Continuous time quantum algorithms

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Quantum systems evolve according to the Schrödinger equation
\[ i \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \]

Such systems can be efficiently simulated by a universal quantum computer when \( H \) has an appropriate form.

Maybe these dynamics can be used to do interesting computations.
I. Quantum walk

\[ H = \]
Undirected graph $G$ with no self loops

**Adjacency matrix:** $A_{jk} = \begin{cases} 1 & (j, k) \in G \\ 0 & \text{otherwise} \end{cases}$

**Laplacian:** $L = A - D$ \[D \text{ diagonal, } D_{jj} = \text{deg}(j)\]

$L$ is positive semidefinite
$L(\sum_j |j\rangle) = 0$
All other eigenvalues are positive (if $G$ is connected)
Random walks/Markov chains are used in many classical algorithms.

**Discrete time random walk**
At each step, equal probability of jumping to each connected vertex

$$p_{a}(t + 1) = \sum_{b: (a, b) \in G} \frac{p_{b}(t)}{\text{deg}(b)}$$

**Continuous time random walk**
Probability per unit time $\gamma$ of jumping to each connected vertex

$$\frac{dp_{a}(t)}{dt} = \sum_{b: (a, b) \in G} \gamma p_{b}(t) - \gamma \text{deg}(a)p_{a}(t)$$

$$= \sum_{b} L_{ab} p_{b}(t)$$
Quantum walk

How to define a quantum analogue of a random walk on an \( N \)-vertex graph \( G \)?

Proposal:
- Basis state \( |a\rangle \) for each vertex \( a \)
- At each step, move to all adjacent sites with equal amplitude

This does not work!

Example:

Walk cannot be unitary.

\[
|4\rangle \rightarrow \frac{1}{\sqrt{2}}(|3\rangle + |5\rangle) \\
|6\rangle \rightarrow \frac{1}{\sqrt{2}}(|5\rangle + |7\rangle)
\]

Meyer 96
Quantum walk

Two alternatives:

1. Introduce extra variables
   State space: Directed edges $|a,b\rangle$

   $|j, L\rangle \rightarrow \frac{1}{\sqrt{2}}(|j - 1, L\rangle + |j - 1, R\rangle)$
   $|j, R\rangle \rightarrow \frac{1}{\sqrt{2}}(|j + 1, L\rangle - |j + 1, R\rangle)$

2. Continuous time
<table>
<thead>
<tr>
<th>Random walk</th>
<th>Quantum walk</th>
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</thead>
<tbody>
<tr>
<td><strong>State space</strong></td>
<td><strong>Basis states</strong></td>
</tr>
<tr>
<td>$N$ vertices $j=1,...,N$</td>
<td>$N$ basis states $</td>
</tr>
<tr>
<td>$p_j = \text{probability of being at vertex } j$</td>
<td>$q_j = \langle j</td>
</tr>
<tr>
<td><strong>Differential equation</strong></td>
<td><strong>Generator</strong></td>
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<tr>
<td>$\frac{dp_j}{dt} = \gamma \sum_k L_{jk} p_k$</td>
<td>$i\frac{dq_j}{dt} = \sum_k H_{jk} q_k$</td>
</tr>
<tr>
<td><strong>Generator</strong></td>
<td><strong>Probability conservation</strong></td>
</tr>
<tr>
<td>$\gamma L, L = \text{Laplacian of } G$</td>
<td>$H = H^\dagger$ $\Rightarrow \frac{d}{dt} \sum_j</td>
</tr>
<tr>
<td><strong>Probability conservation</strong></td>
<td></td>
</tr>
<tr>
<td>$\sum_j L_{jk} = 0 \Rightarrow \frac{d}{dt} \sum_j p_j = 0$</td>
<td></td>
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</tbody>
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**Walk on a line**

**Infinite line:**

\[ i \frac{d}{dt} q_x = q_{x-1} + q_{x+1} \]

Eigenstates of A: \( \langle x| p \rangle = \frac{1}{\sqrt{2\pi}} e^{ipx} \), \(-\pi \leq p \leq \pi\)

Eigenvalues: \( E_p = 2 \cos p \)

Amplitude to go from \( x \) to \( y \):

\[ \langle y| e^{-iAt} |x \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} dp \ e^{ip(y-x) - 2it\cos p} \]

\[ = (-i)^{y-x} J_{y-x}(2t) \]

⇒ Walk propagates with speed 2: in time \( t \), walk moves a distance \( 2t \).

(Classical random walk: in time \( t \), walk moves a distance \( \propto \sqrt{t} \).)
Mixing times

How long does it take for the walk to spread out over the entire graph?

**Classical random walk:** $p$ approaches a limiting distribution as $t \to \infty$

\[
e^{Lt} = \sum_j e^{-E_j t} |\phi_j \rangle \langle \phi_j|
\]

\[
\to |\phi_0 \rangle \langle \phi_0|
\]

\[
= \frac{1}{N} \begin{pmatrix}
1 & \cdots & 1 \\
\vdots & \ddots & \vdots \\
1 & \cdots & 1
\end{pmatrix}
\]

\[
p_a^\infty = \frac{1}{N}
\]

**Mixing time:** $T \propto 1/E_1$
**Quantum walk:** no limiting distribution — dynamics are unitary!

But consider:

\[ q_{ab} = \frac{1}{T} \int_{0}^{T} dt \left| \langle a | e^{-iHt} | b \rangle \right|^2 \]

\[ = \frac{1}{T} \int_{0}^{T} dt \left| \sum_{j,k} \langle a | \phi_j \rangle \langle \phi_j | e^{-iHt} | \phi_k \rangle \langle \phi_k | b \rangle \right|^2 \]

\[ = \frac{1}{T} \int_{0}^{T} dt \left| \sum_{j} e^{-iE_j t} \langle a | \phi_j \rangle \langle \phi_j | b \rangle \right|^2 \]

\[ = \frac{1}{T} \int_{0}^{T} dt \sum_{j,k} e^{-i(E_j - E_k) t} \langle a | \phi_j \rangle \langle \phi_j | b \rangle \langle b | \phi_k \rangle \langle \phi_k | a \rangle \]

for \( T \gg \min_{j,k, E_j \neq E_k} \frac{1}{|E_j - E_k|} \):

\[ q_{ab}^\infty = \sum_{j,k} \delta_{E_j,E_k} \langle a | \phi_j \rangle \langle \phi_j | b \rangle \langle b | \phi_k \rangle \langle \phi_k | a \rangle \]

\[ = \sum_{j} \left| \langle a | \phi_j \rangle \langle \phi_j | b \rangle \right|^2 \]

no degeneracy:

Aharonov, Ambainis, Kempe, Vazirani 00
Hitting times

How long does it take for the walk to reach a particular vertex?

More precisely, we say the hitting time of the walk from $a$ to $b$ is polynomial in $n$ if for some $t=\text{poly}(n)$ there is a probability $1/\text{poly}(n)$ of being at $b$, starting from $a$. 
Theorem: Let $G_n$ be a family of graphs with designated ENTRANCE and EXIT vertices. Suppose the hitting time of the classical random walk from ENTRANCE to EXIT is polynomial in $n$. Then the hitting time of the quantum walk from ENTRANCE to EXIT is also polynomial in $n$ (for a closely related graph).

Proof idea: Analytically continue the classical walk, $t \rightarrow i \, t$. 

Farhi, Gutmann 97
Let $|\psi(0)\rangle = |00\ldots0\rangle$; then $|\psi(t)\rangle = e^{-iAt} |00\ldots0\rangle$.

Probability of reaching opposite corner in time $t$: 
$|\langle\psi(t)|11\ldots1\rangle|^2 = (\sin t)^{2n}$

Classical hitting time is exponential in $n$!

Moore, Russell 02
Black box graph traversal problem

Names of vertices: random $2n$-bit strings ($n=\lceil \log N \rceil$)
Name of ENTRANCE is known
Oracle outputs the names of adjacent vertices
$v_c(a) = c$th neighbor of $a$

Examples:

$v_1(\text{ENTRANCE}) = 0110101$  
$v_1(0110101) = 1001101$
$v_2(\text{ENTRANCE}) = 1110100$  
$v_2(0110101) = \text{ENTRANCE}$
$v_3(\text{ENTRANCE}) = 1111111$  
$v_3(0110101) = 1110100$
$v_4(\text{ENTRANCE}) = 1111111$  
$v_4(0110101) = 1111111$
Exponential speedup
Reduction of the quantum walk

Column subspace

\[
|\text{col } j\rangle = \frac{1}{\sqrt{N_j}} \sum_{a \in \text{column } j} |a\rangle
\]

where

\[
N_j = \begin{cases} 
2^j & 0 \leq j \leq n \\
2^{2n+1-j} & n+1 \leq j \leq 2n+1
\end{cases}
\]

Reduced Hamiltonian

\[
\langle \text{col } j | H | \text{col}(j+1) \rangle
\]

\[
= \begin{cases} 
\sqrt{2} \gamma & 0 \leq j \leq n-1, \\
\gamma & n+1 \leq j \leq 2n \\
2\gamma & j = n
\end{cases}
\]

\[
\gamma = \frac{1}{\sqrt{2}}
\]
**Theorem:** Any classical algorithm that makes at most $2^{n/6}$ queries to the oracle finds the **EXIT** with probability at most $4 \cdot 2^{-n/6}$. 
II. Quantum computation by adiabatic evolution

\[ \frac{1}{\sqrt{N}} \sum_x |x\rangle \to H(t) \to |\text{solution}\rangle \]
Encode the solution of a computational problem in the ground state of a Hamiltonian.

**Example:** $k$-SAT

$\exists x_1, \ldots, x_n \in \{0,1\}$:

$$(x_1 \lor x_3 \lor \neg x_{11}) \land \cdots \land (\neg x_{23} \lor x_{42} \lor \neg x_{17}) = 1$$

Let $h_C = 0$ if clause $C$ is satisfied

$h_C = 1$ if clause $C$ is not satisfied

Minimize $h = \sum_C h_C$

Equivalently, find the ground state of

$H = \sum_x h(x) \left| x \right\rangle \langle x \right|$
The adiabatic theorem

Rough version:
Let \( H(t) \) be slowly varying.
Let \( |\psi(0)\rangle = |E_j(0)\rangle \).
Then \( |\psi(T)\rangle \approx |E_j(T)\rangle \).

More precisely:
Let \( \tilde{H}(s) \) be a smooth function of \( s \in [0,1] \).
Let \( H(t) = \tilde{H}(t/T) \).
Let \( |\psi(0)\rangle = |E_0(0)\rangle \).
Then \( |\psi(T)\rangle \approx |E_0(T)\rangle \) so long as
\[
T \gg \frac{\Gamma(s)}{[E_1(s) - E_0(s)]^2}
\]
where
\[
\Gamma^2(s) = \langle \phi_0(s) | \left( \frac{dH}{ds} \right)^2 | \phi_0(s) \rangle - \langle \phi_0(s) | \frac{dH}{ds} | \phi_0(s) \rangle^2
\]
Adiabatic quantum computation

Let $\tilde{H}(0)=H_B$ be a Hamiltonian whose ground state is easy to prepare.

**Example:** $H_B = -\sum_j \sigma_x^{(j)}$, ground state $\frac{1}{2^n/2} \sum_{z=0}^{2^n-1} |z\rangle$

Let $\tilde{H}(1)=H_P$ be a Hamiltonian whose ground state encodes the solution to the problem.

**Example:** $H_P = \sum_z h(z) |z\rangle \langle z|$ to minimize $h(z)$

Let $\tilde{H}(s)$ interpolate from $H_B$ to $H_P$.

**Example:** $\tilde{H}(s) = (1-s) H_B + s H_P$

Start in $|E_0(0)\rangle$, evolve for time $T$, and measure.
Adiabatic Grover search

Minimize function \( h(z) = \begin{cases} 0 & z = w \\ 1 & z \neq w \end{cases} \)

\[
H_P = -|w\rangle\langle w| \\
H_B = -|s\rangle\langle s| \\
|s\rangle = \frac{1}{\sqrt{N}} \sum_x |x\rangle 
\]

Roland, Cerf 01; van Dam, Mosca, Vazirani 01
Minimize function \( h(z) = \begin{cases} 0 & z = w \\ 1 & z \neq w \end{cases} \)

\[ H_P = -|w\rangle\langle w| \]

\[ H_B = -|s\rangle\langle s| \]

\[ |s\rangle = \frac{1}{\sqrt{N}} \sum_x |x\rangle \]

\[ \tilde{H}(s) = [1-f(s)] H_B + f(s) H_P \]

Roland, Cerf 01; van Dam, Mosca, Vazirani 01
Hard problems

How well does the adiabatic algorithm work on hard problems?

Note: We could learn a lot more if we had even a small quantum computer (say 30 qubits)!

Farhi, Goldstone, Gutmann, Lapan, Lundgren, Preda 02
Theorem: The output of any quantum circuit (acting on the $|0\rangle$ state) can be efficiently simulated by an adiabatic quantum computation with linear interpolation $\hat{H}(s) = (1-s) H_B + s H_P$ where $H_B$ and $H_P$ are sums of Hermitian operators acting on a constant number of qubits.

Proof: Based on Feynman’s proof that any (quantum) computation can be performed by time-independent Hamiltonian evolution.

Also related to the proof that LOCAL HAMILTONIAN is QMA-Complete (Kitaev).

Aharonov, Ta-Shma 03; Aharonov et al., in preparation
Adiabatic computation is robust

**Robustness to control error:** Computation depends on going smoothly from $H_B$ to $H_P$, not on the particular path between them.

**Robustness to thermal noise:** Computation depends on (and is protected by) a gap $E_1 - E_0$. If $k_B T \ll 1/(E_1 - E_0)$ then thermal transitions are suppressed.
Many kinds of Hamiltonian evolution can be efficiently simulated by universal quantum computers.

This allows us to simulate quantum physics much more efficiently than is possible using classical computers.

Hamiltonian evolution can also be used to build quantum algorithms.
- Quantum walks
- Adiabatic quantum computation
- …
Continuous time quantum walks

References

Discrete time quantum walks

Hamiltonian-based search algorithms
Adiabatic quantum computation