Baker-Campbell-Hausdorf Formula

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

Let $H = \sum_k^L H_k$,

Define,

$$U_{\Delta t} = \left[e^{-iH_1 \Delta t} e^{-iH_2 \Delta t} \cdots e^{-iH_L \Delta t} \right] \left[e^{-iH_L \Delta t} e^{-iH_{L-1} \Delta t} \cdots e^{-iH_1 \Delta t} \right]$$

Then,

$$U_{\Delta t} = e^{-2iH\Delta t} + O(\Delta t^3),$$

and,

$$E\left(U_{\Delta t}^m, e^{-2miH\Delta t}\right) \leq m\alpha \Delta t^3,$$

for any positive integer, m, and constant, α.

Quantum Simulation of Schrödinger's Equation

Single particle living on a line, in a one-dimensional potential, $V(x)$, with Hamiltonian,

$$H = \frac{p^2}{2m} + V(x),$$

where p is the momentum operator and x is the position operator.

The eigenvalues of x are continuous, and the system $|\psi\rangle$ resides in an infinite dimensional Hilbert space.

~~Approximately~~

Thus,

$$|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\psi\rangle \, dx.$$

Remember: $|\psi\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\psi\rangle \, dx$.

Only a finite region is of interest, where $-d \leq x \leq d$.
A differential step size Δx is sufficiently small compared to the shortest wavelength in the system.

Thus,

$$|\psi\rangle \approx |\tilde{\psi}\rangle = \sum_{k=-d/\Delta x}^{d/\Delta x} a_k |k\Delta x\rangle.$$

Requires $n = \lceil \log(2d/\Delta x + 1) \rceil$ qubits.

... so replace basis $|k\Delta x\rangle$ with $|k\rangle$,
a computational basis state of n qubits.

Remember:

$$H = \frac{p^2}{2m} + V(x),$$

$$|\tilde{\psi}\rangle = \sum_{k=-d/\Delta x}^{d/\Delta x} a_k |k\Delta x\rangle.$$

In general,

$$H_1 = V(x) \quad \text{and} \quad H_0 = \frac{p^2}{2m}$$

do not commute.

$$\Rightarrow |\tilde{\psi}(t)\rangle = e^{-iHt} |\tilde{\psi}(0)\rangle \quad \text{will be approximated.}$$

Because $|\tilde{\psi}\rangle$ is expressed in eigenbasis of $H_{0,1}$, then $e^{-iH_1\Delta t}$ is realised as,

$$|k\rangle \rightarrow e^{-iV(k\Delta x)\Delta t} |k\rangle$$

Moreover, x and p are related by $U_{FFT}\, x\, U_{FFT}^{\dagger} = p$, so....

Remember: $e^{-iH_1\Delta t}|k\rangle = e^{-iV(k\Delta x)\Delta t}|k\rangle$

$U_{FFT}\, x\, U_{FFT}^{\dagger} = p,$

Therefore,

$$e^{-iH_0\Delta t} = U_{FFT}\, e^{-ix^2\Delta t/2m}\, U_{FFT}^{\dagger}$$

So,

$$e^{-iH_0\Delta t}|k\rangle = U_{FFT}\, e^{-ix^2/2m}\, U_{FFT}^{\dagger}|k\rangle.$$

Efficient Quantum Simulations are possible even for Hamiltonians which act non-trivially on all or nearly all parts of a large system.

Consider the Hamiltonian,

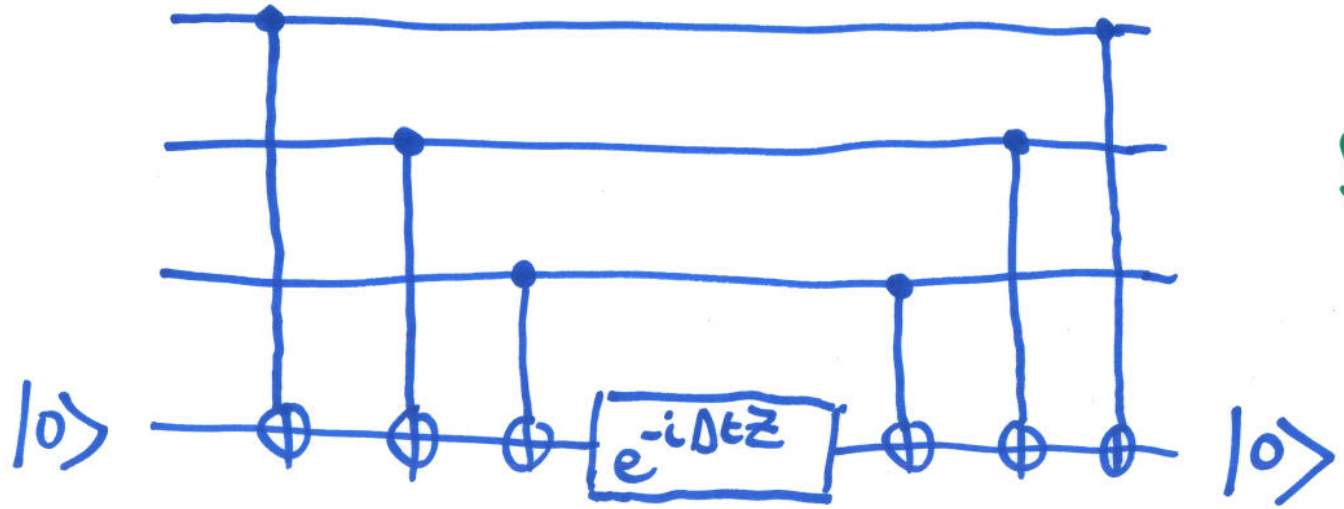
$$H = Z_1 \otimes Z_2 \otimes \ldots \otimes Z_n,$$

acting on an n-qubit system.

It can be simulated efficiently although it interacts with the whole system.

Remember: $H = Z_1 \otimes Z_2 \otimes \ldots \otimes Z_n$.

We desire a simple circuit for $e^{-iH\Delta t}$ for arbitrary Δt.



Simulates $H = Z_1 \otimes Z_2 \otimes Z_3$ for time Δt.

Phase shift applied is $e^{-i\Delta t}$ if the parity of the n qubits is even, otherwise $e^{i\Delta t}$ is applied, so....

classically compute parity,
apply phase shift conditioned on parity
uncompute parity

} works because H acts classically on system

Similarly, ...

any Hamiltonian of the form,

$$H = \bigotimes_{k=1}^{\hat{}} \sigma_{c(k)}^{k} \quad , \qquad \sigma_{c(k)}^{k} \text{ a Pauli matrix or identity,}$$

$c(k) \in \{0,1,2,3\} : \{I, X, Y, Z\}$

can be efficiently simulated

.... X or Y terms can be transformed by single qubit gates to Z operations.

More generally...

It is possible to simulate,

$$H = \sum_{k=1}^{L} H_k ,$$

if the H_k have a tensor product structure, and L is polynomial in #particles, n.

... we only require an efficient circuit to simulate each H_k separately.

e.g. $H = \sum_{k=1}^{n} X_k + Z^{\otimes n}$ could be easily simulated.

Difference between quantum and classical simulation

For quantum, there is no way to obtain (non-trivial) information from an intermediate step without significantly changing the algorithm . .

. . . the final measurement must be chosen to provide desired result.

. . . even though the simulation can be performed efficiently, it is not always possible to efficiently perform a desired measurement

- the algorithm may only be repeated poly times.

Not all Hamiltonians can be efficiently simulated,

... otherwise...

all unitary transformations could be efficiently approximated.

Alternate Universality Construction

Let U be a unitary on n qubits

Define $H = i\ln(U)$.

Then,

H is Hermitian, with eigenvalues in the range 0 to 2π.

H can be written, $H = \sum_g h_g g$, where h_g are real and each g is an n-fold tensor product of $\{I, X, Y, Z\}$.

$e^{-ih_g g\Delta}$ can be implemented using $O(n)$ one and two qubit operations, where $\Delta = 1/k$.

$$e^{-iH\Delta} = \prod_g e^{-ih_g g\Delta} + O(4^n\Delta^2)$$

$$\Rightarrow U = \left[\prod_g e^{-ih_g g\Delta}\right]^k + O(4^n\Delta),$$

so U can be approximated to within $\varepsilon > 0$, using $O(n16^n/\varepsilon)$ one and two qubit operations.

Summary

Universality:

Any unitary on n qubits may be implemented exactly using single qubit and controlled-NOT gates.

Universality with a discrete set:

The Hadamard, phase, controlled-NOT and T gates are universal to within arbitrary accuracy $\varepsilon > 0$.

The Hadamard, phase, C-NOT and Toffoli gates are also universal.

Not all unitaries can be efficiently implemented:

Some unitaries on n qubits require $\Omega(2^n \log(1/\varepsilon)/\log(n))$ gates to approximate to within ε.

Simulation: $H = \sum_k H_k$, a sum of poly terms, where H_k can be efficiently built. Then a QC can efficiently simulate e^{-iHt}.