambda_n} \end{pmatrix}$$

Raise e to the power of a matrix?

- For a Hermitian matrix A, we have $A = UDU^{-1}$ where D is diagonal. Thus we have

$$e^A = \sum_{k=0}^{\infty} \frac{(UDU^{-1})^k}{k!} = Ue^D U^{-1}$$

Requiring H to be Hermitian

- If H is Hermitian, then all its eigenvalues are real

$$
\begin{aligned}
H|v\rangle &= \lambda|v\rangle \\
\langle v|H|v\rangle &= \lambda \\
\langle v|H^*|v\rangle &= \lambda^* \\
H &= H^* \\
\lambda &= \lambda^*
\end{aligned}
$$

- Any Hermitian matrix can be written as $H = UDU^*$ where D is diagonal and U is unitary
- For any Hermitian matrix H, e^{-iHt} is unitary

Requiring H to be Hermitian

- If H is Hermitian, then all its eigenvalues are real

$$
\begin{aligned}
H|v\rangle &= \lambda|v\rangle \\
\langle v|H|v\rangle &= \lambda \\
\langle v|H^*|v\rangle &= \lambda^* \\
H &= H^* \\
\lambda &= \lambda^*
\end{aligned}
$$

- Any Hermitian matrix can be written as $H = UDU^*$ where D is diagonal and U is unitary
- For any Hermitian matrix H, e^{-iHt} is unitary

Requiring H to be Hermitian

- If H is Hermitian, then all its eigenvalues are real

$$
\begin{aligned}
H|v\rangle &= \lambda|v\rangle \\
\langle v|H|v\rangle &= \lambda \\
\langle v|H^*|v\rangle &= \lambda^* \\
H &= H^* \\
\lambda &= \lambda^*
\end{aligned}
$$

- Any Hermitian matrix can be written as $H = UDU^*$ where D is diagonal and U is unitary
- For any Hermitian matrix H, e^{-iHt} is unitary

Requiring H to be Hermitian

- if $|v\rangle$ is an eigenvector of Hermitian H associated with eigenvalue λ, then $|v\rangle$ is an eigenvector of e^{-iHt} associated with eigenvalue $e^{-i\lambda t}$
- Given a unitary matrix U, we can find a Hermitian matrix H such that $U = e^{-iHt}$

Requiring H to be Hermitian

- if $|v\rangle$ is an eigenvector of Hermitian H associated with eigenvalue λ, then $|v\rangle$ is an eigenvector of e^{-iHt} associated with eigenvalue $e^{-i\lambda t}$
- Given a unitary matrix U, we can find a Hermitian matrix H such that $U = e^{-iHt}$

Energies

- The eigenvalues of a Hamiltonian matrix are called energies. These values are amounts of energy that the system can have!
- Let $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be a list of energies of H
- For each energy λ_j, there corresponds to an energy eigenstate $|v_j\rangle$ such that $H|v_j\rangle = \lambda|v_j\rangle$

Energies

- The eigenvalues of a Hamiltonian matrix are called energies. These values are amounts of energy that the system can have!
- Let $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be a list of energies of H
- For each energy λ_j, there corresponds to an energy eigenstate $|v_j\rangle$ such that $H|v_j\rangle = \lambda|v_j\rangle$

Energies

- The eigenvalues of a Hamiltonian matrix are called energies. These values are amounts of energy that the system can have!
- Let $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be a list of energies of H
- For each energy λ_j, there corresponds to an energy eigenstate $|v_j\rangle$ such that $H|v_j\rangle = \lambda|v_j\rangle$

Arbitrary state energies

- Let $|\psi\rangle = \alpha_1|v_1\rangle + \cdots + \alpha_n|v_n\rangle$
- Then

$$e^{-iHt}|\psi\rangle = \alpha_1 e^{-i\lambda_1 t}|v_1\rangle + \cdots + e^{-i\lambda_n t}\alpha_n|v_n\rangle$$

- This means
  - the universe just evolves by picking up phases, each rotating around the unit circle at a speed proportional to its energy.
  - life is a basis-dependent phenomenon
  - we can define energy as the speed at which a quantum state picks up a phase
  - The energy $\sum_j |\alpha_j|^2 \lambda_j$ in the state $|\psi\rangle$ stays the same over time

Arbitrary state energies

- Let $|\psi\rangle = \alpha_1|v_1\rangle + \cdots + \alpha_n|v_n\rangle$
- Then

$$e^{-iHt}|\psi\rangle = \alpha_1 e^{-i\lambda_1 t}|v_1\rangle + \cdots + e^{-i\lambda_n t}\alpha_n|v_n\rangle$$

- This means
  - the universe just evolves by picking up phases, each rotating around the unit circle at a speed proportional to its energy.
  - life is a basis-dependent phenomenon
  - we can define energy as the speed at which a quantum state picks up a phase
  - The energy $\sum_j |\alpha_j|^2 \lambda_j$ in the state $|\psi\rangle$ stays the same over time

Arbitrary state energies

- Let $|\psi\rangle = \alpha_1|v_1\rangle + \cdots + \alpha_n|v_n\rangle$
- Then

$$e^{-iHt}|\psi\rangle = \alpha_1 e^{-i\lambda_1 t}|v_1\rangle + \cdots + e^{-i\lambda_n t}\alpha_n|v_n\rangle$$

- This means
  - the universe just evolves by picking up phases, each rotating around the unit circle at a speed proportional to its energy.
  - life is a basis-dependent phenomenon
  - we can define energy as the speed at which a quantum state picks up a phase
  - The energy $\sum_j |\alpha_j|^2 \lambda_j$ in the state $|\psi\rangle$ stays the same over time

Arbitrary state energies

- Let $|\psi\rangle = \alpha_1|v_1\rangle + \cdots + \alpha_n|v_n\rangle$
- Then

$$e^{-iHt}|\psi\rangle = \alpha_1 e^{-i\lambda_1 t}|v_1\rangle + \cdots + e^{-i\lambda_n t}\alpha_n|v_n\rangle$$

- This means
  - the universe just evolves by picking up phases, each rotating around the unit circle at a speed proportional to its energy.
  - life is a basis-dependent phenomenon
  - we can define energy as the speed at which a quantum state picks up a phase
  - The energy $\sum_j |\alpha_j|^2 \lambda_j$ in the state $|\psi\rangle$ stays the same over time

Arbitrary state energies

- Let $|\psi\rangle = \alpha_1|v_1\rangle + \cdots + \alpha_n|v_n\rangle$
- Then

$$e^{-iHt}|\psi\rangle = \alpha_1 e^{-i\lambda_1 t}|v_1\rangle + \cdots + e^{-i\lambda_n t}\alpha_n|v_n\rangle$$

- This means
  - the universe just evolves by picking up phases, each rotating around the unit circle at a speed proportional to its energy.
  - life is a basis-dependent phenomenon
  - we can define energy as the speed at which a quantum state picks up a phase
  - The energy $\sum_j |\alpha_j|^2 \lambda_j$ in the state $|\psi\rangle$ stays the same over time

Arbitrary state energies

- Let $|\psi\rangle = \alpha_1|v_1\rangle + \cdots + \alpha_n|v_n\rangle$
- Then

$$e^{-iHt}|\psi\rangle = \alpha_1 e^{-i\lambda_1 t}|v_1\rangle + \cdots + e^{-i\lambda_n t}\alpha_n|v_n\rangle$$

- This means
  - the universe just evolves by picking up phases, each rotating around the unit circle at a speed proportional to its energy.
  - life is a basis-dependent phenomenon
  - we can define energy as the speed at which a quantum state picks up a phase
  - The energy $\sum_j |\alpha_j|^2 \lambda_j$ in the state $|\psi\rangle$ stays the same over time

Arbitrary state energies

- Let $|\psi\rangle = \alpha_1|v_1\rangle + \cdots + \alpha_n|v_n\rangle$
- Then

$$e^{-iHt}|\psi\rangle = \alpha_1 e^{-i\lambda_1 t}|v_1\rangle + \cdots + e^{-i\lambda_n t}\alpha_n|v_n\rangle$$

- This means
  - the universe just evolves by picking up phases, each rotating around the unit circle at a speed proportional to its energy.
  - life is a basis-dependent phenomenon
  - we can define energy as the speed at which a quantum state picks up a phase
  - The energy $\sum_j |\alpha_j|^2 \lambda_j$ in the state $|\psi\rangle$ stays the same over time

Ground state

- The energy eigenstate $|v_1\rangle$ corresponds to the lowest energy and is called the ground state
- The value λ_1 is the ground state energy
- The energy eigenstate $|v_2\rangle$ corresponds to the second-lowest energy and is called the first excited state
- If $\lambda_1 = \lambda_2$, then we call this as a ground state degeneracy
- Physical systems likes to minimize their energy and then stay there do nothing
- Ground state is the lowest state they can go

Ground state

- The energy eigenstate $|v_1\rangle$ corresponds to the lowest energy and is called the ground state
- The value λ_1 is the ground state energy
- The energy eigenstate $|v_2\rangle$ corresponds to the second-lowest energy and is called the first excited state
- If $\lambda_1 = \lambda_2$, then we call this as a ground state degeneracy
- Physical systems likes to minimize their energy and then stay there do nothing
- Ground state is the lowest state they can go

Ground state

- The energy eigenstate $|v_1\rangle$ corresponds to the lowest energy and is called the ground state
- The value λ_1 is the ground state energy
- The energy eigenstate $|v_2\rangle$ corresponds to the second-lowest energy and is called the first excited state
- If $\lambda_1 = \lambda_2$, then we call this as a ground state degeneracy
- Physical systems likes to minimize their energy and then stay there do nothing
- Ground state is the lowest state they can go

Ground state

- The energy eigenstate $|v_1\rangle$ corresponds to the lowest energy and is called the ground state
- The value λ_1 is the ground state energy
- The energy eigenstate $|v_2\rangle$ corresponds to the second-lowest energy and is called the first excited state
- If $\lambda_1 = \lambda_2$, then we call this as a ground state degeneracy
- Physical systems likes to minimize their energy and then stay there do nothing
- Ground state is the lowest state they can go

Ground state

- The energy eigenstate $|v_1\rangle$ corresponds to the lowest energy and is called the ground state
- The value λ_1 is the ground state energy
- The energy eigenstate $|v_2\rangle$ corresponds to the second-lowest energy and is called the first excited state
- If $\lambda_1 = \lambda_2$, then we call this as a ground state degeneracy
- Physical systems likes to minimize their energy and then stay there do nothing
- Ground state is the lowest state they can go

Ground state

- The energy eigenstate $|v_1\rangle$ corresponds to the lowest energy and is called the ground state
- The value λ_1 is the ground state energy
- The energy eigenstate $|v_2\rangle$ corresponds to the second-lowest energy and is called the first excited state
- If $\lambda_1 = \lambda_2$, then we call this as a ground state degeneracy
- Physical systems likes to minimize their energy and then stay there do nothing
- Ground state is the lowest state they can go

Ground state

- A ball rolls downhill to reach the ground state with lowest potential energy and the kinetic energy that used to be in the ball dissipates away in the heat
- For quantum systems that we found in Nature, they're often sitting in their ground states. If they weren't, then their interactions with surroundicng systems would tend to carry away excess energy until they were
- the ground state of a hydrogen atom has the electron sitting in the lowest shell (the one closest to the nucleus).
- The first excited state has the electron in the next shell up
- If the atom is in its first excited state, it can drop back down to its ground state via the electron emitting a photon. The photon carries away an amount of energy $\lambda_2 - \lambda_1$
- A hydrogen atom in its ground state can jump up to its first excited state via the electron absorbing a photon (rare)

Ground state

- A ball rolls downhill to reach the ground state with lowest potential energy and the kinetic energy that used to be in the ball dissipates away in the heat
- For quantum systems that we found in Nature, they're often sitting in their ground states. If they weren't, then their interactions with surroundicng systems would tend to carry away excess energy until they were
- the ground state of a hydrogen atom has the electron sitting in the lowest shell (the one closest to the nucleus).
- The first excited state has the electron in the next shell up
- If the atom is in its first excited state, it can drop back down to its ground state via the electron emitting a photon. The photon carries away an amount of energy $\lambda_2 - \lambda_1$
- A hydrogen atom in its ground state can jump up to its first excited state via the electron absorbing a photon (rare)

Ground state

- A ball rolls downhill to reach the ground state with lowest potential energy and the kinetic energy that used to be in the ball dissipates away in the heat
- For quantum systems that we found in Nature, they're often sitting in their ground states. If they weren't, then their interactions with surroundicng systems would tend to carry away excess energy until they were
- the ground state of a hydrogen atom has the electron sitting in the lowest shell (the one closest to the nucleus).
- The first excited state has the electron in the next shell up
- If the atom is in its first excited state, it can drop back down to its ground state via the electron emitting a photon. The photon carries away an amount of energy $\lambda_2 - \lambda_1$
- A hydrogen atom in its ground state can jump up to its first excited state via the electron absorbing a photon (rare)

Ground state

- A ball rolls downhill to reach the ground state with lowest potential energy and the kinetic energy that used to be in the ball dissipates away in the heat
- For quantum systems that we found in Nature, they're often sitting in their ground states. If they weren't, then their interactions with surroundicng systems would tend to carry away excess energy until they were
- the ground state of a hydrogen atom has the electron sitting in the lowest shell (the one closest to the nucleus).
- The first excited state has the electron in the next shell up
- If the atom is in its first excited state, it can drop back down to its ground state via the electron emitting a photon. The photon carries away an amount of energy $\lambda_2 - \lambda_1$
- A hydrogen atom in its ground state can jump up to its first excited state via the electron absorbing a photon (rare)

Ground state

- A ball rolls downhill to reach the ground state with lowest potential energy and the kinetic energy that used to be in the ball dissipates away in the heat
- For quantum systems that we found in Nature, they're often sitting in their ground states. If they weren't, then their interactions with surroundicng systems would tend to carry away excess energy until they were
- the ground state of a hydrogen atom has the electron sitting in the lowest shell (the one closest to the nucleus).
- The first excited state has the electron in the next shell up
- If the atom is in its first excited state, it can drop back down to its ground state via the electron emitting a photon. The photon carries away an amount of energy $\lambda_2 - \lambda_1$
- A hydrogen atom in its ground state can jump up to its first excited state via the electron absorbing a photon (rare)

Ground state

- A ball rolls downhill to reach the ground state with lowest potential energy and the kinetic energy that used to be in the ball dissipates away in the heat
- For quantum systems that we found in Nature, they're often sitting in their ground states. If they weren't, then their interactions with surroundicng systems would tend to carry away excess energy until they were
- the ground state of a hydrogen atom has the electron sitting in the lowest shell (the one closest to the nucleus).
- The first excited state has the electron in the next shell up
- If the atom is in its first excited state, it can drop back down to its ground state via the electron emitting a photon. The photon carries away an amount of energy $\lambda_2 - \lambda_1$
- A hydrogen atom in its ground state can jump up to its first excited state via the electron absorbing a photon (rare)

Addition of Hamiltonians

- In general, a collection of physical subsystems forming a larger system usually have Hamiltonian of the form

$$\hat{H} = \sum_{k=1}^{L} \hat{H}_k$$

where $\hat{H}_k$ is a Hamiltonian acting on a small number of nearby subsystems and L is polynomial in the number of sussystems

Addition of Hamiltonians

- For example $H_{SM} = H_{Kinetic} + H_{EM} + H_{Strong} + H_{Weak}$ where $H_{Kinetic}$ is the Hamiltonian that would act even if there were no forces (corresponding to Newton's First Law of Motion), and H_{EM}, H_{Strong}, and H_{Weak} are the Hamiltonians corresponding to electromagnetism and to the strong and weak nuclear forces respectively
- Unfortunately, genearally we do not have $e^{A+B} = e^A e^B$!
- However, if $AB = BA$, then we have $e^{A+B} = e^A e^B$!

Addition of Hamiltonians

- For example $H_{SM} = H_{Kinetic} + H_{EM} + H_{Strong} + H_{Weak}$ where $H_{Kinetic}$ is the Hamiltonian that would act even if there were no forces (corresponding to Newton's First Law of Motion), and H_{EM}, H_{Strong}, and H_{Weak} are the Hamiltonians corresponding to electromagnetism and to the strong and weak nuclear forces respectively
- Unfortunately, genearally we do not have $e^{A+B} = e^A e^B$!
- However, if $AB = BA$, then we have $e^{A+B} = e^A e^B$!

Addition of Hamiltonians

- For example $H_{SM} = H_{Kinetic} + H_{EM} + H_{Strong} + H_{Weak}$ where $H_{Kinetic}$ is the Hamiltonian that would act even if there were no forces (corresponding to Newton's First Law of Motion), and H_{EM}, H_{Strong}, and H_{Weak} are the Hamiltonians corresponding to electromagnetism and to the strong and weak nuclear forces respectively
- Unfortunately, genearally we do not have $e^{A+B} = e^A e^B$!
- However, if $AB = BA$, then we have $e^{A+B} = e^A e^B$!

Addition of Hamiltonians

- Each $e^{i\hat{H}_j t}$ would be easy to simulate
- Unfortunately, the $\hat{H}_k$ do not necessarily commute which means that

$$e^{i\hat{H}t} \neq e^{i\hat{H}_1 t} \cdot e^{i\hat{H}_2 t} \ldots e^{i\hat{H}_L t}$$

Addition of Hamiltonians

- Each $e^{i\hat{H}_j t}$ would be easy to simulate
- Unfortunately, the $\hat{H}_k$ do not necessarily commute which means that

$$e^{i\hat{H}t} \neq e^{i\hat{H}_1 t} \cdot e^{i\hat{H}_2 t} \ldots e^{i\hat{H}_L t}$$

Approximiations: Trotterization

Theorem 4.3 (**Trotterization**): For Hermitian operators A and B and any real t,

$$\lim_{n\to\infty}\left(e^{iAt/n}\cdot e^{iBt/n}\right)^n = e^{i(A+B)t}$$

Exercise 4.50: Let

$$U_{\Delta t} = \left[e^{-i\hat{H}_1\Delta t}e^{-i\hat{H}_2\Delta t}\dots e^{-i\hat{H}_L\Delta t}\right]\left[e^{-i\hat{H}_L\Delta t}e^{-i\hat{H}_{L-1}\Delta t}\dots e^{-i\hat{H}_1\Delta t}\right]$$

Then

$$E(U_{\Delta t}^m, e^{-2mi\hat{H}\Delta t}) \leq m\alpha\Delta t^3$$

Simulation Algorithm: Inputs

- $\hat{H} = \sum_{k=1}^{L} \hat{H}_k$ where each $\hat{H}_k$ acts non-trivially on a subsystem of size bounded by a constant.
- A description of an easy-to-prepare quantum state $|\psi_0\rangle$
- A positive accuracy δ
- A time t_f of which the evolved state is desired

Simulation Algorithm: Inputs

- $\hat{H} = \sum_{k=1}^{L} \hat{H}_k$ where each $\hat{H}_k$ acts non-trivially on a subsystem of size bounded by a constant.
- A description of an easy-to-prepare quantum state $|\psi_0\rangle$
- A positive accuracy δ
- A time t_f of which the evolved state is desired

Simulation Algorithm: Inputs

- $\hat{H} = \sum_{k=1}^{L} \hat{H}_k$ where each $\hat{H}_k$ acts non-trivially on a subsystem of size bounded by a constant.
- A description of an easy-to-prepare quantum state $|\psi_0\rangle$
- A positive accuracy δ
- A time t_f of which the evolved state is desired

Simulation Algorithm: Inputs

- $\hat{H} = \sum_{k=1}^{L} \hat{H}_k$ where each $\hat{H}_k$ acts non-trivially on a subsystem of size bounded by a constant.
- A description of an easy-to-prepare quantum state $|\psi_0\rangle$
- A positive accuracy δ
- A time t_f of which the evolved state is desired

Simulation Algorithm: Outputs and runtime

- A state $|\hat{\psi}(t_f)\rangle$ such that

$$\left|\langle\hat{\psi}(t_f)|e^{-i\hat{H}t_f}|\psi_0\rangle\right|^2 \geq 1-\delta$$

- Runtime $O(poly(\frac{1}{\delta}, L, t_f))$

Simulation Algorithm: Outputs and runtime

- A state $|\hat{\psi}(t_f)\rangle$ such that

$$\left|\langle\hat{\psi}(t_f)|e^{-i\hat{H}t_f}|\psi_0\rangle\right|^2 \geq 1-\delta$$

- Runtime $O(poly(\frac{1}{\delta}, L, t_f))$

Simulation Algorithm

- Pick a suitable approximation to $e^{-i\hat{H}t_f}$
- For example, using Exercise 4.50, set

$$m \in O\left(\sqrt{\frac{t_f^3}{\delta}}\right), \Delta t \in O\left(\sqrt{\frac{t_f}{\delta}}\right)$$

  so that $m\Delta t = t_f$ and $m(\Delta t)^3 \in O(\delta)$
- Approximate each $\tilde{U}_{\Delta t}$ with accuracy in $O(\frac{\delta}{m})$ which can be done by approximating each $e^{-i\hat{H}_j t}$ with accuracy in $O(\frac{\delta}{L_m})$

Simulation Algorithm

- Pick a suitable approximation to $e^{-i\hat{H}t_f}$
- For example, using Exercise 4.50, set

$$m \in O\left(\sqrt{\frac{t_f^3}{\delta}}\right), \Delta t \in O\left(\sqrt{\frac{t_f}{\delta}}\right)$$

  so that $m\Delta t = t_f$ and $m(\Delta t)^3 \in O(\delta)$
- Approximate each $\tilde{U}_{\Delta t}$ with accuracy in $O(\frac{\delta}{m})$ which can be done by approximating each $e^{-i\hat{H}_j t}$ with accuracy in $O(\frac{\delta}{L_m})$

Simulation Algorithm

- Pick a suitable approximation to $e^{-i\hat{H}t_f}$
- For example, using Exercise 4.50, set

$$m \in O\left(\sqrt{\frac{t_f^3}{\delta}}\right), \Delta t \in O\left(\sqrt{\frac{t_f}{\delta}}\right)$$

  so that $m\Delta t = t_f$ and $m(\Delta t)^3 \in O(\delta)$
- Approximate each $\tilde{U}_{\Delta t}$ with accuracy in $O(\frac{\delta}{m})$ which can be done by approximating each $e^{-i\hat{H}_j t}$ with accuracy in $O(\frac{\delta}{L_m})$

Simulation Algorithm

1. Prepar $|\tilde{\psi}_0\rangle$ with accuracy in $O(\delta)$
2. Set $j = 1$
3. Compute $|\tilde{\psi}_j\rangle = \tilde{U}_{\Delta t}|\tilde{\psi}_{j-1}\rangle$
4. If $j < m$, increment j and goto Step 3. Otherwise output $|\tilde{\psi}_{t_f}\rangle = |\tilde{\psi}_m\rangle = \tilde{U}^m_{\Delta t}|\tilde{\psi}_0\rangle$

Simulation Algorithm

1. Prepar $|\tilde{\psi}_0\rangle$ with accuracy in $O(\delta)$
2. Set $j = 1$
3. Compute $|\tilde{\psi}_j\rangle = \tilde{U}_{\Delta t}|\tilde{\psi}_{j-1}\rangle$
4. If $j < m$, increment j and goto Step 3. Otherwise output $|\tilde{\psi}_{t_f}\rangle = |\tilde{\psi}_m\rangle = \tilde{U}^m_{\Delta t}|\tilde{\psi}_0\rangle$

Simulation Algorithm

1. Prepar $|\tilde{\psi}_0\rangle$ with accuracy in $O(\delta)$
2. Set $j = 1$
3. Compute $|\tilde{\psi}_j\rangle = \tilde{U}_{\Delta t}|\tilde{\psi}_{j-1}\rangle$
4. If $j < m$, increment j and goto Step 3. Otherwise output $|\tilde{\psi}_{t_f}\rangle = |\tilde{\psi}_m\rangle = \tilde{U}^m_{\Delta t}|\tilde{\psi}_0\rangle$

Simulation Algorithm

1. Prepar $|\tilde{\psi}_0\rangle$ with accuracy in $O(\delta)$
2. Set $j = 1$
3. Compute $|\tilde{\psi}_j\rangle = \tilde{U}_{\Delta t}|\tilde{\psi}_{j-1}\rangle$
4. If $j < m$, increment j and goto Step 3. Otherwise output $|\tilde{\psi}_{t_f}\rangle = |\tilde{\psi}_m\rangle = \tilde{U}^m_{\Delta t}|\tilde{\psi}_0\rangle$

Example Simulation Algorithm: *k-local Hamiltonian problem*

INSTANCE: a collection $\{\hat{H}_n\}$ of Hamiltonians each of which acts on at most k qubits; real numbers a, b such that $b - a = O(1/poly(n))$.

QUESTION: is the smallest eigenvalue of $\sum_{j=1}^{n} H_j$ less than a or greater than b, promised that this is the case?

Example Simulation Algorithm: k-SAT

Consider a given boolean formula:

$$C_1 \wedge C_2 \wedge \ldots \wedge C_M$$

over the variables $x_1, x_2, \ldots, x_N$; each C_i is the disjunction $\left(b_{i_1} \vee b_{i_2} \vee \ldots \vee b_{i_k}\right)$ and b_i is either x_i or its negation $\neg x_i$. Our problem is to decide whether there is an assignment to the boolean variables $x_1, x_2, \ldots, x_N$ that satisfies all the clauses simultaneously.

Example Simulation Algorithm: k-SAT

For a clause $C_i = \left(b_{i_1} \vee b_{i_2} \vee \ldots \vee b_{i_k}\right)$ define the local function:

$$f_{C_i}(x_1, x_2, \ldots, x_N) = \prod_{i_j \in \Lambda_+^i} (1 - x_{i_j}) \cdot \prod_{i_j \in \Lambda_-^i} x_{i_j}$$

Λ_-^i, Λ_+^i containing all the indices of the variables that compare negated or not negated in the clause C_i respectively. Given an assignment $(x_1, x_2, \ldots, x_N)$, the function f_{C_i} will return 0 if the clause C_i is satisfied, 1 otherwise.
The cost $V(x_1, x_2, \ldots, x_N)$ of an assignment can be defined therefore in terms of the functions f_{C_i} as:

$$V(x_1, x_2, \ldots, x_N) = \sum_{i=1}^{M} f_{C_i}(x_1, x_2, \ldots, x_N),$$

that is the total number of violated clauses. An instance of k-SAT is satisfiable if there exists a configuration of zero cost.

Example Simulation Algorithm: translating k-SAT to k-local Hamiltonian

To each variable x_i we assign a *qubit*. For the sake of definiteness we will consider spins $(\sigma_1(i), \sigma_2(i), \sigma_3(i))$, $i = 1, 2, \ldots, N$ and their component $\sigma_3(i)$ along the z axis of a given reference frame as computational direction. Furthermore, we decide that if an assignment assigns the value 1 (*true*) to the variable x_i then the corresponding qubit is in the state $\sigma_3(i) = +1$ (spin up) and in the state $\sigma_3(i) = -1$ otherwise. To each clause we associate the Hamiltonian term:

$$H_i = \prod_{i_j \in \Lambda_+^i} \frac{1 - \sigma_3(i_j)}{2} \cdot \prod_{i_j \in \Lambda_-^i} \frac{1 + \sigma_3(i_j)}{2}, \tag{1}$$

which acts non trivially only on k qubits.

Example Simulation Algorithm: translating k-SAT to k-local Hamiltonian

The total Hamiltonian:

$$H = \sum_{i=1}^{M} H_i \tag{2}$$

is k-local and plays the role of a cost function: if an assignment satisfies all the clauses simultaneously then the corresponding energy is zero. Otherwise the energy would be equal to the number of violated clauses, thus > 0.
So we get
INSTANCE: Hamiltonian $H = \sum_{j=1}^{M} P_j$ acting on N qubits, where each P_j is *projector* on a 2^k dimensional subspace of the whole (2^N) dimensional Hilbert space.

QUESTION: Is the ground state energy E_0 of H zero, promised that either $E_0 = 0$ or $E_0 > 1/poly(N)$?

Quantum Adiabatic Computation (QAC)

QAC is based on the well known adiabatic theorem. Given a time $T > 0$ and two Hamiltonians H_I and H_T we consider the time dependent Hamiltonian:

$$H(t) = tH_T + (T - t)H_I,\ 0 \leq t \leq T, \tag{3}$$

or, equivalently,

$$\tilde{H}(s) = H\left(\frac{t}{T}\right),\ 0 \leq s \leq 1.$$

Let us indicate with $|s; e_k(s)\rangle$ the *instantaneous eigenvector* of $\tilde{H}(s)$ corresponding to the *instantaneous eigenvalue* $e_k(s)$ with $e_0(s) \leq e_1(s) \leq \ldots \leq e_n(s)$, $0 \leq s \leq 1$ and by $|\psi(s)\rangle$ the solution of the Cauchy problem:

$$\begin{cases} i\frac{d}{ds}|\psi(s)\rangle = \tilde{H}(s)|\psi(s)\rangle \\ |\psi(0)\rangle = |0; e_0(0)\rangle. \end{cases}$$

Quantum Adiabatic Computation (QAC)

The adiabatic theorem states that, if the time T satisfies $T \gg \frac{\xi}{g_{min}^2}$ where g_{min} is the minimum gap

$$g_{min} = \min_{0 \le s \le 1} (e_1(s) - e_0(s))$$

and

$$\xi = \max_{0 \le s \le 1} \left| \langle s; e_1(s) | \frac{d\tilde{H}}{ds} | s; e_0(s) \rangle \right|,$$

then $|\langle 1; e_0(1) | \psi(1) \rangle|$ can be made arbitrarily close to 1. In other words if we start in the state $|0; e_0(0)\rangle$ we will end up in the ground state $|T; e_0(T)\rangle$ of the target Hamiltonian H_T.

Quantum Adiabatic Computation (QAC)

In practical cases ξ is not too large; thus the size of T is governed by g_{min}^{-2}: the smaller g_{min} the slower must be the change rate of the Hamiltonian if we want to avoid transitions.

Q&A

Q&A?