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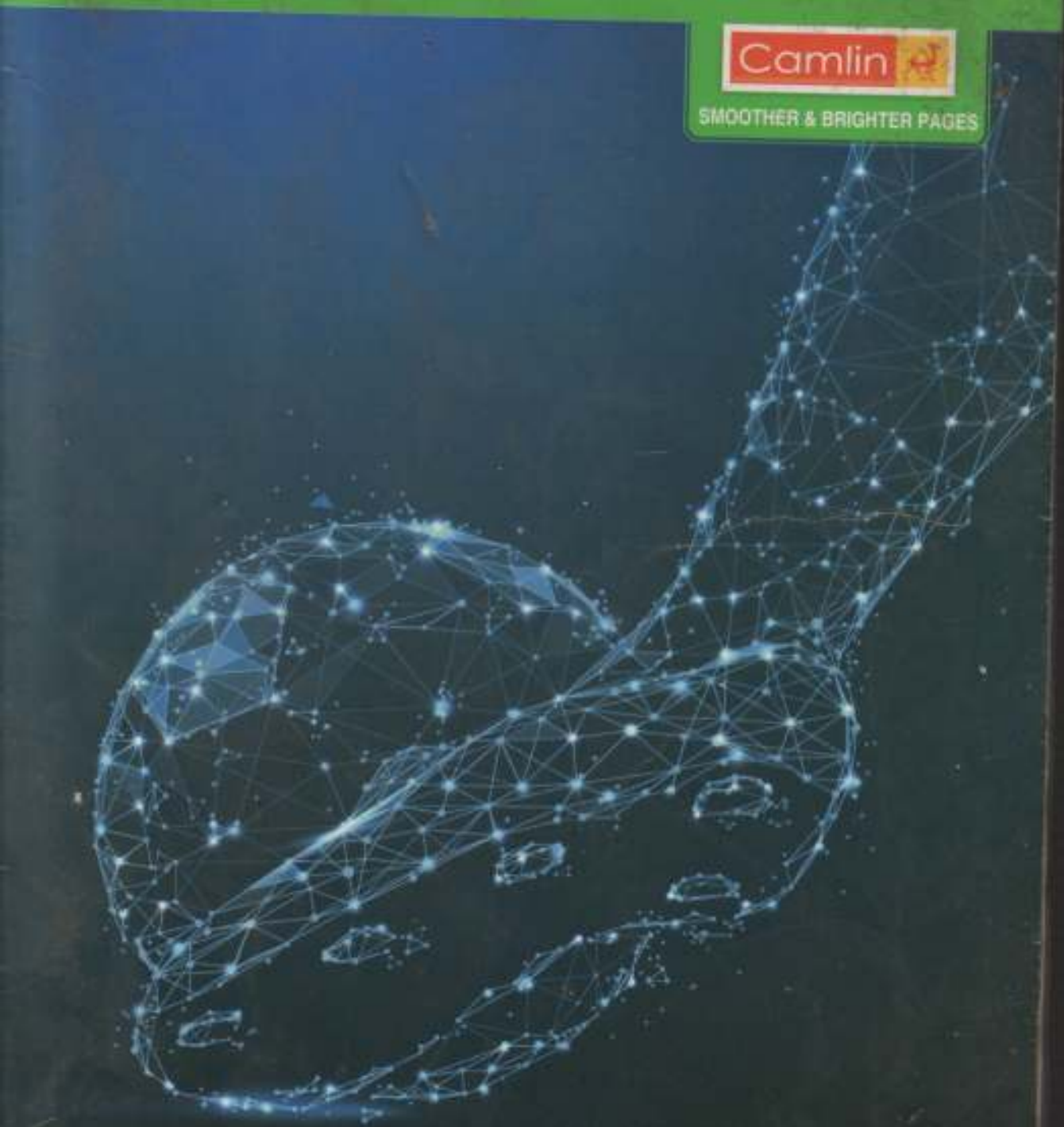

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		QUANTUM COMPUTATION & QUANTUM INFORMATION - Nielsen & Chuang		

Simulation of Quantum Systems

The heart of simulation is the solution of differential equations which capture the physical laws governing the dynamical behavior of a system.

Ex:-

Newton's law : $\frac{d}{dt}\left(m\frac{dx}{dt}\right) = F$

Poisson's eq^n : $-\vec{\nabla}\cdot(k\vec{\nabla}u) = \vec{Q}$

the em vector wave eq^n $\vec{\nabla}\cdot\vec{\nabla}\vec{E} = \epsilon_0\mu_0\frac{\partial^2\vec{E}}{\partial t^2}$

diffusion eq^n $\vec{\nabla}^2\psi = \frac{1}{a^2}\frac{\partial\psi}{\partial t}$

The goal is generally: given an initial state of the system, what is the state at some other time and/or position?

Solutions are usually obtained by approximating the state with a digital representation, then discretizing the differential equation in space and time such that an iterative application of a procedure carries the state from the initial to the final conditions. Importantly, the error in this procedure is bounded, and known not to grow faster than some small power of the # of iterations. Furthermore, not all dynamical systems can be simulated efficiently: generally only those systems which can be described efficiently can be simulated efficiently.

Simulation of quantum systems by classical computers is possible, but generally only very inefficiently. The dynamical behavior of many simple quantum systems is governed by Schrödinger's equation,

$$i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle$$

We'll find it convenient to absorb $\hbar$ into H;

For a typical Hamiltonian of interest to physicists dealing with real particles in space (rather than abstract systems such as qubits, which we have been dealing with), this reduces to

$$i\frac{\partial}{\partial t}\psi(x) = \left[\frac{-1}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x)$$

using a convention known as the position representation $\langle x|\psi\rangle = \psi(x)$. This is an elliptical equation very much like the diffusion equation.

∴

Just simulating Schrödinger's equation is not the especially difficulty faced in simulating quantum systems.

What is the difficulty ?

The key challenge in simulating quantum systems is the exponential # of differential eq^n's which must be solved.

For one qubit evolving according to the Schrödinger eq^n, a system of two differential equations must be solved; for two qubits four equations; and for n qubits, 2^n equations

Sometimes, insightful approximations can be made which reduce the effective # of equations involved, thus making classical simulation of the quantum system feasible.

However, there are many physically interesting quantum systems for which no such approximations are known.

Ex: 4.46

Let ρ be a density matrix describing the state of n qubits. Show that describing ρ requires $4^n - 1$ independent real numbers.

Ans:

# of entries in the density matrix of a n-qubit state $= 2^n \times 2^n$

$= 2^{n+n} = 4^n$

$\text{tr}(\rho) = 1 \Longrightarrow$ The # of independent real numbers required to describe the density matrix is $4^n - 1$.

Quantum computers can efficiently simulate quantum systems for which there is no known efficient classical simulation. Intuitively, this is possible for much the same reason any quantum circuit can be constructed from a universal set of quantum gates. Moreover, just as there exists unitary operations which cannot be efficiently approximated, it is possible in principle to imagine quantum systems with Hamiltonians which cannot be efficiently simulated on a quantum computer.

The quantum simulation algorithm

Classical simulation begins with the realization that in solving a simple differential equation such as $\frac{dy}{dt} = f(y)$, to 1st order, it is known that $y(t+\Delta t) \approx y(t) + f(y)\,\Delta t$.

Similarly, the quantum case is concerned with the solution of $i\frac{d}{dt}|\psi\rangle = H|\psi\rangle$, which, for a time-independent H, is just

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle \qquad \boxed{4.96}$$

Since H is usually extremely difficult to exponentiate (it may be sparse, but it is also exponentially large), a good beginning is the 1st order solution $|\psi(t+\Delta t)\rangle \approx (I - iH\Delta t)|\psi(t)\rangle$.

This is tractable, because for many Hamiltonians H is straightforward to compose quantum gates to efficiently approximate $I - iH\Delta t$. However, such 1st order solutions are generally not very satisfactory.

Efficient approximation of the solution to Eq. 4.96, to high order, is possible for many classes of Hamiltonian.

Ex:- in most physical systems, the Hamiltonian can be written as a sum over many local interactions. Specifically, for a system of n particles,

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

where each H_k acts on at most a constant c number of systems.
and L is a polynomial in n.

Ex:-
the terms H_k are often just two-body interactions such as $X_i X_j$ and one body Hamiltonians such as X_i. Both the Hubbard and Ising models have Hamiltonians of this form. Such locality is quite physically reasonable, and originates in many systems

from the fact that most interactions fall off with increasing distance or difference in Energy. There are sometimes additional global symmetry constraints such as particle statistics.

The important point is:

although e^{-iHt} is difficult to compute, $e^{-iH_k t}$ acts on a much smaller subsystem, and is straightforward to approximate using quantum circuits.

But, because $[H_j, H_k] \neq 0$ in general,

$$e^{-iHt} \neq \Pi_k e^{iH_k t} \; !$$

How then, can $e^{-iH_k t}$ be useful in constructing e^{-iHt} ?

Baker-Campbell-Hausdorff formula

$$e^X e^Y = e^{X+Y+\frac{1}{2}[X,Y]+\frac{1}{12}[X,[X,Y]]-\frac{1}{12}[Y,[X,Y]]+\cdots}$$

for (possibly non-commutative) X and Y in the Lie algebra of a Lie group.

Proof

$$\frac{d}{dt}\left(e^{tX}\right) = \frac{d}{dt}\sum_{n=0}^{\infty}\frac{t^n X^n}{n!} = \sum_{n=0}^{\infty}\frac{n t^{n-1} X^n}{n!}$$

$$= X\sum_{n=1}^{\infty}\frac{t^{n-1}X^{n-1}}{(n-1)!}$$

$$= X\sum_{m=0}^{\infty}\frac{t^m X^m}{m!}, \quad m = n-1$$

$$= X e^{tX}$$

$$\Longrightarrow \boxed{\frac{d}{dt}\left(e^{tX}\right) = X e^{tX}}$$

where t is a real parameter and X is a constant matrix

The derivative of a matrix function $A(t)$ by a scalar t is known as the tangent matrix and is given by

$$\frac{\partial A}{\partial t} = \begin{bmatrix} \frac{\partial a_{11}}{\partial t} & \cdots & \frac{\partial a_{1n}}{\partial t} \\ \vdots & & \vdots \\ \frac{\partial a_{m1}}{\partial t} & \cdots & \frac{\partial a_{mn}}{\partial t} \end{bmatrix}$$

Let $g(t) = e^{tX}$, $h(t) = e^{tY}$

$$f(t) = g(t)h(t) = e^{tX}e^{tY}$$

$$(f(t))_{ij} = (g(t)h(t))_{ij} = \sum_k (g(t))_{ik}(h(t))_{kj}$$

$$\frac{\partial}{\partial t}(f(t))_{ij} = \sum_k \left[\frac{\partial}{\partial t}(g(t))_{ik} h(t)_{kj} + (g(t))_{ik}\frac{\partial}{\partial t}(h(t))_{kj}\right]$$

$$= \sum_k \frac{\partial}{\partial t}(g(t))_{ik} h(t)_{kj} + \sum_k (g(t))_{ik}\frac{\partial}{\partial t}(h(t))_{kj}$$

$$\therefore \frac{\partial}{\partial t}[A(t)B(t)] = \left(\frac{\partial}{\partial t}A(t)\right)B(t) + A(t)\left(\frac{\partial}{\partial t}B(t)\right)$$

Let's define an operator valued function of the variable t,

$$F(t) = e^{tX} Y e^{-tX}$$

Using the Taylor expansion of $F(t)$,

$$F(t) = F(0) + \frac{t}{1!}F^{(1)}(0) + \frac{t^2}{2!}F^{(2)}(0) + \frac{t^3}{3!}F^{(3)}(0) + \cdots$$

* Expand individual terms of the matrix function $F(t)$ in Taylor series,

$$F^{(1)}(t) = X e^{tX} Y e^{-tX} - e^{tX} Y e^{-tX} X$$

$$= X F(t) - F(t) X = [X, F(t)]$$

$$F^{(2)}(t) = [X, F^{(1)}(t)]$$

$$F^{(3)}(t) = [X, F^{(2)}(t)]$$

i.e., $$F^{(n)}(t) = [X, F^{(n-1)}(t)]$$

$$F(t) = e^{tX} Y e^{-tX} \Longrightarrow F(t=0) = Y$$

$\therefore$

$$F^{(1)}(0) = [X, F(0)] = [X, Y]$$

$$F^{(2)}(0) = [X, F^{1}(0)] = [X, [X, Y]]$$

$$F^{(3)}(0) = [X, F^{(2)}(0)] = [X [X, [X, Y]]]$$

$$F(t) = e^{tX} Y e^{-tX}$$

$$= Y + \frac{t}{1!}[X,Y] + \frac{t^2}{2!}[X,[X,Y]] + \frac{t^3}{3!}[X,[X,[X,Y]]] + \frac{t^4}{4!}[X,[X,[X,[X,Y]]]] + \cdots$$

$$= \sum_{n=0}^{\infty} \frac{F_n t^n}{n!}$$

$\Longrightarrow$ Baker - Hausdorff lemma

Setting $t = 1$,

$$e^X Y e^X = Y + [X,Y] + \frac{1}{2!}[X,[X,Y]] + \frac{1}{3!}[X,[X,[X,Y]]] + \cdots + \frac{1}{n!}[\underbrace{X,[X,\cdots[X,Y]\cdots]}_{n\ X's}] + \cdots$$

When $[X,[X,Y]] = 0$,

$$F(t) = e^{tX} Y e^{-tX} = Y + t[X,Y] \quad \text{——— (1)}$$

Define $G(t) := e^{t(X+Y)}$ which satisfies

$$G'(t) = (X+Y)\, e^{t(X+Y)}, \quad G(0) = I \qquad \text{—②}$$

$\frac{d}{dt} e^{tX} = X e^{tX}$

Define $H(t) := e^{tX} e^{tY} e^{-\frac{t^2}{2}[X,Y]}$

$$H'(t) = X H(t) + e^{tX} Y e^{tY} e^{-\frac{t^2}{2}[X,Y]} - e^{tX} e^{tY} t\,[X,Y]\, e^{-\frac{t^2}{2}[X,Y]}$$

Making use of ①

$$e^{tX} Y e^{-tX} = Y + t\,[X,Y]$$

$$\Longrightarrow Y = e^{-tX} Y e^{tX} + e^{-tX}\, t\,[X,Y]\, e^{tX}$$

$$= X H(t) + Y e^{tX} e^{tY} e^{-\frac{t^2}{2}[X,Y]} + t\,[X,Y]\, e^{tX} e^{tY} e^{-\frac{t^2}{2}[X,Y]} - e^{tX} e^{tY}\, t\,[X,Y]\, e^{-\frac{t^2}{2}[X,Y]}$$

Assuming $[Y,[X,Y]]=0$ & we have already assumed $[X,[X,Y]]=0$.

$$\Rightarrow e^{tX}e^{tY} + [X,Y]e^{-\frac{t^2}{2}[X,Y]} = t[X,Y]e^{tX}e^{tY}e^{-\frac{t^2}{2}[X,Y]}$$

$\therefore$

$$\mathcal{H}'(t) = X\mathcal{H}(t) + Y\mathcal{H}(t) = (X+Y)\mathcal{H}(t)$$

$$\mathcal{H}'(t) = (X+Y)\mathcal{H}(t), \quad \mathcal{H}(0) = I$$

Comparing it with ②;

$$\mathcal{G}'(t) = (X+Y)e^{t(X+Y)}, \quad \mathcal{G}(0) = I$$

Uniqueness property of the solution

$$\Longrightarrow \mathcal{H}(t) = \mathcal{G}(t)$$

$$\therefore \quad e^{t(X+Y)} = e^{tX}\, e^{tY}\, e^{-\frac{t^2}{2}[X,Y]}$$

when $[X,[X,Y]] = 0 = [Y,[X,Y]]$

Taking $t = 1$,

$$e^{X+Y} = e^{X} e^{Y} e^{-\frac{1}{2}[X,Y]}$$

If $[X,Y] = 0$, then $e^{X+Y} = e^{X} e^{Y}$.

$$[X,[X,Y]] = [Y,[X,Y]] = 0 \Longrightarrow [X+Y,[X,Y]] = 0$$

$$\therefore \quad e^{X+Y} \cdot e^{+\frac{1}{2}[X,Y]} = e^{X+Y+\frac{1}{2}[X,Y]}$$

When $[X,[X,Y]] = [Y,[X,Y]] = 0$,

the Baker-Campbell-Hausdorff formula becomes,

$$e^X e^Y = e^{X+Y+\frac{1}{2}[X,Y]}$$

Method: 2

$$e^X Y e^{-X} = Y + [X,Y] + \frac{1}{2!}[X,[X,Y]] + \frac{1}{3!}[X,[X,[X,Y]]] + \cdots + \frac{1}{n!}[\underbrace{X,[X,\cdots[X}_{n\ X's},Y]\ .\ ] + \cdots\cdots$$

——— ①

proved in part 1.

$$\frac{d}{dt} e^{A(t)} = \int_0^1 dx\, e^{(1-x)A(t)} \frac{dA}{dt} e^{xA(t)}$$

where $A(t)$ is an arbitrary matrix function of t.

Proof.

$$\frac{d}{dt} e^{A(t)} = \frac{d}{dt}\left[I + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \cdots\right]$$

$$= A' + \frac{A'A + AA'}{2!} + \frac{A'A^2 + AA'A + A^2A'}{3!} + \cdots$$

$$+ \frac{A'A^3 + AA'A^2 + A^2A'A + A^3A'}{4!} + \cdots$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{A^n A' A^m}{(n+m+1)!}$$

$$\int_0^1 dx\, e^{(1-x)A(t)} \frac{dA}{dt} e^{xA} =$$

$$= \int_0^1 dx \left(\sum_{n=0}^{\infty} \frac{(1-x)^n A^n}{n!} \right) A' \left(\sum_{m=0}^{\infty} \frac{x^m A^m}{m!} \right)$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{A^n A' A^m}{n!\, m!} \int_0^1 dx\, (1-x)^n x^m$$

$$I_{n,m} = \int_0^1 (1-x)^n x^m \, dx$$

$$= \left[\frac{(1-x)^n x^{m+1}}{m+1} \right]_0^1 + \int_0^1 n(1-x)^{n-1} \cdot \frac{x^{m+1}}{m+1} dx$$

$$= 0 + \frac{n}{m+1} \int_0^1 (1-x)^{n-1} x^{m+1} \, dx$$

$$= \frac{n}{m+1} I_{n-1,m+1}$$

$$= \frac{n}{m+1} \times \frac{n-1}{m+2} I_{n-2,m+2}$$

$$= \frac{n(n-1) \cdots 1}{(m+1)(m+2) \cdots (m+n)} I_{0,m+n}$$

$$= \frac{n!}{(m+n)\cdots(m+2)(m+1)} \int_0^1 x^{m+n} dx$$

$$= \frac{n!\,m!}{(m+n)!} \left[\frac{x^{m+n+1}}{m+n+1} \right]_0^1$$

$$= \frac{n!\,m!}{(n+m+1)!}$$

$$\int_0^1 (1-x)^n x^m dx = \frac{n!\,m!}{(n+m+1)!}$$

$\therefore$

$$\int_0^1 dx\, e^{(1-x)A(t)} \frac{dA}{dt} e^{xA} = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{A^n A' A^m}{n!\,m!} \cdot \frac{n!\,m!}{(n+m+1)!}$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{A^n A' A^m}{(n+m+1)!} = \frac{d}{dt} e^{A(t)}$$

$$\Longrightarrow \boxed{\frac{d}{dt} e^{A(t)} = \int_0^1 dx\, e^{(1-x)A(t)} \frac{dA}{dt} e^{xA}} \quad \text{—②}$$

$$e^{tX} Y e^{-tX} = Y + \frac{t}{1!}[X,Y] + \frac{t^2}{2!}[X,[X,Y]] + \cdots \quad \text{——③}$$

$\therefore$

$$e^{-X} \frac{d}{dt} e^{X} = \int_0^1 dx\, e^{-xX(t)} \frac{dX}{dt} e^{xX(t)}$$

$$= X' + \frac{1}{2!}[X',X] + \frac{1}{3!}[[X',X],X] + \cdots \quad \text{——④}$$

Let's define,

$$e^{tX} e^{tY} = e^{tG(t)}$$

$$= e^{t[G_1 + tG_2 + tG_3 + \cdots]}$$

$$= e^{tG_1 + t^2G_2 + t^3G_3 + \cdots}$$

$$= e^{G(t)}$$

$$e^{-tY} e^{-tX} \frac{d}{dt} e^{tX} e^{tY} = e^{-g(t)} \frac{d}{dt} e^{g(t)}$$

$$e^{-tY} e^{-tX} \frac{d}{dt} e^{tX} e^{tY} = e^{-tY} e^{-tX} \left[e^{tX} Y e^{tY} + X e^{tX} e^{tY} \right]$$

$$= e^{-tY} Y e^{tY} + e^{-tY} e^{-tX} X e^{tX} e^{tY}$$

$$\left[X, e^{tX}\right] = 0 = \left[Y, e^{tY}\right]$$

$$= Y + e^{-tY} X e^{tY}$$

$$= Y + X + t\left[X, Y\right] + \frac{t^2}{2}\left[Y, \left[Y, X\right]\right] + \cdots$$

— (5)

$$e^{-g(t)} \frac{d}{dt} e^{g(t)} = G' + \frac{1}{2}\left[G', G\right] + \frac{1}{3!}\left[\left[G', G\right], G\right] + \cdots$$

$$G' = G_1 + 2tG_2 + 3t^2 G_3 + \cdots$$

$$\left[G', G\right] = \left[G_1 + 2tG_2 + 3t^2 G_3 + \cdots, tG_1 + t^2 G_2 + t^3 G_3 + \cdots\right]$$

$$= t^2\left[G_1, G_2\right] + 2t^2\left[G_2, G_1\right] + O(t^3)$$

$$= -t^2\left[G_1, G_2\right] + O(t^3)$$

$\frac{1}{3!}\left[[G,G],G\right] = \mathcal{O}(t^3)$ & so we can drop this term.

$$e^{-G(t)}\frac{d}{dt}e^{G(t)} = G_1 + 2tG_2 + t^2\left(3G_3 - \frac{1}{2}\left[G_1,G_2\right]\right) + \mathcal{O}(t^3)$$

——— (6)

Comparing equations (5) and (6),

$$G_1 = X + Y$$

$$G_2 = \frac{1}{2}\left[X,Y\right]$$

$$3G_3 - \frac{1}{2}\left[G_1,G_2\right] = \frac{1}{2}\left[Y,\left[Y,X\right]\right]$$

$$6G_3 = \frac{1}{2}\left[X,\left[X,Y\right]\right] + \frac{1}{2}\left[Y,\left[X,Y\right]\right] + \left[Y,\left[Y,X\right]\right]$$

$$= \frac{1}{2}\left[X,\left[X,Y\right]\right] - \frac{1}{2}\left[Y,\left[Y,X\right]\right]$$

$$\Longrightarrow G_3 = \frac{1}{12}\left(\left[X,\left[X,Y\right]\right] - \left[Y,\left[Y,X\right]\right]\right.$$

$$\therefore \quad e^{tX} e^{tY} = e^{t(X+Y) + \frac{t^2}{2}[X,Y] + \frac{t^3}{12}\left([X,[X,Y]] - [Y,[X,Y]]\right) \cdots}$$

Setting $t=1$, obtains the Baker-Campbell-Hausdorff formula.

$$e^{X} e^{Y} = e^{X+Y+\frac{1}{2}[X,Y] + \frac{1}{12}\left([X,[X,Y]] - [Y,[X,Y]]\right) + \cdots}$$

Method:3

Many functions

Ex: 4.47 For $\mathcal{H} = \sum_k^L H_k$, prove that

$$e^{-i\mathcal{H}t} = e^{-iH_1t}\, e^{-iH_2t} \cdots e^{-iH_Lt} \quad \text{for all } t$$

if $[H_j, H_k] = 0$ for all j,k.

Ans:

$$e^{-i\mathcal{H}t} = e^{-it\sum_k^L H_k} = e^{-it(H_1+H_2+\cdots+H_L)}$$

$$= e^{iH_1t}\cdot e^{it(H_2+H_3+\cdots+H_L)}$$

Since $[H_j, H_k] = 0$ for all j,k. & using the Baker-Campbell-Hausdorff formula.

$$= e^{iH_1t}\, e^{iH_2t} \cdots e^{iH_Lt}$$

Ex 4.48 Show that the restriction of H_k to involve at most c particles implies that in the sum $H = \sum_{k=1}^{L} H_k$, L is upper bounded by a polynomial in n.

Ans: For a system of n particles, the Hamiltonian can be written as

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

where each H_k act on at most a constant c number of systems, and L is a polynomial in n.

The largest # of terms possible is,

$${}^{n}C_1 + {}^{n}C_2 + \cdots + {}^{n}C_c = \sum_{j=1}^{c} {}^{n}C_j = O(n^c)$$

$\therefore$ L is upper bounded by a polynomial in n.

The heart of quantum simulation algorithms is the following asymptotic approximation theorem:

Trotter formula

Let A and B be Hermitian operators. Then for any real t

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

even if A and B do not commute.

It can be generalized to hold for A and B which are generators of certain kinds of semigroups, which corresp. to general quantum operations (Lindblad form is 8.4.1)

Proof.

By definition,

$$e^{iAt/n} = I + \frac{iAt}{n} + O\left(\frac{1}{n^2}\right)$$

$\therefore$

$$e^{iAt/n}\, e^{iBt/n} = I + \frac{1}{n} i(A+B)t + O\left(\frac{1}{n^2}\right)$$

If X and Y commute the Binomial theorem can be proved by induction for $(X+Y)^n$.

$$(X+Y)^n = \sum_{k=0}^{n} {}^nC_k X^{n-k} Y^k$$

Since I & $A+B$ commute,

$$\left(I + \frac{1}{n} i(A+B)t\right)^n = \sum_{k=0}^{n} \binom{n}{k} \frac{1}{n^k} \left(i(A+B)t\right)^k$$

$$\left(e^{iAt/n}\, e^{iBt/n}\right)^n = I + \sum_{k=1}^{n} \binom{n}{k} \frac{1}{n^k} \left[i(A+B)t\right]^k + O(1/n)$$

Q.

$$\binom{n}{k}\frac{1}{n^k} = \frac{n!}{(n-k)!\,k!} * \frac{1}{n^k} = \frac{n(n-1)\cdots(n-(k-1))}{k! * n^k}$$

$$= \left[1\left(1-\tfrac{1}{n}\right)\left(1-\tfrac{2}{n}\right)\cdots\left(1-\tfrac{(k-1)}{n}\right)\right]/k!$$

$$= \left[1+O(1/n)\right]/k!$$

$\therefore$

$$\lim_{n\to\infty}\left(e^{iA t/n}\, e^{iBt/n}\right)^n = \lim_{n\to\infty}\sum_{k=0}^{\infty}\frac{i(A+B)t)^k}{k!}\left(1+O(1/n)\right) + O(1/n)$$

$$= \sum_{k=0}^{\infty}\frac{\left(i(A+B)t\right)^k}{k!} = e^{i(A+B)t}$$

Baker - Campbell - Hausdorf formula

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

Stato 30/10/2021

Prof

$$e^{A\Delta t}\, e^{B\Delta t}\, e^{-\frac{1}{2}[A,B]\Delta t^2} = \left(I + A\Delta t + \frac{A^2\Delta t^2}{2} + O_A(\Delta t^3)\right) \times$$

$$\left(I + B\Delta t + \frac{B^2\Delta t^2}{2} + O_B(\Delta t^3)\right) \times$$

$$\left(I - \frac{1}{2}[A,B]\Delta t^2 + O(\Delta t^4)\right)$$

$$= I + (A+B)\Delta t + \left(AB + \frac{A^2}{2} + \frac{B^2}{2} - \frac{1}{2}[A,B]\right)\Delta t^2 + O_1(\Delta t^3)$$

$$= I + (A+B)\Delta t + \frac{(2AB + A^2 + B^2 - AB + BA)}{2}\Delta t^2 + O_1(\Delta t^3)$$

$$= I + (A+B)\Delta t + \frac{(A^2 + AB + BA + B^2)}{2}\Delta t^2 + O_1(\Delta t^3)$$

$$= I + (A+B)\Delta t + \frac{(A+B)^2\Delta t^2}{2} + O_1(\Delta t^3)$$

$$e^{(A+B)\Delta t} = I + (A+B)\Delta t + \frac{(A+B)^2 \Delta t^2}{2} + \frac{(A+B)^3 \Delta t^3}{3!} + \cdots$$

$$= I + (A+B)\Delta t + \frac{(A+B)^2 \Delta t^2}{2} + O_2(\Delta t^3)$$

$$= I + (A+B)\Delta t + \frac{(A+B)^2 \Delta t^2}{2} + O_1(\Delta t^3) - O_1(\Delta t^3) + O_2(\Delta t^3)$$

$$= e^{A\Delta t} e^{B\Delta t} e^{-\frac{1}{2}[A,B]\Delta t^2} - O_1(\Delta t^3) + O_2(\Delta t^3)$$

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

Proof

① $e^{}$

$$e^{i(A+B)\Delta t} = e^{iA\Delta t}\, e^{iB\Delta t} + O(\Delta t^2)$$

$$e^{i(A+B)\Delta t} = e^{iA\Delta t/2}\, e^{iB\Delta t}\, e^{iA\Delta t/2} + O(\Delta t^3)$$

Proof

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

$$= e^{iA\Delta t}\, e^{iB\Delta t}\left(I + O(\Delta t^2)\right) + O(\Delta t^3)$$

$$= e^{iA\Delta t}\, e^{iB\Delta t} + O(\Delta t^2)$$

(2) $e^{iA\Delta t/2}\, e^{iB\Delta t}\, e^{iA\Delta t/2} = \left(I + \frac{iA\Delta t}{2} + \frac{1}{2!}\left(\frac{iA\Delta t}{2}\right)^2 + O(\Delta t^3)\right)$

$$\times \left(I + \frac{iB\Delta t}{2} + \frac{1}{2!}\left(\frac{iB\Delta t}{2}\right)^2 + O(\Delta t^3)\right)$$

$$\times \left(I + \frac{iA\Delta t}{2} + \frac{1}{2!}\left(\frac{iA\Delta t}{2}\right)^2 + O(\Delta t^3)\right)$$

$$= I + i(A+B)\Delta t + \frac{i^2(A^2+AB+BA+B^2)\Delta t^2}{2} + O(\Delta t^3)$$

$$= I + i(A+B)\Delta t + \frac{(i(A+B)\Delta t)^2}{2} + O(\Delta t^3)$$

$$= e^{i(A+B)\Delta t} + O(\Delta t^3)$$

Ex: 4.50

$U_{\Delta t} =$

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(b) Pro

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Ex. 4.50 Let $H = \sum_k^L H_k$ and define

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

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

(b) Prove that for a +ve integer m,

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

for some constant α,

using the results:

$$|P_U - P_V| = |\langle\psi|U^\dagger M U|\psi\rangle - \langle\psi|V^\dagger M V|\psi\rangle|$$
$$\leq 2E(U,V)$$

where,

$$E(U,V) = \max_{|\psi\rangle\neq 0} \|(U-V)|\psi\rangle\| = \|U-V\|$$

$$E\left(U_m U_{m-1} \cdots U_1, V_m V_{m-1} \cdots V_1\right) \leq \sum_{j=1}^{m} E(U_j, V_j)$$

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

$$= e^{-iH_1\Delta t} \cdots e^{-iH_{L-1}\Delta t} e^{-iH_L\Delta t} e^{-iH_L\Delta t} e^{-iH_{L-1}\Delta t} \cdots e^{-iH_1\Delta t}$$

$$e^{i(A+B)\Delta t} = e^{iA\Delta t/2} e^{iB\Delta t} e^{iA\Delta t/2} + O(\Delta t^3)$$

$$= e^{-iH_1\Delta t} \cdots e^{-iH_{L-2}\Delta t} \left(e^{-2i(H_{L-1}+H_L)\Delta t} + O(\Delta t^3) \right) \cdots e^{-iH_1\Delta t}$$

(b) E(

$$= e^{-iH_1\Delta t} \cdots e^{-iH_{L-2}\Delta t} e^{-2i(H_{L-1}+H_L)\Delta t} e^{-iH_1\Delta t} \cdots e^{-iH_1\Delta t}$$

$$+ O(\Delta t^3)$$

$$\vdots$$

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

(b) $$E\left(U_{\Delta t}, e^{-2iH\Delta t}\right) = \max_{|\psi\rangle \neq 0} \frac{\|(U-V)|\psi\rangle\|}{} = \|U - V\|$$

$$= O(\Delta t^3)$$

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

$$O(\Delta t^3) = \alpha\, \Delta t^3.$$

Algorithm : Quantum Simulation

Inputs :

① A Hamiltonian $H = \sum_k H_k$ acting on a N-d system, where each H_k acts on a small subsystem of size independent of N

② An initial state $|\psi_0\rangle$ of the system at $t=0$

③ A +ve, non-zero accuracy δ

④ A time t_f at which the evolved state is desired.

Outputs : A state $|\tilde{\psi}(t_f)\rangle$ such that

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

Runtime : ?

Procedure:

Choose a representation such that the state $|\tilde{\psi}\rangle$ of $n = \text{poly}(\log_a N)$ qubits approximates the system and the operators $e^{-iH_k \Delta t}$ have efficient quantum circuit approximations.

Select an approximation method (for example

$$e^{i(A+B)\Delta t} = e^{iA\Delta t} e^{iB\Delta t} + O(\Delta t^2)$$

$$e^{i(A+B)\Delta t} = e^{iA\Delta t/2} e^{iB\Delta t} e^{iA\Delta t/2} + O(\Delta t^3)$$

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

equations 4.103–4.105) and Δt such that the expected error is acceptable (and $j\Delta t = t_g$ for an integer j); construct the corresponding quantum circuit $U_{\Delta t}$ for the iterative step, and do:

① $|\tilde{\Psi}_0\rangle \longleftarrow |\Psi_0\rangle$; $j = 0$ initialize state

② $\longrightarrow |\tilde{\Psi}_{j+1}\rangle = U_{\Delta t} |\tilde{\Psi}_j\rangle$ iterative update

③ $\longrightarrow$ $j = j+1$; goto ② until $j\Delta t \geq t_f$ loop

④ $\longrightarrow$ $|\tilde{\Psi}(t_f)\rangle = |\tilde{\Psi}_j\rangle$

Quantum simulation of Schrödinger's equation

Consider a single particle living on a line, in a 1-d potential $V(x)$, governed by the 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 state $|\psi\rangle$ resides in an infinite dimensional Hilbert space; in the x-basis, it can be written as:

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

In practice, only some finite region is of interest, which we may take to be the range $-d \le x \le d$.

Furthermore, it is possible to choose a differential step size Δx sufficiently small compared to the shortest wavelength in the system such that

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

provides a good physical approximation of $|\psi\rangle$ then state can be represented using $n = \log_2\left[2d/\Delta x + 1\right]$ qubits

$$2^n = \frac{2d}{\Delta x} + 1 \longrightarrow n = \log_2\left(\frac{2d}{\Delta x} + 1\right)$$

We simply replace the basis $|k\Delta x\rangle$ (an eigenstate of the operator) with $|k\rangle$, a computational basis state of n qubits.

Note: Only n qubits are required for this simulation, whereas classically 2^n complex numbers could have to be kept track of, thus leading to an exponential resource saving when performing the simulation on a quantum computer..

Computation of $|\tilde{\Psi}(t)\rangle = e^{-iHt}|\tilde{\Psi}(0)\rangle$ must utilize one of the approximations of equations 4.103 – 4.105

$$e^{i(A+B)\Delta t} = e^{iA\Delta t} e^{iB\Delta t} + O(\Delta t^2)$$

$$e^{i(A+B)\Delta t} = e^{iA\Delta t/2} e^{iB\Delta t} e^{iA\Delta t/2} + O(\Delta t^3)$$

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

because in general $H_1 = V(x)$ does not commute with $H_0 = p^2/2m$.

Thus we must be able to compute $e^{-iH_1\Delta t}$ and $e^{-iH_0\Delta t}$.

Because $|\tilde{\Psi}\rangle$ is expressed in the eigenbasis of H_1, $e^{-PH_1\Delta t}$ is a diagonal transformation of the form

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

It is straightforward to compute this, since we can compute $V(k\Delta x)\Delta t$.

~~Because~~ x and p are conjugate variables related by a quantum Fourier transform $U_{FFT} x U_{FFT}^\dagger = p$ and thus

$e^{UAU^\dagger} = U e^A U^\dagger$ for an unitary operator U

ILA (7)
Taylor series expansion

$$e^{-iH_0\Delta t} = e^{-i\frac{p^2}{2m}\Delta t} = e^{-i\left(U_{FFT} x^2 U_{FFT}^\dagger\right)\frac{\Delta t}{2m}}$$

$$= e^{U_{FFT}\left(-ix^2\Delta t/2m\right)U_{FFT}^\dagger}$$

$$= e^{-ix^2\Delta t/2m}$$

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

to compute $e^{-iH_0\Delta t}$ do,

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

- Example: Hamiltonians which acts non-trivially on all or nearly all parts of a large system.

Suppose we have the Hamiltonian

$$H = Z_1 \otimes Z_2 \otimes \cdots \otimes Z_n$$

which acts on an n-qubit system.

What we desire is a simple quantum circuit which implements e^{-iHt} for arbitrary values of Δt.

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = |0\rangle\langle 0| - |1\rangle\langle 1|$$

$Z|0\rangle = |0\rangle$

$Z|1\rangle = -|1\rangle$

$e^{-i\theta Z}|0\rangle = (\cos\theta I - i\sin\theta Z)|0\rangle = e^{-i\theta}|0\rangle$

$e^{-i\theta Z}|1\rangle = (\cos\theta I - i\sin\theta Z)|1\rangle = e^{i\theta}|1\rangle$

Although the Hamiltonian involves all the qubits in the system, it does so in a classical manner: the phase shift applied to the system is e^{-iAt} if the parity of the n qubits in the computational basis is even; otherwise, the phase shift should be e^{iAt}.

∴

Simple simulation of H is possible by first classically computing the parity (storing the result in an ancilla qubit), then applying the appropriate phase shift conditioned on the parity, then uncomputing the parity (to erase the ancilla).

Fig 4.19

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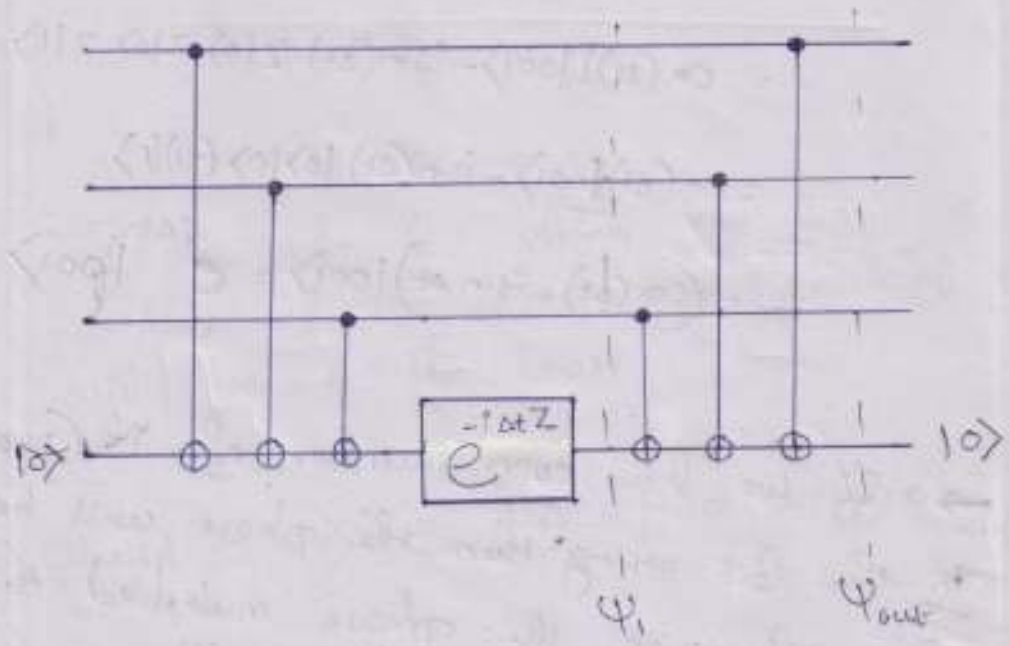
Ex:-

$Z^2 = I$

e^{-iHA}

$e^{|110\rangle}$

Fig 4.19 Quantum circuit for simulating the Hamiltonian, $H = Z_1 \otimes Z_2 \otimes Z_3$ for time Δt.



Ex:- Let $|\psi_{in}\rangle = |1\,1\,0\rangle$

$$Z^2 = I \Longrightarrow (Z \otimes Z \otimes Z)^2 = I$$

$$e^{-iH\Delta t}|110\rangle = e^{-i(Z\otimes Z\otimes Z)\Delta t}|110\rangle = \left(\cos(\Delta t) I - i\sin(\Delta t)(Z\otimes Z\otimes Z)\right)|110\rangle$$

$$= \cos(\Delta t)|110\rangle - i\sin(\Delta t)\, Z|1\rangle Z|1\rangle Z|0\rangle$$

$$= \cos(\Delta t)|110\rangle - i\sin(\Delta t)(-1)|1\rangle(-1)|1\rangle(+1)|0\rangle$$

$$= \left[\cos(\Delta t) - i\sin(\Delta t)\right]|110\rangle = e^{-i\Delta t}|110\rangle$$

$$e^{-iH\Delta t}|0\,0\rangle = e^{-i(Z\otimes Z\otimes Z)\Delta t}|001\rangle$$

$$= \left(\cos(\Delta t)I - i\sin(\Delta t)(Z\otimes Z\otimes Z)\right)|001\rangle$$

$$= \cos(\Delta t)I|001\rangle - i\sin(\Delta t)\, Z|0\rangle Z|0\rangle Z|1\rangle$$

$$= \cos(\Delta t)|001\rangle - i\sin(\Delta t)\,|0\rangle|0\rangle(-1)|1\rangle$$

$$= \left(\cos(\Delta t) + i\sin\Delta t\right)|001\rangle = e^{i\Delta t}|001\rangle$$

→ If we have even number of 1's (parity) in the bit string then the phase will be $e^{-i\Delta t}$, otherwise the phase multiplied to the corresp. bit string will be $e^{i\Delta t}$.

← The circuit in Fig. 4.19 does parity checks with CNOTs:

If in the bit string we have an even number of 1's, the target (ancillary) qubit will be in $|0\rangle$ state.

$$|\psi_i\rangle = |\text{even parity}\rangle \otimes e^{-iZ\Delta t}|0\rangle = |\text{even parity}\rangle \otimes e^{-i\Delta t}|0\rangle$$

If in the bit string we have an odd number of 1's, the target (ancilla) qubit will be in $|1\rangle$ state:

$$|\psi_1\rangle = |\text{odd parity}\rangle \otimes e^{-iZ\Delta t}|1\rangle = |\text{odd parity}\rangle \otimes e^{i\Delta t}|1\rangle$$

$$|\psi_2\rangle = |\text{odd parity}\rangle \otimes e^{i\Delta t}|0\rangle$$

* Extending the same procedure allows us to simulate more complicated extended Hamiltonians.

i.e.,

We can efficiently simulate any Hamiltonian of the form

$$H = \bigotimes_{k=1}^{n} \sigma_{c(k)}^{k}$$

where,

$\sigma_{c(k)}^{k}$: Pauli matrix (or the identity) acting on the k^{th} qubit, with $c(k) \in \{0,1,2,3\}$ specifying one of $\{I, X, Y, Z\}$.

The qubits upon which the identity operation is performed can be discarded, and X or Y terms can be transformed by single qubit gates to Z operations. This leaves us with a Hamiltonian of the form $H = Z_1 \otimes Z_2 \otimes \cdots \otimes Z_n$ which is simulated as described in this section.

Ex: 4.51 Construct a quantum circuit to simulate the Hamiltonian $H = X_1 \otimes Y_2 \otimes Z_3$, performing the unitary transform $e^{-i\Delta t H}$ for any Δt.

Ans:

$$X = HZH$$

$$R_z(\pi/2) \times R_z(-\pi/2) = \left(\frac{I - iZ}{\sqrt{2}}\right) \times \left(\frac{I + iZ}{\sqrt{2}}\right)$$

$$= \frac{1}{2}\left((I - iZ)(X + iXZ)\right) = \frac{1}{2}\left(X + iXZ - iZX + ZXZ\right)$$

$$= \frac{1}{2}\left(X - 2iZX - Z^2X\right)$$

$$= \frac{1}{2}\left(-2iZX\right) = i(-iY) = Y$$

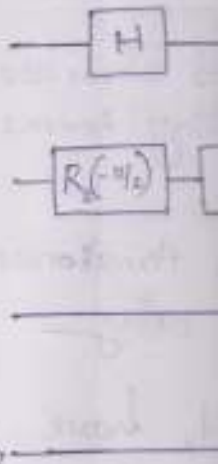
$$Y = R_z(\pi/2)\, HZH\, R_z(-\pi/2)$$

The Hamiltonian can be described as,

$$H = X_1 \otimes Y_2 \otimes Z_3$$

$$= H_1 Z_1 H_1 \otimes R_z(\pi/2) H_2 Z_2 H_2 R_z(-\pi/2) \otimes Z_3$$

$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad \& \quad H^2 = I \quad \& \quad H^\dagger = H = H^{-1}$$



$R_z(\pi/2)\,H$ is unitary

$$e^{UAU^\dagger} = U e^{A} U^\dagger$$

$$e^{iH\Delta t} = e^{-i(X_1 \otimes Y_2 \otimes Z_3)\Delta t}$$

$$= e^{-i\left(H_1 Z_1 H_1 \otimes R_z(\pi/2) H_2 Z_2 H_2 R_z(-\pi/2) \otimes Z_3\right)\Delta t}$$

$$= e^{-i\left(H_1 \otimes R_z(\pi/2) H_2 \otimes I\right)\left(Z_1 \otimes Z_2 \otimes Z_3\right)\left(H_1 \otimes H_2 R_z(-\pi/2) \otimes I\right)\Delta t}$$

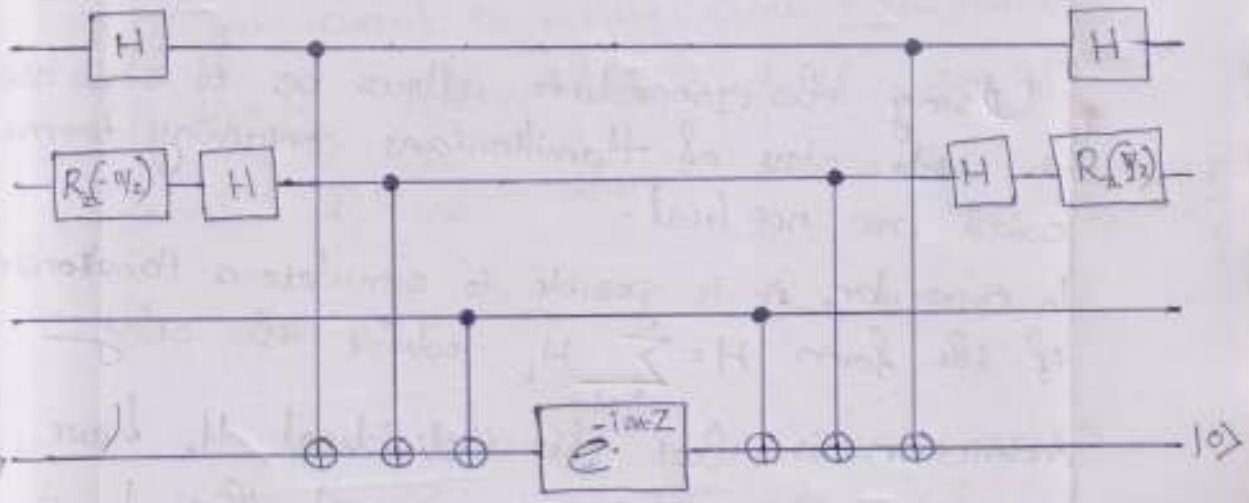
$$= e^{-i(Z_1 \otimes Z_2 \otimes Z_3)\Delta t}\left(H_1 \otimes H_2 R_z(-\pi/2) \otimes I\right)$$

$$= \left(H_1 \otimes R_z(\pi/2) H_2 \otimes I\right) e^{\left(H_1 \otimes H_2 R_z(-\pi/2) \otimes I\right)}$$

$(A \otimes B)^\dagger = A^\dagger \otimes B^\dagger$? $(H \otimes R_z\, H \otimes I)^\dagger = H^\dagger \otimes (R_z H)^\dagger \otimes I^\dagger = H \otimes H^{-1} R_z^{-1} \otimes I^{-1} = H^{-1} \otimes (R_z H)^{-1} \otimes I^{-1} = (H \otimes R_z H \otimes I)^{-1}$

$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$

$\Rightarrow H \otimes R_z H \otimes I$ is unitary


H
H
$R_x(-\pi/2)$
H
H
$R_x(\pi/2)$
$e^{-i\alpha Z}$
|0⟩

* Using this procedure allows us to simulate a wide class of Hamiltonians containing terms which are not local.

In particular, it is possible to simulate a Hamiltonian of the form $H = \sum_{k=1}^{L} H_k$ where the only restriction is that the individual H_k have a tensor product structure, and that L is polynomial in the total # of particles n.

All that is required is that there be an efficient circuit to simulate each H_k separately.

Ex:-
the Hamiltonian $H = \sum_{k=1}^{n} X_k + Z^{\otimes n}$ can be easily simulated using these techniques.

Such Hamiltonians typically do not arise in Nature.

If you want to evolve some Hamiltonian $H = H_1 + H_2$ where H_1 and H_2 are of the form $\bigotimes_{k=1}^{n} \sigma_{c(k)}^{k}$, then we can decompose the evolution as

$$e^{-iHt} = e^{-i(H_1+H_2)t} = \lim_{n\to\infty} \left(e^{-iH_1 t/n} e^{-iH_2 t/n} \right)^n$$

and each of those small steps $e^{-iH_i t/n}$ can be implemented with the previous circuit