Reading, Analyzing, and Simulating Quantum Circuits

(With speculation on the status of “quantum supremacy”)

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Is Nature Lexical?

I.e., can all natural processes be simulated in proportional time by computers using today's programming languages?

Pro:

- "It From Bit." "Unreasonable Effectiveness of Mathematics."
- *Church-Turing Thesis* extended to physics and **feasible** computation (as formalized e.g. by the polynomial-time class P).
- Stephen Wolfram's cellular automata universe; others' models...
- The classical Simulation Hypothesis presumes it.

Con:

- "Nature isn't classical, dammit!" (Richard Feynman, whole quote)
- Experience with exponential blowups in simulations.
- "It From Qubit."

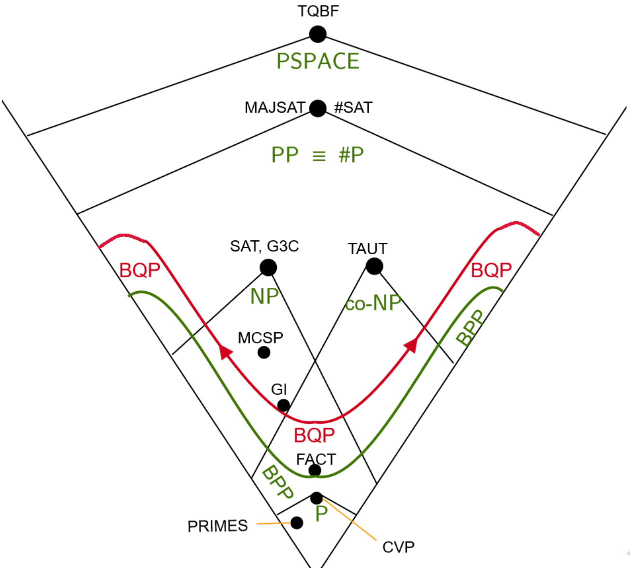
The Reach of Mathematics

- Can **define and analyze** entities that cannot be computed.
  - $V = \{$true statements about integers in formal arithmetic (PA)$\}$.
  - Tarski, 1923: definable in set theory but not within PA itself.
- Can compute entities in some cases but not others.
  - $A = \{$provable statements of PA$\}$. (Gödel, Turing, Church, 1930s)
- Can compute other entities but **not in feasible time**.
  - $B = \{$true statements of PA using $+, =$ but not $\cdot\}$.
  - Decidable by Presburger, 1929; infeasible by Fischer and Rabin, 1974.
- For other entities we strongly doubt feasibility:
  - $Q = \{$true sentences using only $(\wedge, \vee, \neg, \exists, \forall)\}$. (PSPACE-complete)
  - SAT $= \{$true sentences using only $(\wedge, \vee, \neg, \exists)$. (NP-complete)
  - We know $\mathsf{P} \subseteq \mathsf{NP} \subseteq \mathsf{PSPACE}$ but have not proved $\mathsf{P} \neq \mathsf{PSPACE}$.
- So Math can outpace its own calculations, but can Nature?

Concreteness and Complexity

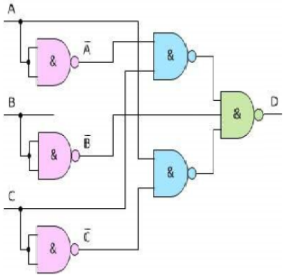
- Perfect chess and Go on $n \times n$ boards are PSPACE-complete (under extensions of common rules limiting the length of games).
- On concrete 8×8 (respectively, 19×19)boards, **perfection** remains a challenge.
  - Perfect chess has been **tablebased** for up to 7 pieces on the board.
  - A laptop holding 32-piece tables would collapse to a black hole.
- Will we ever compute the Ramsey number $R(6,6)$? (Erdős quote)
  - We know $102 \leq R(6,6) \leq 162$.
  - $R(5,5)$ still open, recently tightened to $43 \leq R(5,5) \leq 46$.
  - Is there a cosmic shortcut? Maybe if NP = P super-concretely??
- **Factoring** m-bit numbers seems concretely hard **in most cases**.
- Belief in asymptotic classical time lower bound $2^{\tilde{\Omega}(m^{1/3})}$.
  - But no wide-ranging *hardness* result. (Maybe exponent is 1/4? 1/5?)
- Hence a shock in 1993-94 when Peter Shor put factoring into **BQP**.
- Realizable by **quantum circuits** of size $\tilde{O}(m^2)$.

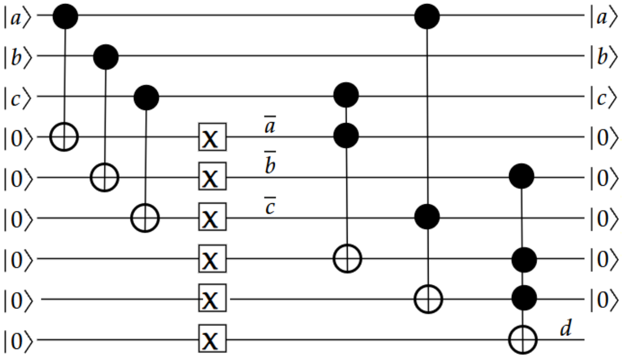
The Complexity Class Neighborhood



Classical and Quantum Circuits

$d = f(a,b,c) = \overline{\wedge}\,(c\ \overline{\wedge}\ \bar{a}, \bar{b}, a\ \overline{\wedge}\ \bar{c})$ $\quad$ $\mathbf{X}$ = NOT, $\bullet\!\!-\!\!\oplus$ = controlled-NOT





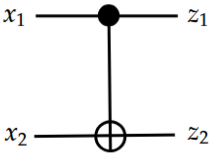
Quantum circuit computes the **reversible** Boolean function
$F(a,b,c,e_1,e_2,e_3,e_4,e_5,e_6) = (a,b,c,e_1,e_2,e_3,e_4,e_5,e_6 \oplus f(a,b,c))$.
Underlying: a vector of $N = 2^9 = 512$ dimensions.

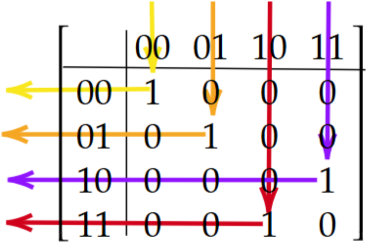
Quantum Coordinates and the CNOT Gate

By **linearity**, an n-qubit circuit is determined by its actions on the 0-1 **standard basis** vectors $e_{0^n} = [1,0,0,\dots,0]^T$ thru $e_{1^n} = [0,0,0,\dots,1]^T$.

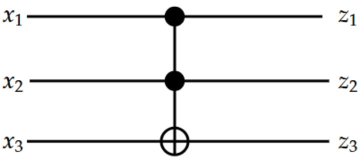
For $n = 2$, $e_{00} = \begin{bmatrix}1\\0\\0\\0\end{bmatrix}$, $e_{01} = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$, $e_{10} = \begin{bmatrix}0\\0\\1\\0\end{bmatrix}$; and $e_{11} = \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$ (in "big-endian" order). Then **CNOT**$e_{00} = e_{00}$ and **CNOT**$e_{01} = e_{01}$, while **CNOT**$e_{10} = e_{11}$ and **CNOT**$e_{11} = e_{10}$. **Feynman path** visualization:

$$\begin{bmatrix}1 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 1\\0 & 0 & 1 & 0\end{bmatrix}$$





Toffoli Gate ($n = 3$, $N = 2^n = 8$)



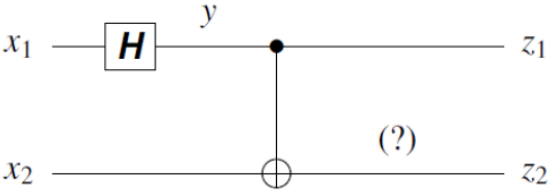
	000	001	010	011	100	101	110	111
000	1	0	0	0	0	0	0	0
001	0	1	0	0	0	0	0	0
010	0	0	1	0	0	0	0	0
011	0	0	0	1	0	0	0	0
100	0	0	0	0	1	0	0	0
101	0	0	0	0	0	1	0	0
110	0	0	0	0	0	0	0	1
111	0	0	0	0	0	0	1	0

In **Dirac notation**, e_x is written $|x\rangle$. So we have **Tof** $|000\rangle = |000\rangle$ thru **Tof** $|101\rangle = |101\rangle$, while **Tof** $|110\rangle = |111\rangle$ and **Tof** $|111\rangle = |110\rangle$.

Note that fixing $x_3 = 1$ makes $z_3 = x_1 \barwedge x_2$. Since NAND is a universal gate, this already suffices to show that quantum circuits simulate classical ones. Their extra power comes from one more gate.

Hadamard Gate, Nondeterminism, and Entanglement

Hadamard gate H $= \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ "emits" a free Boolean variable y.



On input $|00\rangle$, $y = 0$ leads to output $z_1 = 0$, $z_2 = 0$, while $y = 1$ leads to $z_1 z_2 = 11$. The other combinations 01 and 10 cannot happen. *Matrices:*

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}.$$

Measurement and Sampling

- **Measuring** the state vector $|\phi\rangle = [a_0, a_1, \ldots, a_{N-1}]^T$ of all n qubits returns some i, $0 \leq i \leq N-1$, with probability $|a_i|^2$. You can say it returns e_i, $|i\rangle$, or the i-th binary string $z_i \in \{0,1\}^n$.
- This entails that $|\phi\rangle$ is a Euclidean **unit vector**, so that the probabilities sum to 1.
- **Unitary** matrices A, meaning $AA^* = I$, preserve unit vectors.
- Measuring the **entangled** state $\frac{|00\rangle+|11\rangle}{\sqrt{2}}$ returns $|00\rangle$ with probability 0.5 or $|11\rangle$ with probability 0.5, but never $|01\rangle$ or $|10\rangle$.
- So an n-qubit circuit C, on any input $|x\rangle$, gives rise to a distribution $D_{C,x}$ on $\{0,1\}^n$ to sample from.
- Google's *quantum supremacy* methodology creates a family of C such that non-negligible values of $D_{C,-}$ are hard to find classically.
- **Shor's algorithm** creates $D_{C,x}$ such that sampling often gives z from which the period r of $f_a(u) = a^u \bmod x$ can be classically inferred, which in turn often enables factoring x.

Some More Gates

$$\mathsf{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \mathsf{Y} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \mathsf{Z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

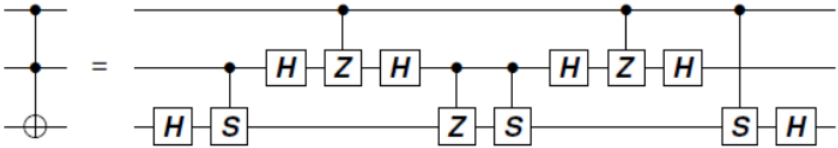
$$\mathsf{S} = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}, \quad \mathsf{T} = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}, \quad \mathsf{R_8} = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/8} \end{bmatrix},$$

$$\mathsf{SWAP} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad \mathsf{CZ} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \quad \mathsf{CS} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & i \end{bmatrix}.$$

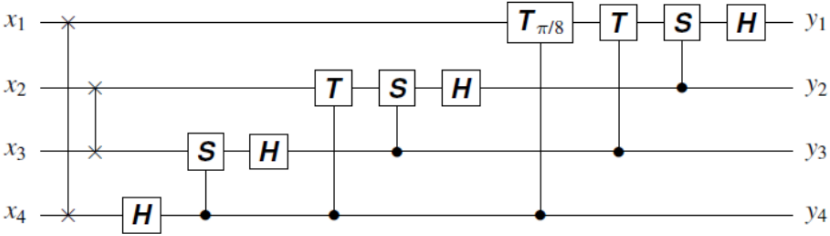
- The gates $\mathsf{H}, \mathsf{X}, \mathsf{Y}, \mathsf{Z}, \mathsf{S}, \mathsf{CNOT}, \mathsf{CZ}$ generate *Clifford circuits*, which are simulatable in polynomial time. **(Time improved by us.)**
- Adding any of T, $\mathsf{R_8}$, CS, or Tof gives the full power of BQP.
- Note: $\mathsf{T}^2 = \mathsf{S}$, $\mathsf{S}^2 = \mathsf{Z}$, $\mathsf{Z}^2 = \mathsf{I} = \mathsf{H}^2$, and $\mathsf{CS}^2 = \mathsf{CZ}$.

Two Notable Circuits

H and **CS** alone can simulate the Toffoli gate:

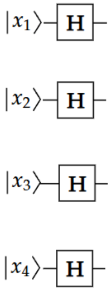


The 4-qubit **Quantum Fourier Transform** == the 16×16 **Discrete Fourier Transform**. In general, $\mathbf{QFT}_n$ needs $O(n^2)$ basic gates.



Juxtaposition and Tensor Product

Many QCs begin with m Hadamard gates on each of m qubits



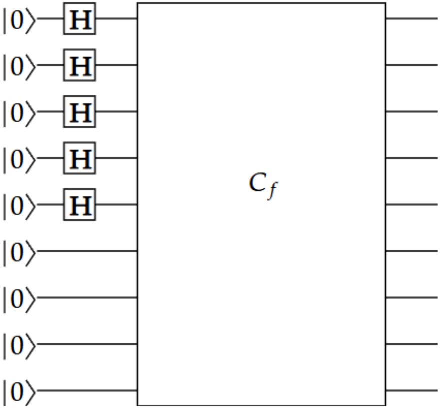
$\frac{1}{4}$

$\mathbf{H}^{\otimes 4}$	0000	0001	0010	0011	0100	0101	0110	0111	1000	1001	1010	1011	1100	1101	1110	1111
0000	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0001	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
0010	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1
0011	1	−1	−1	1	1	−1	1	−1	1	−1	−1	1	1	−1	1	−1
0100	1	1	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1
0101	1	−1	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1	−1	1
0110	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1	1	1
0111	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1	−1	1	1	−1
1000	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1
1001	1	−1	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1	−1	1
1010	1	1	−1	−1	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1
1011	1	−1	−1	1	1	−1	1	−1	−1	1	1	−1	−1	1	1	−1
1100	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1
1101	1	−1	1	−1	−1	1	−1	1	−1	1	−1	1	1	−1	1	−1
1110	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1	1	1	−1	−1
1111	1	−1	−1	1	−1	1	1	−1	−1	1	1	−1	1	−1	−1	1

- Is this “4” units of work? Or “16”? Or “256”?
- On one hand, the rule $\mathbf{H}^{\otimes n}[u,v] = \frac{1}{\sqrt{n}}(-1)^{u \bullet v}$ for entries is simple.
- On the other, some claim this involves splitting off 2^n branches of a multiverse.

Hadamard Transforms and Functions

Suppose $C_f(x, y) = (x, y \oplus f(x))$ computes the reversible form of f. Then



computes what I call the **functional superposition**

$$\frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle \otimes |f(x)\rangle.$$

- Maybe this has exponentially many “jaggies”?
- *We’ve now seen all the ingredients of Shor’s Algorithm.*

Three Universal Libraries, Phase Angles, and Noise

- The gate set H + CNOT + T is **efficiently metrically universal**, meaning that any feasible quantum circuit of size s can be approximated to within entrywise error ϵ by a circuit of these gates only in size $O(s) \cdot (\log \frac{s}{\epsilon})^{O(1)}$. (See Solovay-Kitaev theorem.)
- Programmed improvement by Peter Selinger and Neil Ross.
- The gate set H + Tof is not metrically universal—it has no complex scalars—but it is **computationally universal**: It can maintain real and complex parts of quantum states in double-rail manner.
- The gate set H + CS is efficiently metrically universal.
- Thus we don't need arbitrarily fine-angled *gates* to compute $\mathbf{QFT}_n$ finely enough with $\tilde{O}(n^2)$ basic gates.
- But fine angles exist in the output and may be especially vulnerable to noise.

Demo of Simulation Code and Its Blue-Sky Ideas

Theorem (Regan-Chakrabarti-Guan): Given an n-qubit circuit C with h nondeterministic (Hadamard) gates, we can efficiently compute [...]:

- A product polynomial $p_C(x_1, \ldots, x_n; \mathbf{y_1}, \ldots, \mathbf{y_h}; z_1, \ldots, z_n)$.
- An additive polynomial $q_C(x_1, \ldots, x_n; \mathbf{y_1}, \ldots, \mathbf{y_h}; z_1, \ldots, z_n; w_1, \ldots)$.
- A Boolean representation ϕ_C with various auxiliary variables. **Used by the simulator.**

Idea 1: Bounds from algebraic-geometric invariants of ∂p_C? **Hard...**

2. Can **SAT solvers**—or really #SAT counters—heuristically evaluate C? **They perform poorly.**

3. Simplify intermediate states via logic? **Not promising so far...**

4. Maybe program **non-physical** approximations? **Hmmmmm...**

5. Iteratively program **tensor network and SVD approximations**... **On the agenda...**

I. Feynman Path Polynomials and Logical Formulas

Let C have "minphase" $K = 2^k$ and let F embed K-th roots of unity ω.

- H + Tof has $k = 1$, $K = 2$.
- H + CS has $k = 2$, $K = 4$.
- H + CNOT + T has $k = 3$, $K = 8$.

Theorem (RC 2007-09, extending Dawson et al. (2004) over $\mathbb{Z}_2$)

Any QC C of n qubits quickly transforms into a polynomial $P_C = \prod_g P_g$ over gates g and a constant $R > 0$ such that for all $x, z \in \{0,1\}^n$:

$$\langle z \mid C \mid x \rangle = \frac{1}{R} \sum_{j=0}^{K-1} \omega^j (\# y : P_C(x,y,z) = \iota(\omega^j)) = \frac{1}{R} \sum_y \omega^{P_C(x,y,z)},$$

where C has h nondeterministic (Hadamard) gates and $y \in \{0,1\}^h$.

Additive Case (Cf. Bacon-van Dam-Russell [2008])

Theorem (RC (2007-09), RCG (2018))

Given C and K, we can efficiently compute a polynomial $Q_C(x_1,\dots,x_n,y_1,\dots,y_h,z_1,\dots,z_n,w_1,\dots,w_t)$ of degree $O(1)$ over $\mathbb{Z}_K$ and a constant R' such that for all $x,z \in \{0,1\}^n$:

$$\langle z \mid C \mid x\rangle = \frac{1}{R'}\sum_{j=0}^{K-1}\omega^j(\#y,w : Q_C(x,y,z,w)=j) = \frac{1}{R'}\sum_{y,w}\omega^{Q_C(x,y,z,w)},$$

where Q_C has the form $\sum_{gates\ g} q_g + \sum_{constraints\ c} q_c$.

- Gives a particularly efficient reduction from BQP to #P.
- In P_C, illegal paths that violate some constraint incur the value 0.
- In Q_C, any violation creates an additive term $T = w_1 \cdots w_{\log_2 K}$ using fresh variables whose assignments give all values in $0 .. K-1$, which *cancel*. (This trick is my main original contribution.)

Constructing the Polynomials

- Initially $P_C = 1$, $Q_C = 0$.
- For Hadamard on line i (u_i—H–), allocate new variable y_j and do:

$$\begin{aligned} P_C &\; *= \; (1 - u_i y_j) \\ Q_C &\; += \; 2^{k-1} u_i y_j. \end{aligned}$$

- CNOT with incoming terms u_i on control, u_j on target: u_i stays, $u_j := 2u_i u_j - u_i - u_j$. No change to P_C or Q_C.
- S-gate: Q_C adds u_i^2.
- CS-gate: Q_C adds $u_i u_j$.
- Thereby CS escapes the easy case over $\mathbb{Z}_4$ (with $k = 2$).
- TOF: controls u_i, u_j stay, target u_k changes to $2u_i u_j u_k -$ $u_i u_j$ $- u_k$.
- T-gate also goes cubic.

Logical Simulation

Theorem (C. Guan in RCG 2018)

Given C, n, K, h as above, we can quickly build a Boolean formula ϕ_C in variables $y_1, \dots, y_h$, together with substituted-for $x_1, \dots, x_n$, $z_1, \dots, z_n$, and other "forced" variables such that for all $x, z \in \{0,1\}^n$:

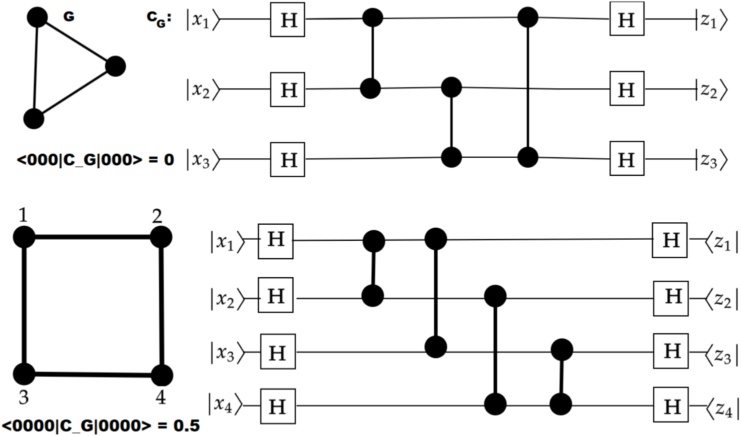
$$\langle z \mid C \mid x \rangle = \frac{1}{R} \sum_{j=0}^{K-1} \omega^j \cdot \#sat(\phi_C).$$

- The ϕ is a conjunction of "controlled bitflips" $p' = p \oplus (u \wedge v)$.
- Easy to transform into 3CNF (i.e., "3SAT" form). **(show demo)**
- For $K = 2, 4$ (i.e., for H + Tof and H + CS), we get the acceptance *probability* as a simple difference:

$$|\langle z \mid C \mid x \rangle|^2 = \frac{1}{R} \left(\#sat(\phi_C) - \#sat(\phi'_C) \right).$$

II. Strong Simulation of Graph State Circuits

Computing amplitudes $\langle z \mid C \mid x \rangle$ for Clifford circuits C can be efficiently reduced to computing $\langle 0^n \mid C_G \mid 0^n \rangle$ for **graph-state circuits** C_G of graphs G, using H and CZ gates, as exemplified by:

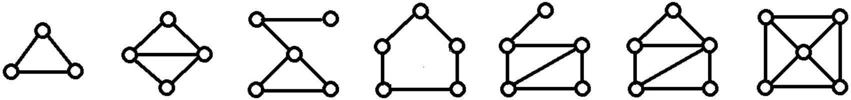


Improved From $O(n^3)$ to $O(n^{2.37155...})$

Theorem (Guan-Regan, 2019)

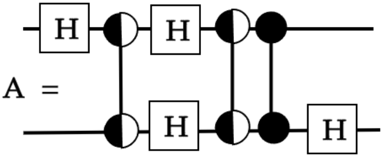
For n-qubit stabilizer circuits of size s, $\langle z \mid C \mid x\rangle$ can be computed in $O(s + n^\omega)$ time, where $\omega \leq 2.37155...$ is the exponent of multiplying $n \times n$ matrices.

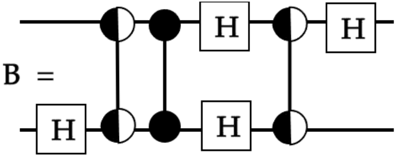
- Although C has $K = 2$, proof needs to use quadratic forms over $\mathbb{Z}_4$. And LDU decompositions over $\mathbb{Z}_2$ by Dumas-Pernet [2018].
- **Corollary:** Counting solutions to quadratic polynomials $p(x_1, \dots, x_n)$ over $\mathbb{Z}_2$ is in $O(n^{2.37155...})$ time.
- Improves $O(n^3)$ time of Ehrenfeucht-Karpinski (1990).
- See Beaudrap and Herbert [2021] for other time/size/#H tradeoffs.
- Can we recognize G with $\langle 0^n \mid C_G \mid 0^n\rangle = 0$ more quickly still?

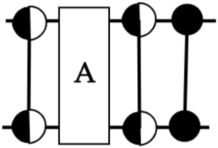


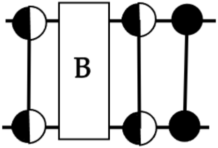
From Graphs to Polymatroids

- A self-loop on node i becomes a Z-gate on qubit line i.
- An S-gate on line i would then be a "half loop."
- A CS gate would then be a "half edge."
- Formalizable as a **polymatroid** (PM). Into universal QC now.
- John Preskill's notes show that the following four widgets, together with their conjugations by $\mathsf{H} \otimes \mathsf{H}$, suffice:









New Heuristic Forms to Investigate

- Would be a "PM State Circuit"—except for all those H gates in the middle.
- Can we move them to the sides, as with graph state circuits?
- If not, are there other useful canonical forms, a-la this?
- How about the power of PM state circuits by themselves?
- Are they more amenable to algebraic or logical model-counting heuristics than general quantum circuits?
- Chaowen and I also considered graphs that can have:
  - Loops not attached to a vertex, called *circles*.
  - Numbered copies of the empty graph, called *wisps*.
  - Wisps of negative sign, called *negative isols*.
- They can be formalized via (*graphical*) 2-polymatroids. Call them "(G)2PMs."
- We took them in a different direction.

Singular Value Decomposition

Unlike with diagonalization, this is *always* possible:

SVD Theorem: For every $m \times n$ matrix A we can efficiently find:

- an $m \times m$ unitary matrix U,
- an $m \times n$ pseudo-diagonal matrix Σ with non-negative entries $\Sigma[i,i] = \sigma_i$, and
- an $n \times n$ unitary matrix V,

such that $A = U\Sigma V^*$. Furthermore, we can arrange that $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{\min(m,n)}$, and in consequence:

- $||A||_F = \sqrt{\sum_i \sigma_i^2}$,
- $||A||_2 = \sigma_1$,
- $A^*A = V\Sigma^T U^* U\Sigma V^* = V \operatorname{diag}(\sigma_i^2) V^*$, and
- $AA^* = U\Sigma V^* V\Sigma^T U^* = U \operatorname{diag}(\sigma_i^2) U^*$,

so that the squares of the σ_i and associated vectors give the spectral decompositions of the Hermitian PSD matrices A^*A and AA^*, respectively.

III. SVD and Tensor Network Ideas

- Show SVD and truncation idea.
- SVD in Image Compression.
- Strategy for simulating quantum circuits via *classical* **tensor networks** and **SVD truncation**.
- Most workable scheme?
- How this might be programmed.

What Is the Status?

- Can quantum hardware open up and widen a gap over classical?
- Can more-clever classical simulations always catch up?
- What does Nature do, anyway? Is it the "rose" in Umberto Eco's maxim *Stat rosa pristina nomine, nomina nuda tenemus*—?
- If so, are human brains left behind with Turing's vision? In verse:

"It From Bit" we once proclaimed,
but now the Bit has bit the dust
of whizzing quantum chips that gamed
coherence, to evade the trust
that the Word framed creation's hour:
Mother Nature fully lexical.
Why not evolve us that same power?
It is a status most perplexical.