Simulating Physical Systems
on a Quantum Computer

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Topics:

- Quantum computers and physical systems
- Systems with local finite degrees of freedom
- Systems characterized by conjugate variables
- Bosonic systems
- Unphysical Hamiltonians
- Fermionic systems
- Open questions

Simulating quantum systems on a classical machine

Richard Feynman (1982)

> A system with n particles, each, say, given as a 2-level system is described by 2^n complex coefficients. In order to simulate the time-dynamics we have to keep track of these 2^n coefficients in time which takes exponentially much space.

But at the end, we do a measurement, say, on a single qubit, do we really need to keep track of all these 2^n coefficients?

= The question of the power of quantum computation…..

Universality

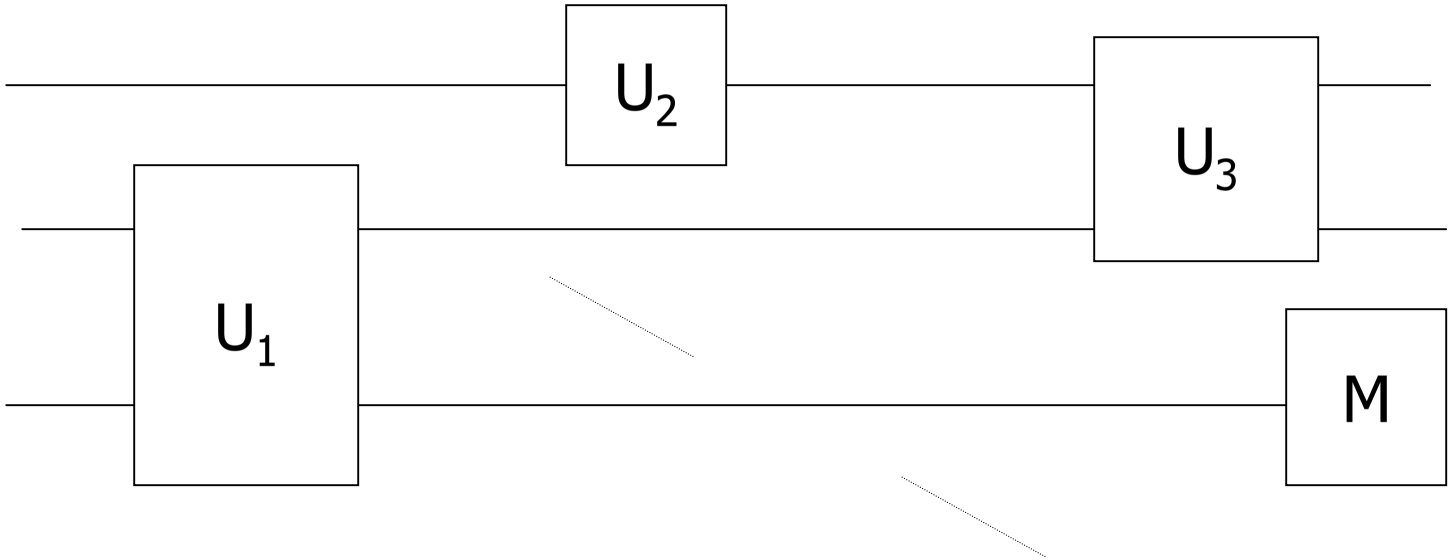
Richard Feynman (1982):

"What, in other words, is the universal quantum simulator? ….If you had discrete quantum systems, what other discrete quantum systems are exact imitators of it, and is there a class against which everything can be matched?"

Involves the question of efficiency: given a physical system with n d-level particles; can we simulate the time-dynamics of this system on our universal quantum computer in a polynomial number of steps in n?

Explore a set of physical quantum systems…..

The quantum computer model



- Hilbert space, a tensor product of two-dimensional spaces
- Use 2 qubit gates between any 2 qubits and 1 qubit gates
- 1-qubit measurements in computational basis.
- Simulation cost: count the number of 1 and 2 qubit gates; is it polynomial in n?

Systems with finite local degrees of freedom

Dynamics of a physical system given by time-independent Hamiltonian $H=H^{\dagger}$ (H Hermitian) which gives rise to a unitary time-evolution $U=e^{iHt}$

- Hilbert space K has a tensor product structure where each term in the product has a small finite dimension.
$K=K_1 \otimes K_2 \otimes \ldots \otimes K_n$ where $\dim(K_i)=c_i$
- The Hamiltonian H is a sum of interactions involving a a small constant number of local Hilbert spaces K_i:
$H=\sum_i H_i$, where H_i acts on, say, a small constant number of spaces K_j. A local Hamiltonian.

Example

Crystal structure with nuclear spins of atoms on lattice sites. Interactions between the spins is short range. For example, the J-coupling between neighboring nuclear spins: $H=a_1 X \otimes X + a_2 Y \otimes Y + a_3 Z \otimes Z$.

The problem:

1) Match qubits with local Hilbert spaces K_i
2) Express e^{iHt} in a sequence of local gates: dependence on accuracy of simulation, time t and number of qubits n.

Small time-step method

H=A+B, where [A,B]=AB-BA ≠0

Use Baker-Campbell-Hausdorff formula for small t:

$$e^{(A+B)t} = e^{At}e^{Bt}e^{-[A,B]t^2/2} + O(t^3)$$

Take a large integer k, such that t/k << 1: we write

$U^t = e^{iHt} = \left(e^{i(A+B)t/k}\right)^k$ and we simulate

$U^{t/k} = e^{i(A+B)t/k}$ by $\tilde{U}^{t/k} = e^{iAt/k}e^{iBt/k}$

Simulate A and B for a short time t/k in alternating fashion.

Approximation error

||A|| is operator norm:
$||A||=\max_{\omega}|| A|\omega> ||$

$$||U^{t/k} - \tilde{U}^{t/k}|| = O((t/k)^2) \Rightarrow$$

$$||U^{t} - \tilde{U}^{t}|| = O(k(t/k)^2) = O(t^2/k) \equiv \delta$$

Now consider a general local qubit Hamiltonian $H = \sum_{j=1}^{poly(n)} H_j$

We approximate $e^{iHt/k}$ by $\tilde{U}^{t/k} = e^{iH_1 t/k} e^{iH_2 t/k} \ldots . e^{iH_p t/k}$

Simulation cost (when each H_i acts on a 2-qubit Hilbert space):
To obtain a final accuracy δ, we use k poly(n)= $O(t^2/\delta)$poly(n) 2-qubit gates.

Note t^2 dependence...

Systems with continuous conjugate variables

1. Observables of position x and momentum p of a particle.
2. Bosonic systems, see further
2. Phase difference and number of Cooper pairs tunneled in superconducting Josephson junction.

$$[\hat{x}, \hat{p}] = iI \qquad |x\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dp e^{ipx} |p\rangle$$

$$\hat{x}|x\rangle = x\,|x>,$$
$$\hat{p}\,|p> = p\,|p>$$

Consider $H=H_1(p)+H_2(x)$ (drop ˆs on operators)

Example: a quantum particle in a potential, i.e. $H_2(x)=V(x)$ (the potential) and $H_1(p)=p^2/2m$ where m is the mass.

Simulation

Discretize Hilbert space: |x>, x=0…2^n-1. $\hat{x}|x\rangle = x\,|x>$
and let the p-basis be related to the x-basis by a discrete Fourier transform:

$$|x\rangle = \frac{1}{\sqrt{2^n}} \sum_{p=0}^{p=2^n-1} e^{2\pi i p x / 2^n} |p\rangle$$

As before, slice up simulation in small time-steps t/k

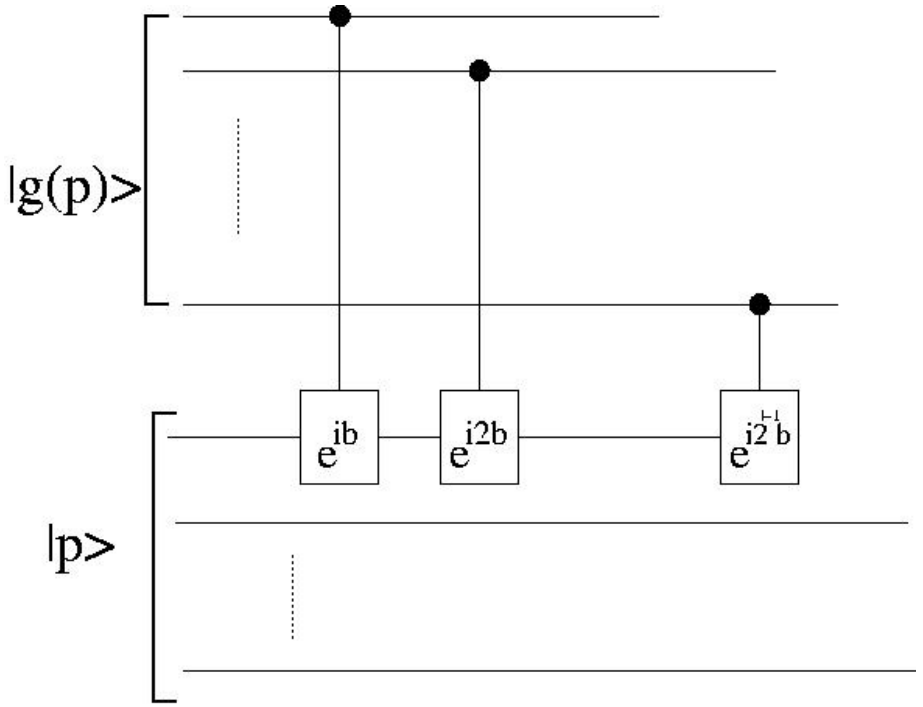
$$U^{t/k} = e^{iH_1(p)t/k} e^{iH_2(x)t/k} + O((t/k)^2)$$

, and implement with

$$\left(U_{FT} \begin{pmatrix} e^{iH_1(0)t/k} & & 0 \\ & \ddots & \\ 0 & & e^{iH_1(2^n-1)t/k} \end{pmatrix} U_{FT}^{-1} \begin{pmatrix} e^{iH_2(0)t/k} & & 0 \\ & \ddots & \\ 0 & & e^{iH_2(2^n-1)t/k} \end{pmatrix} \right)$$

Diagonal Phaseshifts

We can compute $g(p) \approx H_1(p)$ t/k given p, i.e. $|p\rangle|0\rangle \to |p\rangle|g(p) \oplus 0\rangle$ where, say, g(p) is given with l bits.
Then we can use the following circuit:



b is the control bit.
The circuit uses
l controlled 1-qubit
phaseshifts.

Total Cost of Simulation

Run for time t, obtain accuracy δ (omitting error due to discretization):

Number of elementary gates= $O(t^2/\delta)$ $(O(n^2)+2l)$

phaseshifts

#gates for Fourier transform

Many particle system with $[x_i,p_j]=[p_i,p_j]=0$ for $i \neq j$,

$$H = \sum_{i=1}^{m} H_i(p_i) + V(x_1, x_2, \ldots, x_m)$$

Basis for Hilbert space is $|x_1, x_2, \ldots, x_m\rangle$

Bosons

For example, photons….

Creation and annihilation operators of a particular mode (characterized by polarization and wave-vector)

$a^\dagger|n\rangle=(n+1)^{1/2}|n+1\rangle$, $a|n\rangle=n^{1/2}|n-1\rangle$ and their commutation relations $[a, a^\dagger]=1$.

Furthermore, a and $a^\dagger$ commute with creation and annihilation operators b, $b^\dagger$ of a different mode.

Take

$$x_a = \frac{1}{\sqrt{2}}(a + a^+), \qquad [x, p] = iI$$

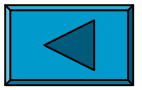
$$p_a = \frac{1}{i\sqrt{2}}(a - a^+)$$

Hermitian conjugate variables…

Bosonic representation

Take a basis for finite Hilbert space, $|x_a\rangle = |0,\ldots,2^n-1\rangle$
Or for more modes, $|x_a\rangle$ 🗁 $|x_b\rangle$.....
Goal: simulate bosonic interactions (possibly between different modes) with a number of elementary gates that is polynomial in n. Large n limit, simulation should capture some of the continuum dynamics.

In conjugate variable representation, these interactions can be simulated efficiently:



Displacement: $$H = \alpha_1 i(a - a^+) + \alpha_2 (a + a^+) = \sqrt{2}(\alpha_2 x_a - \alpha_1 p_a),$$

Phaseshifter: $$H = a^+ a = \frac{1}{2}(x_a^2 + p_a^2 - 1),$$

Some Linear Optics Interactions

'Squeezer': $H = ab + a^+b^+ = x_a x_b - p_a p_b,$

Beamsplitter: $H = ab^+ + a^+b = x_a x_b + p_a p_b$

But other interactions such as $H = x_a p_a + p_a x_a$ may be harder…

Are we expecting too much, if we ask for a polynomial (in n) simulation here?

Energy of system ⇩ number of levels ⇩ 2^n

Energy to physically operate on system ⇩ 2^n

Special 'Unphysical' systems

H=Z⊗Z⊗…⊗Z

'Unphysical', since interaction involves all n qubits

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$Z^{\otimes n} \mid x >= (-1)^{\oplus_i x_i} \mid x >$$

This suggests:

$$\mid x > \otimes \mid 0 > \rightarrow \mid x > \otimes \mid 0 \oplus_j x_j > \xrightarrow{e^{iZt} \text{ on last qubit}}$$

$$e^{i(-1)^{\oplus_j x_j} t} \mid x > \otimes \mid 0 \oplus_j x_j > \rightarrow e^{i(-1)^{\oplus_j x_j} t} \mid x > \otimes \mid 0 >$$

Cost: 2n 2-qubit CNOT gates+1 1-qubit rotation

‘Unphysical’ systems

Similar for H’=X⊗Z⊗I⊗…⊗Y etc, $X=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, Y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$

since $e^{iH't} = U^{-1} e^{i(Z\otimes Z\otimes I\otimes\ldots\otimes Z)t} U$

where U is a tensorproduct of 1 qubit operations $U_1 \ldots U_n$ rotating Z to X and Y, for example $U_1^{-1} Z U_1 = X$ with

$U_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$ The Hadamard transformation

Concatenation with the previous techniques allows a simulation of Hamiltonians which are sums of polynomially many terms, each of which has a polynomial time circuit such as H’

Fermions

Example: (spinless) electrons on a lattice. The operator $a_i^\dagger$ (a_i) creates (annihilates) an electron at lattice site i. Since electrons are fermions, no two electrons can occupy the same state (here the same lattice site). Thus we can associate their presence/absence at a lattice site with a 2-level system.

(Compare with bosons in which many particles can be created in the same mode and therefore Hilbert space of a single mode is large.)

Because of anti-commutation relations among a_i ,$a_i^\dagger$, a_j and $a_j^\dagger$, i.e. $a_i a_j + a_j a_i = 0$, $a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0$, $a_i^\dagger a_j + a_j a_i^\dagger = I\delta_{ij}$, we can choose

$$a_i \mid x >= 0, \quad \text{when } x_i = 0$$

Non-local phase: 'the sign problem'

$$a_i \mid x >= (-1)^{\oplus_{k=1}^{i-1} x_k} \mid x_1 \ldots x_{i-1}, \overline{x}_i, x_{i+1} \ldots x_n >$$

Fermionic interactions

Simulate time-evolution generated by $H = \sum_{i=1}^{n} a_i^+ a_i$
(counting the electrons)

$[a_i^+ a_i, a_j^+ a_j] = 0$ Check with anti-commutation relations...

Thus $e^{iHt} = e^{iH1t} e^{iH2t} \ldots e^{iHnt}$ where $H_i = a_i^+ a_i$

Since $a_i^\dagger a_i |x\rangle = 0$ if $x_i = 0$ and $a_i^\dagger a_i |x\rangle = |x\rangle$ when $x_i = 1$,
We can represent $a_i^\dagger a_i$ as (I-Z)/2 acting on the ith qubit.

Thus we can implement the time-evolution by a sequence of 1-qubit rotations $e^{i(I-Z)t/2}$

Simple...(no global phases)

2-particle tunneling interaction

Simulate time-evolution generated by $H = \sum_{(i,j)\in L} (a_i^+ a_j + a_j^+ a_i)$
(electrons hopping over a lattice L)

Consider a single Hermitian term (i < j):

$$H_{ij} \mid x >= a_i^+ a_j + a_j^+ a_i \mid ...x_i..x_j... >$$

$$a_i^+ a_j + a_j^+ a_i \mid ...0_i..0_j... >= 0, a_i^+ a_j + a_j^+ a_i \mid ...1_i..1_j... >= 0$$

$$a_i^+ a_j + a_j^+ a_i \mid ...0_i..1_j... >= (-1)^{\oplus_{k=i}^{j-1} x_k} \mid ...1_i..0_j... >,$$

$$a_i^+ a_j + a_j^+ a_i \mid ...1_i..0_j... >= -(-1)^{\oplus_{k=i}^{j-1} x_k} \mid ...0_i..1_j... >$$

In terms of Pauli matrices…

We can rewrite this in terms of Pauli matrices as:

$$H_{ij}\,|x\rangle = \frac{1}{2}(X_i \otimes X_j + Y_i \otimes Y_j)(Z_{i+1} \otimes .. \otimes Z_{j-1})\,|x\rangle$$

Non-local!

An 'unphysical' Hamiltonian with commuting terms, so we can simulate each term separately with the procedure that we have given previously 

Simulation cost of a pairwise interaction: 4n CNOT+10 single qubit interactions.

The total Hamiltonian H which is the sum of the pairwise interactions can then be simulated with the small timestep method.

Comments

- Other physical (parity preserving) interactions can be simulated similarly.
- Faster simulation (O(log(n)) by cleverer encoding (Bravyi/Kitaev).

Open questions

We have seen that a variety of physical systems can be efficiently simulated on a quantum computer. The related question about universality is also of great interest:
Can we find physical quantum systems whose natural dynamics gives rise to a stronger quantum computation model?
From what we have seen the answer is NO.
An alternative description of quantum computation may be useful to understand the power of QCs.

- What simulations do physicists carry out on their PCs? Simulations of noisy systems, systems at finite temperature, calculations of correlation functions….
- Simulation of relativistic field theories, lattice gauge theories…?
- Question about starting states: for example, prepare Gaussian wavepacket for quantum particle in a potential.