BIRTH OF QC IDEA

- SIMULATING PHYSICAL PROCESSES

- RICHARD FEYNMAN

  "SIMULATING PHYSICS WITH COMPUTERS, 1982"

"Nature isn't classical, dammit, and if you want to make a simulation of nature you'd better make it quantum-mechanical

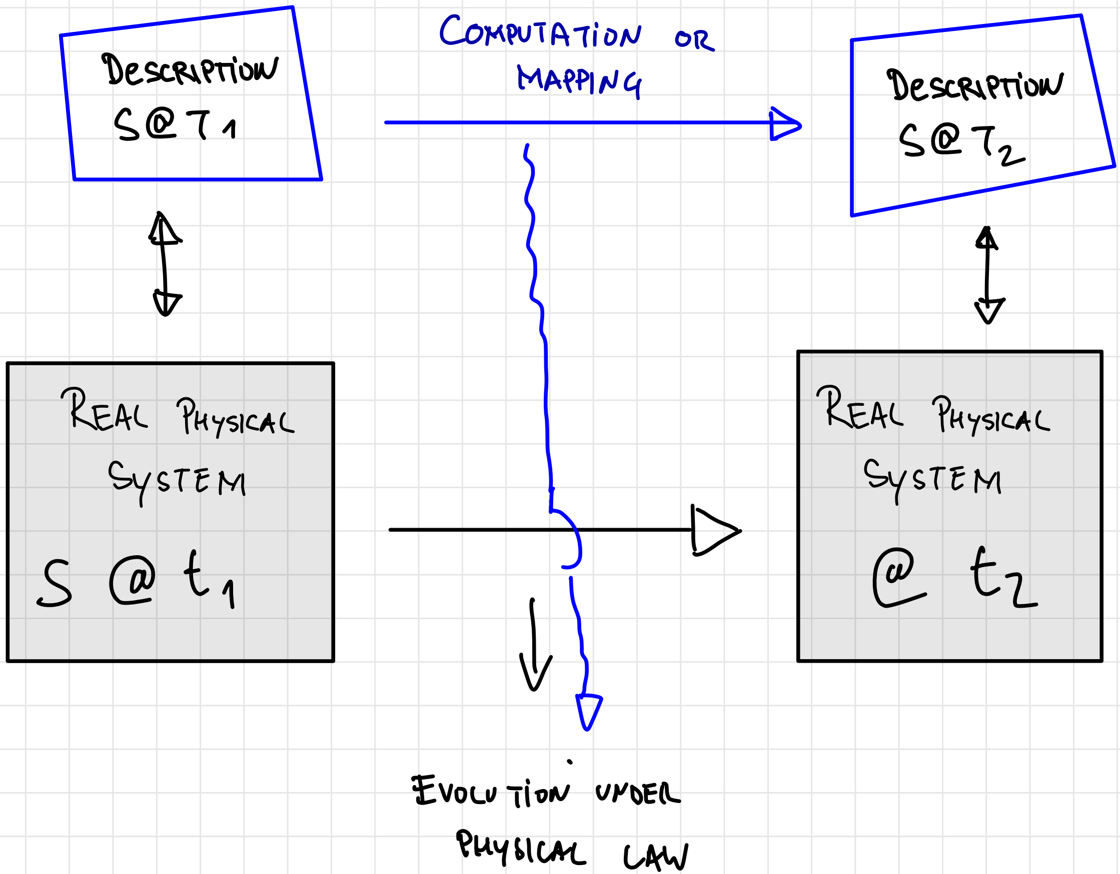
and by golly, it's a wonderful problem because it does not look so easy"

- YURI MANIN
  "COMPUTABLE AND UNCOMPUTABLE" 1980

- PAUL BENIOFF 1980/1982

- DAVID DEUTSCH 1985
  QUANTUM TURING MACHINE

But what does "simulating nature" mean



CLASSICAL SYSTEMS (E.G. SECOND ORDER ODE IN $\mathbf{x}(t) \in \mathbb{R}^3$

$$M[\mathbf{x}(t), \dot{\mathbf{x}}(t), \ddot{\mathbf{x}}(t), t] = 0$$)

QUANTUM SYSTEMS... DESCRIBED BY WAVEFUNCTION (STATE VECTOR) $|\psi(t)\rangle$

FOR PHYSICISTS

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

$\sqrt{-1}$

REDUCED PLANCK CONSTANT

WE WILL SET IT TO 1...

HAMILTONIAN

$\Rightarrow$ GENERATOR OF DYNAMICS

WHAT DO WE DO WITH SCHRÖDINGER'S EQUATION

$|\psi(t_1)\rangle \xrightarrow[\text{Evolution specified by } H]{} |\psi(t_2)\rangle$

Solve the Schrödinger equation

1-D INTUITION

$$i\frac{\partial x(t)}{\partial t} = \alpha x(t)$$

$$\boxed{\begin{aligned} f'(x) &= \alpha f(x) \\ \int f'(x)\,dx &= \int \alpha f(x)\,dx \\ f(x) &= \exp(\alpha x) + C \end{aligned}}$$

$x(t)$ is an exponential

$$x(t) = \exp(\alpha i t) + C$$

$$\underline{\underline{x(t_2) = \exp(\alpha i \Delta t)\, x(t_1)}}$$

$\Delta t = t_2 - t_1 \ldots$

$$|\psi(t_2)\rangle = \int i H |\psi(t)\rangle\, dt$$

Assume H is diagonal $H = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_N \end{pmatrix}$, $\Delta t = t_2 - t_1$

$$|\psi(t_2)\rangle = \begin{pmatrix} \exp(i\lambda_1 \Delta t) & & & \\ & \exp(i\lambda_2 \Delta t) & & \\ & & \ddots & \\ & & & \exp(i\lambda_N \Delta t) \end{pmatrix} |\psi(t_1)\rangle$$

OFC, WORKS IN ALL BASES... RECALL FUNCTIONS OF OPERATORS

YOU JUST NEED TO KNOW HOW TO COMPUTE FUNCTIONS OF OPERATORS...

① SPECTRAL THEOREM + DIAGONAL CASE

$$= \quad |\Psi(t_2)\rangle = \exp(-i H \Delta t) \, |\Psi(t_1)\rangle$$

$$\exp(-i H \Delta t) = \exp\left(i \, U \, \mathrm{diag}(-\vec{\lambda}) \, U^{\dagger} \Delta t\right)$$

$$= U \exp\left(i \, \mathrm{diag}(-\vec{\lambda}) \Delta t\right) U^{\dagger}$$

$$= U \underbrace{\mathrm{diag}\left(e^{-i\lambda_1 \Delta t}, \ldots, e^{-i\lambda_n \Delta t}\right)}_{\text{unitary operator!}} U^{\dagger}$$

② OR DIRECTLY VIA TAYLOR SERIES...

HAMILTONIAN SIMULATION :

- given H, $|\psi(t_1)\rangle$, $\Delta t = t_2 - t_1$

COMPUTE: $|\psi(t_2)\rangle := \exp(-iH\Delta t)\,|\psi(t_1)\rangle$

"Classically" "QUANTUMLY"

THERE IS ALSO THE TIME – INDEPENDENT SCHRÖDINGER EQUATION:

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

EIGENVALUE EQUATION

"energy" = eigenvalue! $\in \mathbb{R}$ (because $H = H^\dagger$)

- TYPICAL PROBLEM: FIND (LOW-ENERGY, GROUND) EIGENSTATES OF H.
- ACTUALLY, DETECTING WHETHER GROUND ENERGY (= SMALLEST EIGENVALUE) IS BELOW SOME η IS VERY (QMA) HARD
- SUPER IMPORTANT! HAM. SIM. WILL BE INSTRUMENTAL FOR THIS TOO.
- MUCH OF THE REMAINDER OF THE COURSE WILL BE ABOUT THIS

HAMILTONIAN SIMULATION:

- given H, $|\psi_1\rangle$, over n QUBITS, $\Delta t = t_2 - t_1$

COMPUTE: $|\psi_2\rangle := \exp(-i H \Delta t)|\psi_1\rangle$

"Classically"

TAKES $\Omega(\dim(H)) = \Omega(\exp(n))$

TO EVEN WRITE DOWN $|\psi_2\rangle$ AS A VECTOR...

"QUANTUMLY"

WELL... DEPENDS ON WHAT WE MEAN.

HAMILTONIAN SIMULATION ON A QC

INPUT : • An n- qubit quantum register in STATE $|\psi_1\rangle$

(SOMETIMES , U s.t. $U|\vec{0}\rangle = |\psi_1\rangle$)

• (a) SUCCINT DESCRIPTION OF H (CLASSICAL)

(b) AN ORACLE FOR COMPUTING ENTRIES OF H (USUALLY SPARSE)

→ time t

OUTPUT : n- qubit quantum register IN THE STATE $|\tilde{\psi}_2\rangle$

S.T. $\| |\psi_2\rangle - |\tilde{\psi}_2\rangle \|_2 \leq \varepsilon$ (SUFFICIENTLY CLOSE)

SEE N&C 9.2, 9.2.2

SANITY: GIVEN H, U S.T. $U|0\rangle = |\psi\rangle$, t THERE IS A "BRUTE FORCE" Q. ALGORITHM WITH (HIGH) EXP. RUNTIME..

GOAL: ALGORITHMS WITH $\mathrm{poly}(n)$ $\left(\mathrm{polylog}(N)\right)$ RUNTIME...

NEXT:

EFFICIENT ALGORITHMS FOR LOCAL HAMILTONIANS (TROTTERIZATION BASED)

TIME PERMITTING: ALGORITHMS FOR SPARSE HAMILTONIANS AND "$\log(1/\varepsilon)$" METHODS

PATH TO TROTTERIZATION - BASED ALGORITHMS FOR QUANTUM SIMULATION

1) HAMILTONIAN SIMULATION FOR $\mathcal{H} = Z$, $\mathcal{H} = X$

o→ DIGRESSION: GLOBAL VS RELATIVE PHASE

2) HAMILTONIAN SIMULATION FOR "PAULI STRINGS", E.G. $\mathcal{H} = X \otimes Y \otimes \mathbb{1} \otimes Z^{\otimes k} \otimes X$

3) FROM PAULI STRINGS TO ARBITRARY HAMILTONIANS VIA TROTTERIZATION

o→ DIGRESSION: VECTOR SPACES OF OPERATORS

SIMULATING SIMPLEST HAMILTONIANS

SIMPLE(ST) HAMILTONIANS

. ASSUME $G = \{ H, \text{CNOT}, \text{CZ}, Z_\phi \}$ $\qquad Z_\phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$

1) SIMULATING $\mathcal{H} = Z \quad \left[= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right]$

$\Rightarrow$ IT IS IN OUR TOOLBOX (GATE SET)

$$\exp(-i Z t) = \underbrace{\exp(-it)}_{\text{GLOBAL PHASE}} \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & \exp[2it] \end{bmatrix}}_{Z_{2t}}$$

USUALLY : $\exp\left(-i Z \frac{\theta}{2}\right) = Z_\theta$. "UP TO GLOBAL PHASE"

"angle"

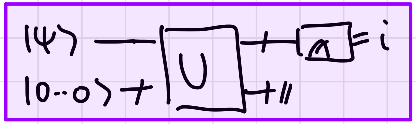
GLOBAL PHASE ... RECALL

DIGRESSION

- QUANTUM STATE $\longrightarrow$ UNIT VECTOR IN $\mathbb{C}^n$ IS NOT 1-1

"OBSERVABLE PROPERTY" $\longrightarrow$ $\exists$ PHYSICAL MEANS TO MEASURE

HOWEVER $\quad |\psi\rangle \quad$ VS $\quad e^{i\theta}|\psi\rangle = |\psi'\rangle$



$\forall\,\theta,\ \forall\,U$

$$P_\psi(i) = \left|[\langle i|\otimes\mathbb{1}]\,U\,[|\psi\rangle\otimes|0..0\rangle]\right|^2 = |e^{i\theta}|\left|[\langle i|\otimes\mathbb{1}]\,U\,[|\psi\rangle\otimes|0..0\rangle]\right|^2 = \left|[\langle i|\otimes\mathbb{1}]\,U\,[e^{i\theta}|\psi\rangle\otimes|0..0\rangle]\right|^2 = P_{\psi'}(i)$$

- $U \simeq e^{i\theta}U$ IN THE SAME WAY $\left(\exp(iHt) \simeq \exp(iHt + i\lambda\mathbb{1}) = \underbrace{\exp(i\lambda t)}\cdot\mathbb{1}\cdot\exp(iHt)\right)$

  - CONSTANT SHIFT OF ENERGIES
  - CHANGE OF UNIT.

$U|\psi\rangle$ VS $e^{i\theta}U|\psi\rangle$ RESULTS IN SAME STATE UP TO GLOBAL PHASE

NOT UNITARIES.. "SPECIAL UNITARY GROUP" $SU(N)$

GLOBAL PHASE... RECALL...

DIGRESSION

TO AVOID CONFUSION... RELATIVE V.S. GLOBAL PHASE

- $Z|0\rangle = |0\rangle$; $Z|1\rangle = \underline{(-1)}|1\rangle$ NOT A GLOBAL PHASE OF UNITARY

$|\psi\rangle + e^{i\theta}|\psi^\perp\rangle$ "RELATIVE PHASE" IN STATE

$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$

$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

$Z|+\rangle = |-\rangle$

ORTHOGONAL...
OUTCOMES DIFFER MAXIMALLY.

ALSO:

MATHEMATICALLY : $\mathbb{1} \otimes [e^{i\theta} U]$ = GLOBAL PHASE

$\mathbb{1} \oplus [e^{i\theta} U]$ = RELATIVE PHASE $\Rightarrow$ $\left[\begin{array}{c|c} \mathbb{1} & 0 \\ \hline 0 & e^{i\theta} U \end{array}\right] = \text{ctrl-}e^{i\theta} U$

eg: $-\mathbb{1} = \mathbb{1}$; but.. $\text{ctrl-}(-\mathbb{1}) = Z \otimes \mathbb{1}$!!

DIGRESSION

- CAN BE CONFUSING. COMPUTE ALL THE WAY WITH FULL PHASES & ALL WILL BE OK.

- "PROJECTIVE HILBERT SPACE" & $SU(N)$

- DENSITY MATRIX FORMALISM

$$
\begin{tikzcd}
|\psi\rangle \arrow[r] \arrow[d, "U"'] & |\psi\rangle\langle\psi| \arrow[d, "\mathcal{U}"] \\
U|\psi\rangle \arrow[r] & \mathcal{U}(|\psi\rangle\langle\psi|) = U|\psi\rangle\langle\psi|U^\dagger
\end{tikzcd}
$$

TRACE-1 POSITIVE-SEMIDEFINITE OPERATOR

NB:

$$e^{i\theta}|\psi\rangle \to \left(e^{i\theta}|\psi\rangle\right)\left(\langle\psi|e^{-i\theta}\right) = \cancel{\left(e^{i\theta}\cdot e^{-i\theta}\right)}\,|\psi\rangle\langle\psi|$$

TRUE 1-1 CORRESPONDENCE

SIMPLE(ST) HAMILTONIANS

$G = \{ H, CNOT, CZ, Z_\phi \}$ $\quad Z_\phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$

1) $\mathcal{H} = Z \longrightarrow \exp(i Z \theta/2) = Z_\theta$ (UP TO GLOBAL PHASE)

2) $\mathcal{H} = P \qquad P \in \{ \underset{}{\overset{\text{TRIV}}{\mathbb{1}}}, X, Y, \underset{\text{BID}}{Z} \}$

> LEMMA "BASIS CHANGE": $\forall\ U, W \in U(N),\ \exp(i U W U^\dagger t) = U \exp(i W t) U^\dagger$

$\Rightarrow H Z_\phi H = X_\phi \Rightarrow \exp(-i X \frac{\theta}{2}) = H Z_\theta H \ldots$

NB U, U' S.T. $\exists\ W \in U(N)$, $U = W U' W^\dagger \Leftrightarrow U, U'$ HAVE SAME SPECTRUM.

$\Rightarrow$ CAN SWITCH BETWEEN ALL PAULIES.

SIMPLE(ST) HAMILTONIANS

$G = \{ H, CNOT, CZ, Z_\phi \}$ $\quad Z_\phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$

1) $\mathcal{H} = Z \longrightarrow \exp(i Z \theta/2) = Z_\theta$ (UP TO GLOBAL PHASE)

2) $\mathcal{H} = P \qquad P \in \{ \overset{\text{TRIV}}{\mathbb{1}}, X, Y, \underset{\text{DID}}{Z} \}$

LEMMA "BASIS CHANGE": $\forall\ U, W \in U(N),\ \exp(i U W U^\dagger t) = U \exp(i W t) U^\dagger$

3) $\mathcal{H} = \mathbb{1}^{\otimes k} \otimes P \otimes \mathbb{1}^{\otimes n-k-1}$

LEMMA LOCAL ACTION:

$$\forall H \quad \exp[-i\, \mathbb{1}^{\otimes k-1} \otimes H \otimes \mathbb{1}^{\otimes n-k+1}\, t] = \mathbb{1}^{\otimes k-1} \otimes \exp[-iH t] \otimes \mathbb{1}^{\otimes n-k+1}$$

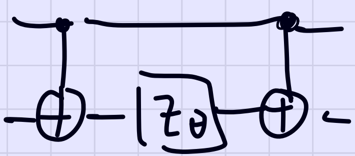
SIMPLE HAMILTONIANS:

2) "TWO-BODY TERMS"...

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

$$\boxed{\exp\left(-i \; Z\otimes Z \; \tfrac{\theta}{2}\right)} = \begin{pmatrix} \exp(-i\theta/2) & & & \\ & \exp(+i\theta/2) & & \\ & & \exp(+i\theta/2) & \\ & & & \exp(-i\theta/2) \end{pmatrix} = \exp(-i\theta/2) \begin{bmatrix} 1 & & & \\ & \exp(\theta i) & & \\ & & \exp(\theta i) & \\ & & & 1 \end{bmatrix}$$

$$\|$$



$$= |0\rangle\langle 0| \otimes Z_\theta + |1\rangle\langle 1| \otimes (X Z_\theta X) = \left[\begin{array}{c|cc} Z_\theta & \multicolumn{2}{c}{0} \\ \hline 0 & e^{i\theta} & 0 \\ & 0 & 1 \end{array}\right]$$

EQUAL

$$X Z_\theta X = \begin{pmatrix} e^{i\theta} & \\ & 1 \end{pmatrix} \underset{\text{UP TO PHASE}}{=} \begin{pmatrix} 1 & \\ & e^{-i\theta} \end{pmatrix}$$

WITH BASIS CHANGE:

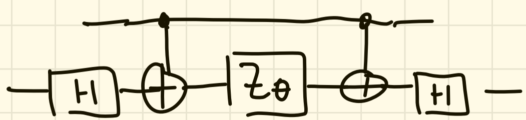
$$\boxed{\mathcal{H} = Z \otimes X} \ldots = (\mathbb{1} \otimes H)(Z \otimes Z)(\mathbb{1} \otimes H)$$

HAMILTONIAN

HADAMARD. RECALL $HZH = X \ldots$

BECAUSE $H = H^\dagger$!!

$\Rightarrow$



WITH LOCALITY & SWAPPING MY WORRIES AWAY ...

$$\boxed{\mathcal{H} = X \otimes \underline{\underline{\mathbb{1}}} \otimes Y} \ldots$$

$$(SWAP_{1,2} \otimes \mathbb{1})\, \mathcal{H}\, (SWAP_{1,2} \otimes \mathbb{1}) = \mathbb{1} \otimes X \otimes Y$$

RECALL: $H Z_\theta H = X_\theta$

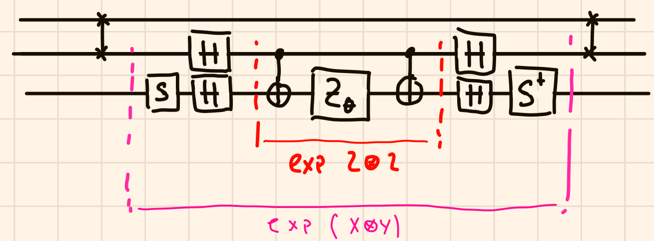
BUT ALSO $S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$

$= Z_{\pi/2}$

$Y_\theta = S.H.Z_\theta.H.S^\dagger$

$\overset{\shortparallel}{H^\dagger}$

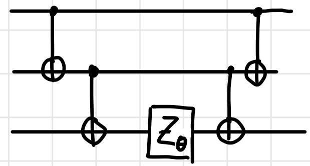
$\exp(i\mathcal{H}(\theta/2)) =$



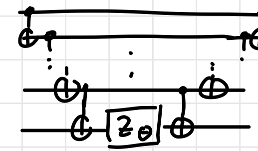
For N-body Pauli products...

Z-strings

$$\exp\left(i\, Z\otimes Z\otimes Z\, \theta/2\right) =$$



$$\ldots \quad \exp\left(i\, Z^{\otimes n}\theta/2\right) =$$



- Z-string + local basis change = any Pauli string in $\{X, Y, Z\}$
- Z-string + local change + swaps = any Pauli string (in $\{\mathbb{1}, X, Y, Z\}$)

$\Rightarrow$ Ham simulation for all Pauli strings

DIGRESSION

SOME TIME EVOLUTIONS ARE MORE "NATURAL" / EXPERIMENTALLY FRIENDLY

LEADING TO EXPERIMENTALLY FRIENDLY GATES

X-Y INTERACTION $H = -(X \otimes X + Y \otimes Y) \Rightarrow \quad iSWAP = e^{i\pi/4} \begin{bmatrix} 1 & & & \\ & 0 & i & \\ & i & 0 & \\ & & & 1 \end{bmatrix}$

MØLMER - SØRENSEN:

$$H = X_i \otimes X_j \quad \& \quad H = \sum_{i,j \in S} X_i \otimes X_j$$

SIMULTANEOUS

$$H = \sum_i X_i \qquad \left(\exp \Sigma x = \Pi \exp x \right)$$

MORE ON THIS IN LATER LECTURES

MORE ON SOME OF THESE LATER.

BUT $\boxed{\text{TAKE HOME MESSAGE:}}$

: CNOT + Z_ϕ + H SUFFICE FOR

$\exp(i\theta P)$, P = "PAULI STRING" $P_1 \otimes P_2 \otimes \cdots \otimes P_n$

$P_k \in \{\mathbb{1}, X, Y, Z\}$

<u>DIRECTLY</u>, $O(n)$ two qubit + $O(n)$ SINGLE QUBIT...

BTW: Z_ϕ CAN BE EFFICIENTLY APPROXIMATED TO ANY PRECISION

WITH $\{H, \pi/8\}$

PAULI STRINGS ARE SPECIAL...

- A BASIS FOR <u>ALL</u> $2^n \times 2^n$ COMPLEX MATRICES
- $\mathcal{L}(\mathbb{C}^{2^n}) = \{ \mathbb{O} : \mathbb{C}^{2^n} \to \mathbb{C}^{2^n} \,/\, \text{linear} \}$ IS ITSELF A VECTOR SPACE
- UNITARY SPACE: $A, B \in \mathcal{L}(\mathbb{C}^{2^n})$ $\langle A, B \rangle_F = \mathrm{Tr}(A^\dagger B)$; $\mathrm{Tr}(A \otimes B) = \mathrm{Tr}(A) \cdot \mathrm{Tr}(B)$
- $P = P_1 \otimes \cdots P_n$ $\quad P_i \in \{ \mathbb{1}, X, Y, Z \}$ $\quad$ NB: $\mathrm{Tr}(P_i P_j) = 2\,\delta_{ij}$

$\Rightarrow \langle \vec{P}, \vec{P}' \rangle = 0$ unless $\vec{P} = \vec{P}'$

$\langle \vec{P}, \vec{P} \rangle = 2^n$, always ... note $\exists\ 4^n = 2^{n \times 2}$ of them...

$\Rightarrow$ complete basis

$$\Rightarrow \quad M = \sum_{\vec{P} \in \mathcal{P}} c_{\vec{P}} \vec{P} \qquad \vec{P} = \text{string}$$

$$\mathcal{P} = \{ \vec{P} \}$$

HERMITIAN MATRICES / OPERATORS (HAMILTONIANS)

$\mathrm{Herm}(\mathbb{C}^{2^n}) \subseteq \mathcal{L}(\mathbb{C}^{2^n})$ ALSO A VECT SPACE

$$H = \sum_{\vec{p} \in \mathcal{P}} \alpha_{\vec{p}} P \quad \& \quad \boxed{\alpha_{\vec{p}} \in \mathbb{R}.}$$

THE SET OF n-qubit COMPLEX HAMILTONIANS (HERMITIAN OP) s.

IS A 4^n-dimensional **REAL** HILBERT SPACE ... GO FIGURE

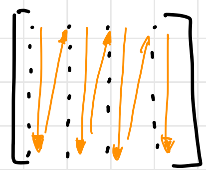
ALL HAMILTONIANS CAN BE EXPRESSED AS WEIGHTED SUMS ($w \in \mathbb{R}$) OF PAULI-STRINGS

$$\boxed{H = \sum \alpha_{\vec{e}}\, P^{\vec{e}}, \quad \vec{e} \in \{\underset{\mathbb{1}}{0}, \underset{X}{1}, \underset{Z}{2}, \underset{Y}{3}\}^n, \quad \alpha_{\vec{e}} \in \mathbb{R}}$$

DIGRESSION

ANOTHER WAY TO UNDERSTAND ALL THIS

$$\text{Vec}: \mathbb{C}^{n \times n} \longrightarrow \mathbb{C}^{n^2}$$



$$\longrightarrow \begin{bmatrix} \text{Column}_1 \\ \text{column}_2 \\ \vdots \\ \text{column}_n \end{bmatrix}$$

$$\text{vec}(\alpha A + \beta B) = \alpha \, \text{vec}(A) + \beta \, \text{vec}(B)$$

$$\text{Tr}(A^\dagger B) = \langle \text{vec}(A) | \text{vec}(B) \rangle$$

PAULI STRINGS $\longrightarrow$ "colum-basis"

BUT DOES NOT MAKE MATH SIMPLER...

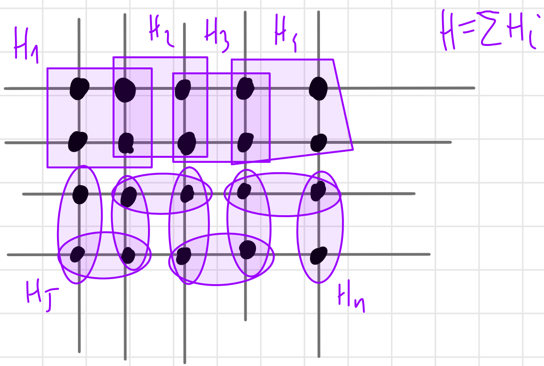
PHYSICALLY & COMPUTATIONALLY (MOST) RELEVANT HAMILTONIANS

K-LOCAL HAMILTONIANS $\quad H = \sum H_i \quad H_i$ is k-LOCAL / k-BODY

LOCALITY HAS MANY MEANINGS

-> NON-LOCALITY OF QM
-> RELATIVISTIC LOCALITY

GEOMETRIC LOCALITY



HERE: n-qubit $H = \sum H_i$
IS k-LOCAL IF EACH
H_i "ACTS NON-TRIVIALLY ON $\leq k$ - SITES

$$H = \sum_i H_i = \sum_{\vec{e}} \alpha_{\vec{e}} \, P^{\vec{e}}$$

each $P^{\vec{e}}$ has $\geq n-k$ identity ops.

(NEARLY) ALL SPIN HAMILTONIANS YOU WILL HAVE SEEN ARE LOCAL:

(1) ISING: $H = \sum_{i,j} w_{ij} \, X_i \otimes X_j + \sum_k h_j \, X_k$

(2) HEISENBERG $H = -\frac{1}{2} \sum \left(J_x \, X_i \otimes X_j + J_z \, Z_i \otimes Z_j + J_y \, Y_i \otimes Y_j + h Z_j \right)$
(ALSO GEOMETRICALLY LOCAL)

(3) X-Y MODEL $H = -\sum J_{ij} \left(X_i \otimes X_j + Y_i \otimes Y_j \right)$

(4) AKLT

(5) KITAEV HAMILTONIAN $H = -\sum_i J_i \bigotimes_{j \in N_i^x} X_j + \bigotimes_{j \in N_i^y} Y_j$ (LATTICE)

$|N_i^{X/Y}| = 4$ or SIMILAR

K-LOCAL HAMILTONIANS HAVE $\binom{n}{k} 4^k$ terms at most

- POLYNOMIAL IN n .. V.S. GENERAL 4^n ... CHANCE !!

FROM SIMULATING PAULI-STRINGS TO LOCAL HAMILTONIANS IN POLY-TIME

So... $H = \sum H_j$ $\qquad H_i = \alpha \cdot$ PAULI STRING $\vec{P}$

$\Rightarrow \exp(\alpha t \vec{P})$ ⇐ THIS WE KNOW HOW TO DO.

NOW $\exp[-iHt] = \exp(-i \sum H_j t)$

$= \exp\left(-\sum (iH_j t)\right) \stackrel{?}{=}$ Hmmm.. $e^{x+y} = e^x \cdot e^y =$ sooo .. $= \prod_j \exp(-iH_j t)$ DONE.

FAIL.

$\mathrm{EXP}(A+B) = \mathrm{EXP}(A)\cdot \mathrm{EXP}(B)$ IFF $AB=BA$ ...

FOR COMMUTING HAMILTONIANS HAM SIM IS <u>EASY</u>:

IMPLEMENT HAMSIM FOR EACH TERM (PAULI STRING) SEPARATELY IN ANY ORDER.

ASSUME $[A,B] = AB - BA \neq 0$

$\exp(A)\cdot\exp(B) = \exp(C)$ $\quad C = A + B + \frac{1}{2}[A,B] + \frac{1}{12}[A,[A,B]] - \frac{1}{12}[B,[A,B]] \dots$

(BAKER-CAMPBELL-HAUSDORFF FORMULA) ...

ZASSENHAUS:

$$\exp(t(X+Y)) = \exp(tX)\exp(tY)\,\exp\left(-\frac{t^2}{2}[X,Y]\right)\exp\left(\frac{t^3}{6}(\dots)\right)\dots$$

FIRST ORDER TROTTER - SUZUKI APPROXIMATION

1) $$e^{A+B} = e^{A} \cdot e^{B} + \underset{\substack{\uparrow \\ \text{error} \\ \text{operator}}}{\mathcal{E}} \quad ; \quad \|\mathcal{E}\| \in O\left(\|A\| \cdot \|B\|\right)$$

$$= \left[\left[e^{A+B}\right]^{\frac{1}{k}}\right]^{k} = \left(e^{\frac{A}{k}+\frac{B}{k}}\right)^{k} = \left(e^{\frac{A}{k}} \cdot e^{\frac{B}{k}} + \underline{\underline{\mathcal{E}_k}}\right)^{k}$$

$$\|\mathcal{E}_k\| \in O\left(\|A\| \cdot \|B\| / k^{2}\right)$$

LM. Let $U = U_k U_{k-1} \cdots U_1$ $\quad \tilde{U} = \tilde{U}_k \tilde{U}_{k-1} \cdots \tilde{U}_1$; $\forall k \ \|U_k - \tilde{U}_k\| \leq \mathcal{E}$

THEN $\|U - \tilde{U}\| \leq k \cdot \mathcal{E}$

$$\left\| e^{\frac{A}{r}} \cdot e^{\frac{B}{r}} - e^{\frac{A+B}{r}} \right\| \in O\left(\frac{1}{r^2}\right) \qquad (\text{assuming } \|A\| = \|B\| = 1)$$

$$\Rightarrow \left\| \prod \left(e^{\frac{A}{r}} \cdot e^{\frac{B}{r}}\right) - e^{A+B} \right\| \in O\left(r \times \frac{1}{r^2}\right) = \underline{\underline{O\left(\frac{1}{r}\right)}}$$

$\Rightarrow$ GOES TO $\emptyset$ IN r

$\Rightarrow$ GENERALIZING TO $H = \sum_j H_j$

$$e^{-iHt} = \left(\prod_j e^{-iH_j \frac{t}{r}}\right)^r + O\left(\frac{t^2}{r}\right)$$

make it small

$$= \left(\prod_j e^{-iH_j \Delta t}\right)^{\frac{t}{\Delta t}} + O(t\,\Delta t)$$

small

SINCE ERROR IS $O\left(\frac{t^2}{r}\right)$ IF $r \in O\left(\frac{t^2}{\varepsilon}\right)$

WE OBTAIN $O(1/\varepsilon)$ IN APPROXIMATION

time of evolution

locality of Hamiltonian (Gate cost of Pauli string simulation)

COMPLEXITY : $O\left(t^2/\varepsilon \times k \times \ell\right)$ $\quad \ell \in O(n)$

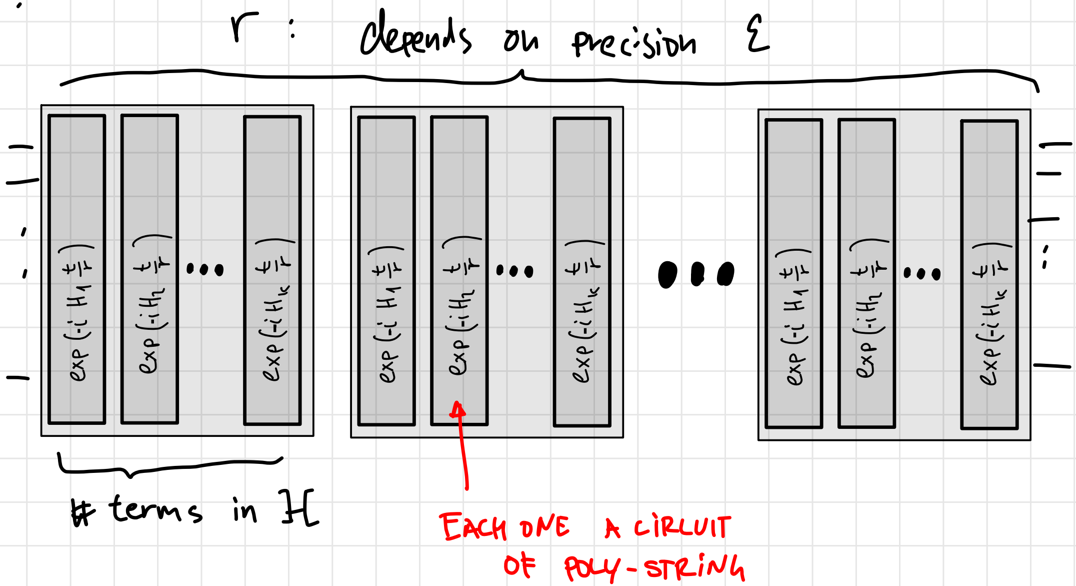
error

terms in H

IT IS POSSIBLE TO DO BETTER IN t &
EXPONENTIALLY BETTER IN ε

. .

CIRCUIT:



r : depends on precision ε
exp(-i H_1 t/r)
exp(-i H_2 t/r)
exp(-i H_k t/r)
# terms in H
EACH ONE A CIRCUIT OF POLY-STRING

STILL $O\left(t^2/\varepsilon \times k \times \ell\right)$ IS POLYNOMIAL IN n

FOR ALL LOCAL HAMILTONIANS SINCE $k \in O(\mathrm{poly}(n))$ IN THAT CASE AND $\ell \in O(1)$

SIMPLE, NEEDS NO ANCILLA QUBITS

OUTLOOK: MORE GENERAL Q. SIMULATION

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

- e.g. $H(t) = \left(1-\frac{t}{T}\right)H_0 + \frac{t}{T}H_T \Rightarrow$ ADIABATIC Q.C., ADIABATIC OPTIMIZATION

e.g. $H_0 = X^{\otimes n}$; $\underbrace{H_T = \sum w_{ij} Z_i Z_j}$

$\Downarrow$

NP-HARD!

ADIABATIC THEOREM

$$|\psi^{H_0}_{g.s.}\rangle \xrightarrow{H(0)\,\cdots\, H(T)} |\psi^{H_T}_{g.s.}\rangle$$

IF SLOW ENOUGH

OUTLOOK: MORE GENERAL Q. SIMULATION

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

- e.g. $H(t) = \left(1-\frac{t}{T}\right)H_0 + \frac{t}{T}H_T$

HAMILTONIAN SIMULATION: TROTTERIZATION

INTUITION: - DISCRETIZE TIME: $t_0, t_1 \ldots t_F$, CONSIDER $H_{t_j} = \left(1-\frac{t_j}{T}\right)H_0 + \frac{t_j}{T}H_T$ TIME-INDEP

- SEQUENTIALLY SIMULATE $H_{t_0}, H_{t_1} \ldots H_{t_F}$.

- EACH WILL CONSIST IN $\left[\exp(i H_0 \delta t') \cdot \exp(i H_T \delta t')\right]$ TERMS WITH DIFFERENT TIMES

IMPROVEMENTS & GENERALIZATIONS

(1) EFFICIENCY IN ALL PARAMETERS, ESPECIALLY ERROR $O(1/\varepsilon)$

(2) MORE GENERAL HAMILTONIANS

BOTH (1) & (2) MOVE US AWAY FROM TROTTERIZATION METHODS

AND TO DIFFERENT MODELS

BEYOND LOCAL HAMILTONIANS

SPARSE HAMILTONIANS. H is s-(row/column)-SPARSE if EACH ROW/COLUMN HAS AT MOST s NON-ZERO ELEMENTS

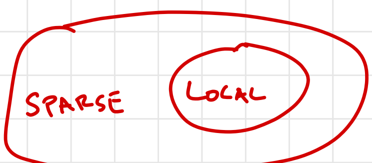
SPARSE: either $s \in O(1)$ OR $s \in O(\text{polylog}(\dim H)) = O(\text{poly}(n))$ ← # qubits

$\text{polylog} = \text{poly}(\log(x))$, e.g. $\log^4(x)$

NOTE: STILL $O(\exp(n))$ non-zero elements possible!

E.G. DIAGONAL MATRIX ... 2^n elements, 1-SPARSE

Local Hamiltonian poly(n) - sparse (but also only poly(n) elements in PAULI BASIS)



PROVE LOCAL ARE SPARSE

HOW DO YOU "LOAD" EXP. MANY COEFFICIENTS??

HOW DO WE 'INPUT' THE MATRIX? (c.f. TROTTERIZATION METHODS)

DEF: "SPARSE (ACCESS) ORACLE"

$|i,j\rangle|0\rangle \to \boxed{M} \to |i,j\rangle|m_{ij}\rangle$ but also:

$|j,\ell\rangle|0\rangle \to \boxed{LocM} \to |j,\ell\rangle|\nu_\ell^j\rangle$

$\ell \in \{0..d-1\}$

ν_ℓ^j = row of ℓ^{th} non-zero element of j^{th} column

NOTE: SPARSE ORACLE ALSO INCLUDES "EFFICIENTLY ROW COMPUTABLE" MATRICES.

BIG PICTURE OF NEW METHODS: "LINEAR-ALGEBRAIC" QC ..

IDEA:
$$\exp(iHt) = \sum \alpha_j H^j$$
$$= \text{FOURIER}$$
$$= \text{OTHER FORMAL SERIES} \dots$$

NB EVEN IF ACCES to $f(H)$ (inveritble)

$\exists\, g$ st $g(f(H)) \approx \exp(iHt)$

WHAT DOES QC GIVE ME?

$U = U_1 U_2 \dots U_n$ .. products... of unitaries

BIG PICTURE OF NEW METHODS: "LINEAR-ALGEBRAIC" QC . .

INGREDIENTS

(1) A TYPE OF "BLOCK - ENCODING"

(2) APPROXIMATIONS OF FUNCTIONS OF (BLOCKS) OF OPERATORS
VIA AN EFFECTIVE FORMAL SERIES

Intuition:

$\forall$ MATRIX A $\exists$ U S.T.

$$U = \begin{pmatrix} \tilde{A} & \cdot \\ \cdot & \cdot \end{pmatrix}; \quad \tilde{A} = \alpha A$$

BLOCK ENCODING.

BIG PICTURE OF NEW METHODS: "LINEAR-ALGEBRAIC" QC . .

INGREDIENTS

(1) A TYPE OF "BLOCK - ENCODING"

(2) APPROXIMATIONS OF FUNCTIONS OF (BLOCKS) OF OPERATORS VIA AN EFFECTIVE FORMAL SERIES

Intuition:

$$\begin{pmatrix} A & \cdot \\ \cdot & \cdot \end{pmatrix}^k = \begin{pmatrix} A^k + \text{rest?} & \cdot \\ \cdot & \cdot \end{pmatrix} \qquad f(x) = \sum \alpha_j x^j \ . . .$$

$$\sum_j \alpha_j \begin{pmatrix} A & \cdot \\ \cdot & \cdot \end{pmatrix}^j = \begin{pmatrix} \sum \alpha_j A^j + \text{rest?} & \cdot \\ \cdot & \cdot \end{pmatrix}$$

LINEAR COMBINATION OF (POWERS) UNITARIES

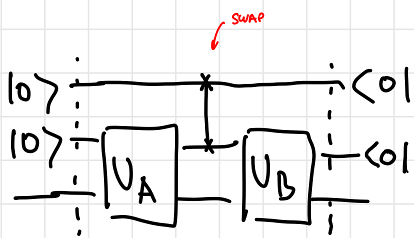
FOR (POWER) SERIES NEED: <u>POWERS</u> & <u>SUMS</u>

PRODUCTS

MULTI QUBIT BLOCK ENCODING ALLOWS MULTIPLICATION

NB

$$U_A = \begin{pmatrix} A & * \\ * & * \end{pmatrix} \iff (\langle 0| \otimes \mathbb{1})\, U\, (|0\rangle \otimes \mathbb{1})$$



U_{AB}

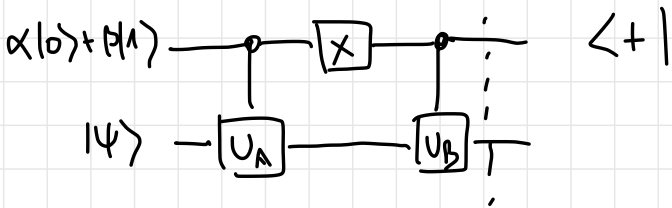
$$(\langle 00| \otimes \mathbb{1})\, U_{AB}\, (|00\rangle \otimes \mathbb{1}) = BA$$

SUMS:

$$U_{A+B} = U_A + U_B$$

NOT IN QC! DETERMINISTICALLY...

CONSIDER ctrl-U_A & ctrl-U_B



$$\alpha|0\rangle U_A|\psi\rangle + \beta|1\rangle U_B|\psi\rangle$$

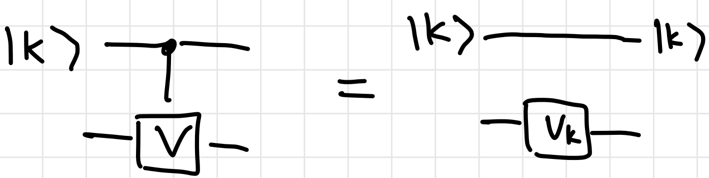
$$\xrightarrow{\langle +|} \frac{1}{\sqrt{2}}\left(\left(\alpha U_A + \beta U_B\right)|\psi\rangle\right)$$

A NEW PARADIGM (2012, 2014)

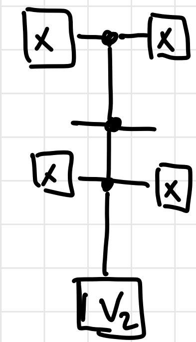
- Suppose $V_0 \ldots V_{M-1}$ are known unitaries..

$(0\,1\,0) = 2$

- Can construct muti-controlled-V:



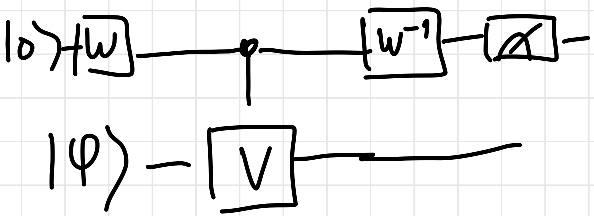
How? Eg.



V_2 fires oly on input "2"

- Assume $\sqrt{\alpha_0} \dots \sqrt{\alpha_{M-1}}$ are amplitudes, $|\psi\rangle = \sum \sqrt{\alpha_i}\,|i\rangle$, $\alpha_j \geq 0$ $\downarrow$ For simplicity

  and have $W|\vec{0}\rangle = |\psi\rangle$; $W^{-1}|\psi\rangle = |\vec{0}\rangle$



"PROJECT ONTO $|0\rangle$"

$$\sum \sqrt{\alpha_j}\,|j\rangle V_j|\varphi\rangle \rightarrow \sum_j \sqrt{\alpha_j}\,|0\rangle\underbrace{\langle\psi|j\rangle}_{\sqrt{\alpha_j}} V_j|\varphi\rangle = |0\rangle \sum \alpha_j V_j\,|\varphi\rangle$$

LINEAR COMBINATION OF UNITARIES. Let $A = \sum \alpha_j V_j$ Then prob $P(|0\rangle) = \dfrac{\|A|\varphi\rangle\|^2}{(\sum|\alpha_j|)^2}$

BY COMBINING BLOCK-ENCODED MULTIPLICATION & LCU
WE CAN, PROBABILISTICALLY IMPLEMENT FUNCTIONS OF
THE BLOCK-ENCODED OPERATOR

→ OBVIOUSLY TAYLOR. BUT BETTER METHODS EXIST.

THEOREM (Gilyen)

GIVEN U_M A BLOCK ENCODING OF M, AND f - AN S-DEGREE POLYNOMIAL (WITH SOME CONSTRAINTS) WE CAN IMPLEMENT $V_{f(M)}$, A BLOCK ENCODING OF $f(M)$ USING S CALLS TO U_M, U_M^{-1}, 1 CALL TO CTRL-U_M AND A SMALL NUMBER OF OTHER 2-QUBIT GATES

⇒ the degree exponentially improves approximation...

BUT HOW DO WE BLOCK ENCODE SPARSE ORACLES?

BLOCK ENCODING OF SPARSE MATRICES

(de Wolf lecture notes)

→ Szegedy construction

SPARSE ORACLE d-SPARSE A:

$$\mathrm{Loc}A : |j, \ell\rangle \to |j, \nu(j,\ell)\rangle$$

ℓ-th NON-ZERO ENTRY

+ READOUT . . .

$$W_1 |0\rangle|\vec{0}^{n}\rangle|j\rangle = \frac{1}{\sqrt{d}} |0\rangle \sum_{\substack{k=0 \\ k:\, A_{k,j}\neq 0}}^{d-1} |k\rangle|j\rangle$$

POSITIONS OF
LOCATIONS OF
NON ZERO entries
in rows &
COLUMNS

$$W_3 |0\rangle|\vec{0}^{n}\rangle|i\rangle = \frac{1}{\sqrt{d}} |0\rangle \sum_{\ell:\, A_{i\ell}\neq 0} |i\rangle|\ell\rangle$$

$$W_2 : |0\rangle|k,j\rangle \to A_{k,j}|0\rangle|k,j\rangle + \sqrt{1-|A_{kj}|^2}\,|1\rangle|k,j\rangle$$

(ASSUME $\|A\|_1 < 1$)

amplitude imprinting ..

THEN IT IS EASY TO PROVE THAT

$U = W_3^{-1} W_2 W_1$ IS SUCH THAT

$$\Big(\underset{\substack{\uparrow \\ n+1}}{\langle \vec{0} |} \otimes \mathbb{1} \Big) \, U \, \Big(|\vec{0}\rangle \otimes \mathbb{1} \Big) = \frac{A}{d}$$

APPLICATIONS

- essentially optimal HAM. SIM.

  $\tau = d \times \|H\|_{max} \times t$

  - $\Omega\left(\tau + \frac{\log(1/\varepsilon)}{\log\log(1/\varepsilon)}\right)$

  - achieved in 2016.

TROTTERIZATION STIC

ADVATAGE IN # ANCILLAS.

- "QUANTUM LINEAR ALGEBRA"

  Effectively cal implement $f(M)|\psi_{in}\rangle$

  - $f(M)$ can be M^{-1}
  - Low-rank projection
  - MOORE-PENROSE