New Developments and Ideas at the Interface between Physics and Computer Science

Eduardo Mucciolo
Department of Physics
University of Central Florida

Overview

- Background and motivation: computation and physics
- Entanglement and irreversibility in circuits
- Ground-state computing and vertex models
- Tensor networks

Computer Science & Physics

The first thing to know:

> "Computer science is no more about computers than astronomy is about telescopes." (Edsger Dijkstra)

My take:

> Computer science is a branch of mathematics that studies what is computable and how it can be computed.

But computations require real-world physical phenomena to be implemented!

Computer science and physics are closely connected.

First connection: Physical laws impose practical limitations on computation.

Computation → Information Processing → Physical World

Example: Landauer's principle (1961)

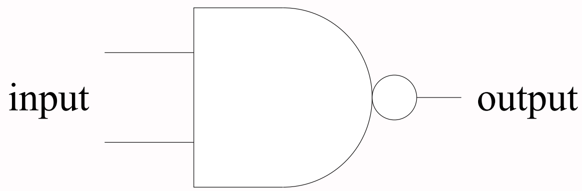
Any logically irreversible manipulation of information, such as the erasure of a bit must be accompanied by a corresponding entropy increase.

[adapted from C. H. Bennett, Stud. Hist. Philos. Sci. B **34**, 501 (2003).]

$$\Delta S \geq k_B \ln 2 \quad \longrightarrow \quad \Delta E \geq k_B T \ln 2$$

energy cost of bit erasure

But it is not only erasure that costs energy:



NAND gate

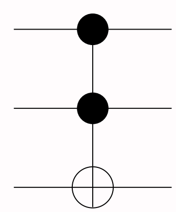
A bit has disappeared!

Irreversibility in logic gates too!

Actually, the connection between computational and irreversibility raised an interesting question:

Is it possible to compute reversibly?

Yes! (C. Bennett, 1973)



Toffoli gate $(\Delta E \geq 0)$

<u>catch</u>: many more auxiliary bits are needed

There is another connection between physics and computer science:

Second connection: **Physics provides models of computation**

- Transistor-based circuit model (current standard)

algorithm → [set of arithmetic operations → set of logic gates] → transistor operations

- Quantum-hardware based circuit model (q. computing)

algorithm → set of quantum and classical abstract operations → quantum and classical hardware operations

There are other physical models of computation…

… including ***ground-state models***

Mizel, Mitchell, Cohen, Phys. Rev. Lett. (2000)

> The result of the computation is encoded on the ground state of a physical system.

Finding the ground state becomes the computation!

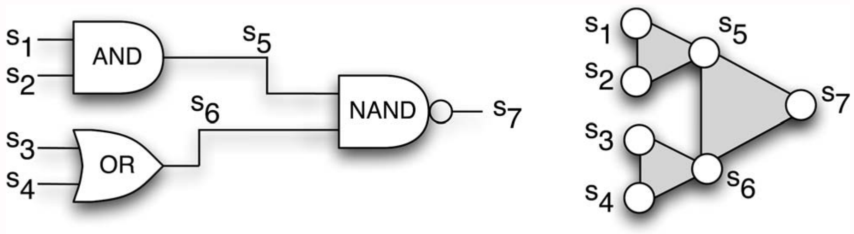
Two formulations:

(1) Choose a system whose interactions enforce a pre-established algorithm.

or

(2) Choose a system whose interactions enforce the problem to be solved.

Example of (1): Enforcing a pre-established algorithm



Crosson, Bacon & Brown, Phys. Rev. E (2010).

$$E_C(s_1,s_2,s_3,s_4,s_5) = \overbrace{\Delta(s_3+s_4+s_6-s_3s_4-2s_3s_6-2s_4s_6+2s_3s_4s_6)}^{\text{OR}}$$
$$+\underbrace{\Delta(s_5+s_1s_2-2s_1s_2s_5)}_{\text{AND}}+\underbrace{\Delta(1-s_7-s_5s_6+2s_5s_6s_7)}_{\text{NAND}}.$$

s_1, s_2, s_3, s_4 : fixed

s_5, s_6, s_7 : free

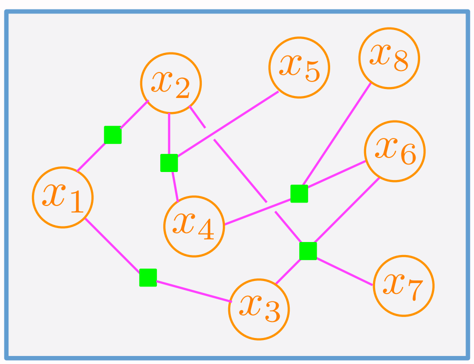
When $E_C = 0$ $\longrightarrow$ s_5, s_6, s_7 : computed ✓

Example (2): Enforcing the problem to be solved

k-SAT problem (satisfiability of a conjunctive normal form):

$$F(x_1, x_2, \ldots, x_N) = (\bar{x}_1 \vee x_2) \wedge (\bar{x}_2 \vee x_4 \vee x_5) \wedge (x_4 \vee \bar{x}_8 \vee \bar{x}_6) \wedge (x_7 \vee x_6 \vee x_2 \vee \bar{x}_3) \wedge (\bar{x}_3 \vee x_1)$$

- To each binary variable, associate a “bit” (e.g., a spin 1/2)
- To each clause, assign a many-body interaction term
- Add all interaction terms to create a total-energy cost function
- The ground state (lowest energy configuration) satisfies (or not!) all clauses simultaneously

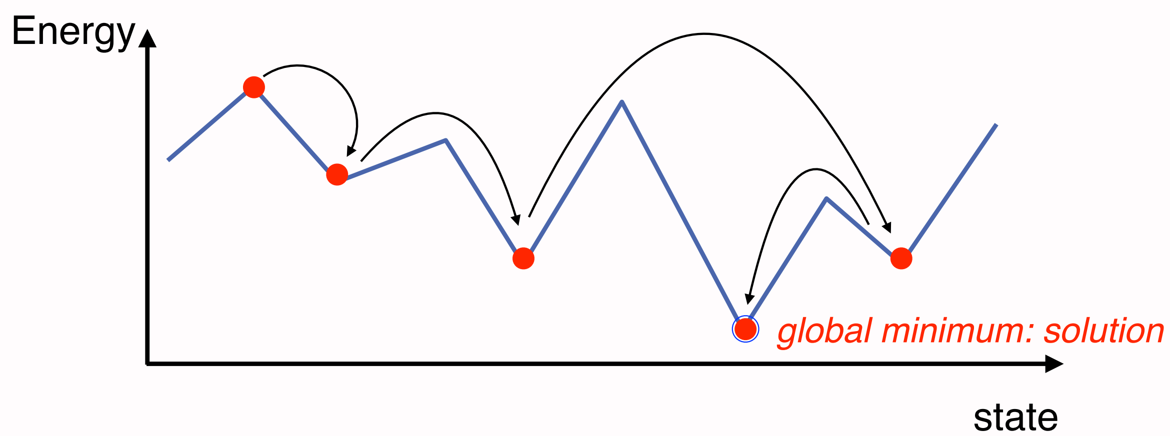


$$\begin{aligned} E_{\text{tot}} \quad &= \quad E_{2-\text{b}}(x_1, x_2) + E_{2-\text{b}}(x_1, x_3) \\ &\quad + E_{3-\text{b}}(x_2, x_4, x_5) + E_{3-\text{b}}(x_4, x_8, x_6) \\ &\quad + E_{4-\text{b}}(x_7, x_6, x_2, x_3) \end{aligned}$$

How can one reach the ground state?

Simulated annealing: slow cooling

Kirkpatrick, Gelatt Jr., Vecchi, Science (1983)



slow cooling + thermal fluctuations

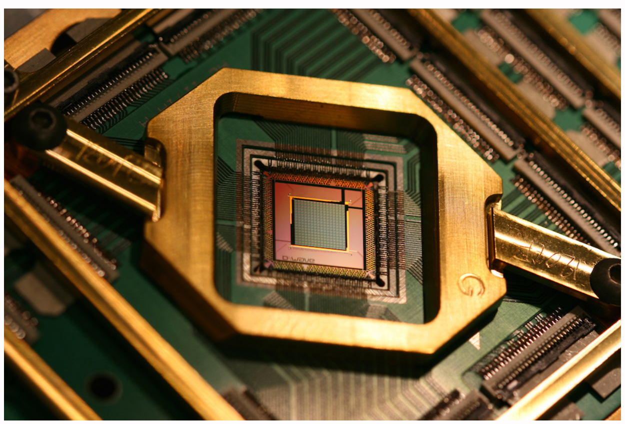
Quantum annealing: slow reshaping of the Hamiltonian

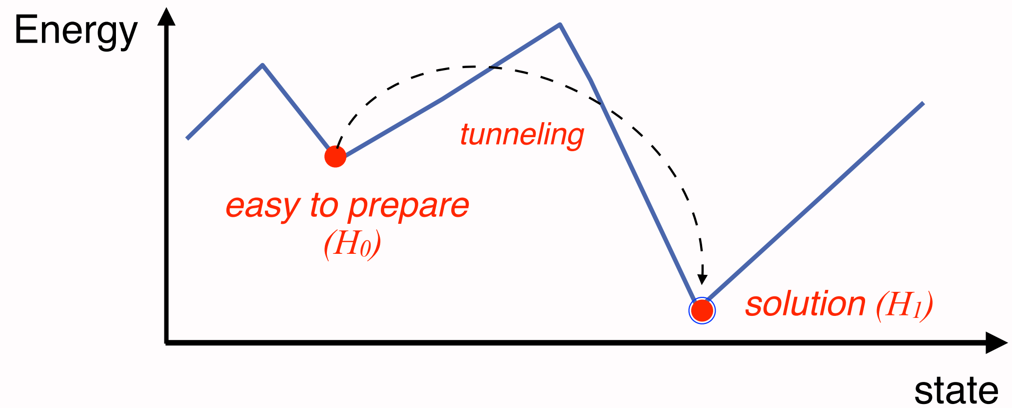
Apolloni, Carvalho, de Falco,
Stochastic Process Appl. (1989)

Finnila, Gomez, Sebenik, Stenson, Doll
Chem. Phys. Lett. (1990)

Kadowaki, Nishimori
Phys. Rev. E (1998)

Farhi, Goldstone, Gutmann, Laplan, Lundgren, Preda
Science 292, 472 (2001)





D-Wave Systems

adiabatic evolution

$$\boxed{H(t) = (1 - t/\tau)H_0 + (t/\tau)H_1}$$

Numerical Simulation:

What is the main problem with these approaches?

Most ground-state encodings create physical systems that are too complex!

They lead to glassy behavior and phase transitions!

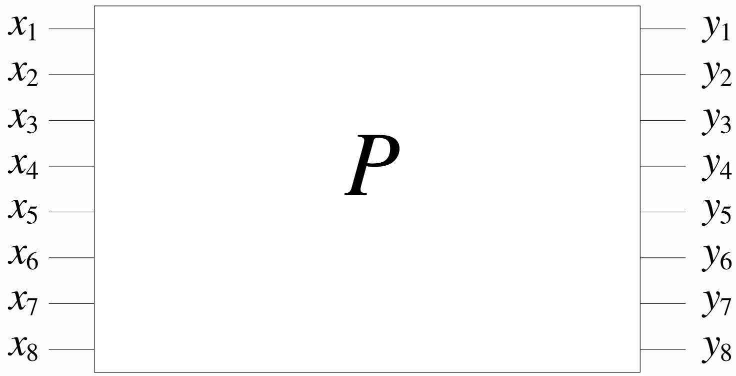
Both features slow down the annealing process…

Our group may have found a way around (more on that soon)

There is yet another connection between physics and computer science:

Third connection: Physics concepts can shed light on the complexity of computations.

Consider a black-box computation implemented with reversible gates.



How hard is it to reverse it?

Why is this an important question? Cryptography!

Our group has found an answer (more on that soon as well)

Our group has been developing applications of physics-inspired methods and ideas to computation:

Chamon & Mucciolo, *Virtual parallel computing and a search algorithm using matrix product states* (Phys Rev Lett, 2012)

Chamon & Mucciolo, *Rényi entropies as a measure of the complexity of counting problems* (J Stat Mech, 2013)

Chamon, Hamma & Mucciolo, *Emergent irreversibility and entanglement spectrum statistics* (Phys Rev Lett, 2014)

Shaffer, Chamon, Hamma & Mucciolo, *Irreversibility and entanglement spectrum statistics in quantum circuits* (J Stat Mech, 2014)

Chamon, Mucciolo, Ruckenstein & Yang, *Quantum vertex model for reversible classical computing* (Nat Comm, 2017)

Yang, Kourtis, Chamon, Mucciolo & Ruckenstein, *Iterative compression-decimation scheme for tensor network optimization* (arXiv, 2017)

Boston-Orlando collaboration

Irreversibility & Entanglement Spectrum in Reversible Circuits

- Consider a set of quantum bits (qubits): $\{|\psi_i\rangle\}_{i=1,\ldots,n}$
- Start each one in a superposition state: $|\psi_i\rangle = \sin(\theta_i)|0\rangle_i + \cos(\theta_i)|1\rangle_i$
- The initial state of the system is a product state (no entanglement): $|\Psi\rangle_{\text{initial}} = |\psi_1\rangle \otimes |\psi_2\rangle \cdots \otimes |\psi_n\rangle$
- Apply the black-box circuit (a given sequence of reversible gates): $U_{\text{circuit}} = U_m \cdot U_{m-1} \cdots U_1$
- The system will evolve into an entangled state: $$|\Psi_{\text{final}}\rangle = \sum_{x_1,\ldots,x_n} A(x_1,\ldots,x_n)|x_1\rangle \otimes \cdots |x_n\rangle$$

Is it possible to reverse the system back to a disentangled state, without referring to the circuit?

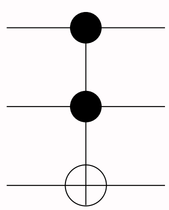
The answer: It depends on the type of circuit!

What we found:

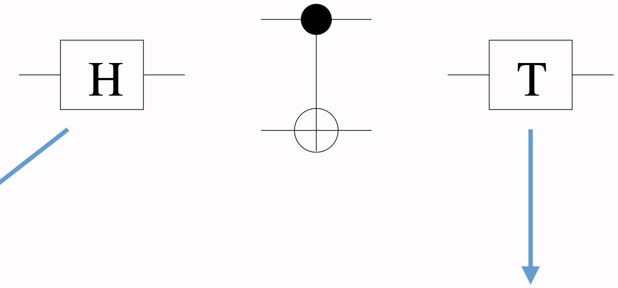
For circuits containing a *universal* set of gates: **NO**

For circuits containing a *non universal* set of gates: **YES**

For classical reversible circuits, the Toffoli gate is universal:



For quantum circuits, Hadamard, CNOT, and T gates form a universal set:



$$|0\rangle \rightarrow \boxed{\text{H}} \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

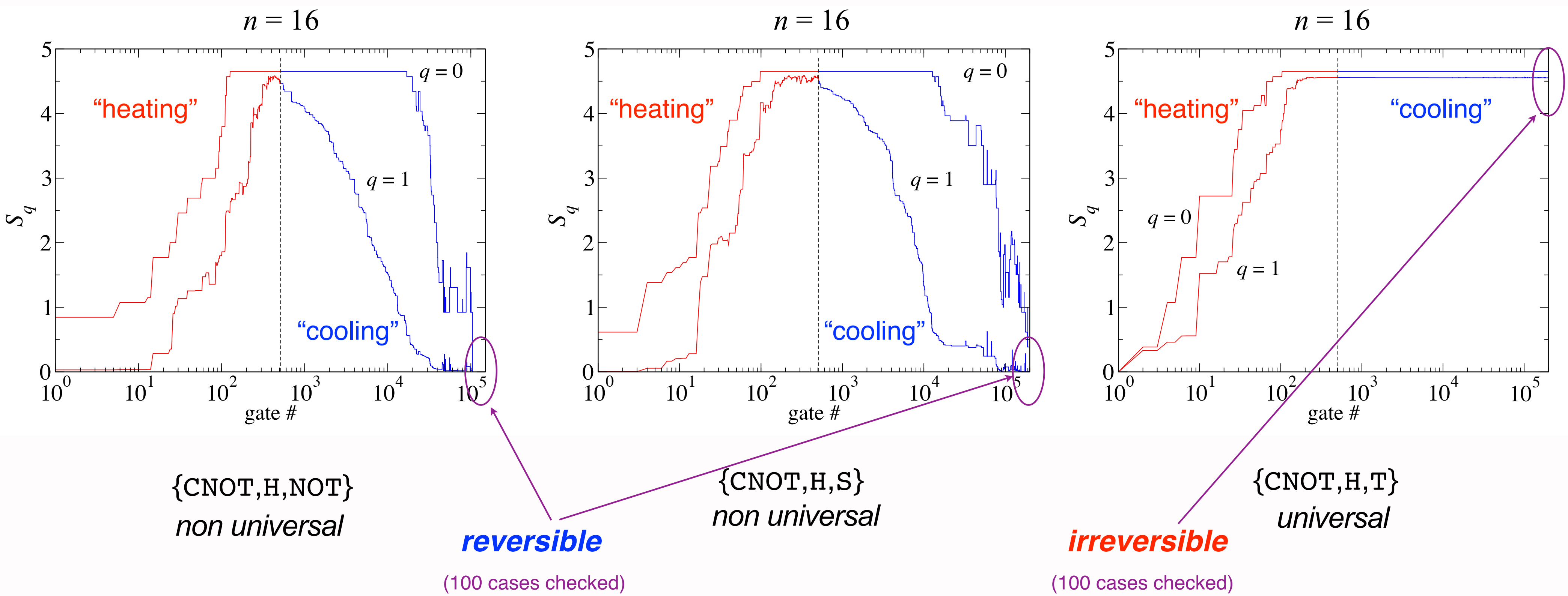
$$|1\rangle \rightarrow \boxed{\text{H}} \rightarrow \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

$$|0\rangle \rightarrow \boxed{\text{T}} \rightarrow |0\rangle$$

$$|1\rangle \rightarrow \boxed{\text{T}} \rightarrow e^{i\pi/4}\,|1\rangle$$

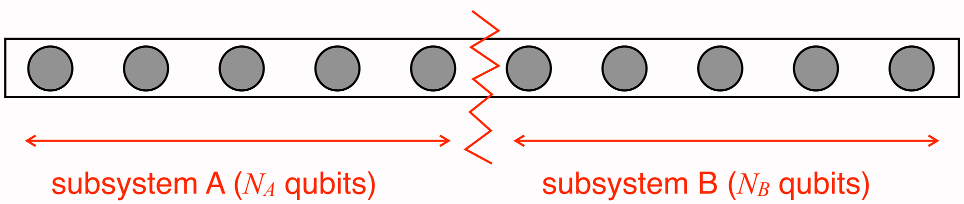
How did we check reversibility and irreversibility?

Trial and error: We followed the entanglement entropy as we tried a random sequence of gates (Metropolis algorithm)



But what if we don’t know anything about the circuit? How could we tell?

> The entanglement spectrum reveals the difficulty in reversing the evolution!



$\rho_A = \mathrm{tr}_B[\rho]$ reduced density matrix

$\hookrightarrow$ eigenvalues $\{\lambda_1, \lambda_2, \cdots, \lambda_{2^{N_A}}\}$

$$\left\{ \begin{array}{l} \lambda_n \geq 0 \\ \displaystyle\sum_{n=1}^{2^{N_A}} \lambda_n = 1 \end{array} \right.$$

entanglement entropy $S_1 = -\sum_{n=1}^{2^{N_A}} \lambda_i \ln \lambda_i$

Entanglement spectrum statistics:

ratio of consecutive spacings:

$$s_n = \frac{\lambda_n - \lambda_{n+1}}{\lambda_{n-1} - \lambda_n} \longrightarrow$$

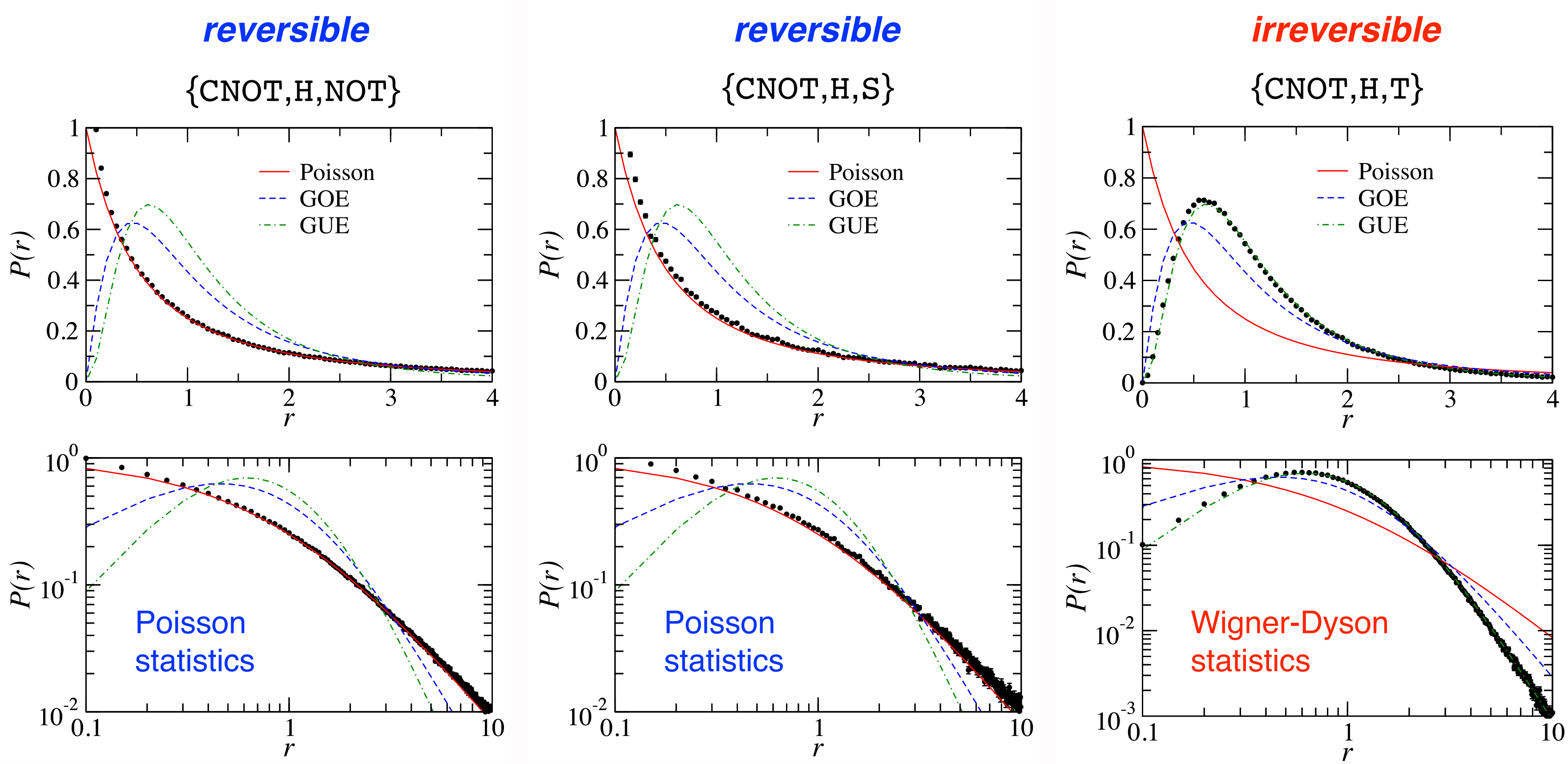
$$\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots \Rightarrow 0 \leq s_n < \infty$$

distribution of ratios:

$$P(s) = \frac{1}{2^{N_A}} \left\langle \sum_{n=1}^{2^{N_A}} \delta(s - s_n) \right\rangle$$

<u>Results</u>: The quantum state of the system reveals the nature of the circuit!

But you need to look deep inside to find it.



5000 samples

$N_A = N/2 = 8$

The statistics of the entanglement spectrum fluctuations

reveal the nature of the circuit and the difficult to reverse it.

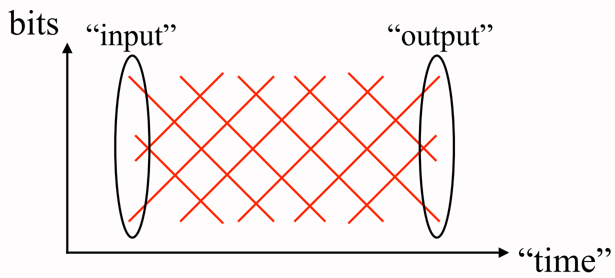
Wigner-Dyson $\longleftrightarrow$ irreversible $\longleftrightarrow$ universal gates

Poisson $\longleftrightarrow$ reversible $\longleftrightarrow$ non universal gates

Mapping Reversible Classical Circuits into Vertex Models

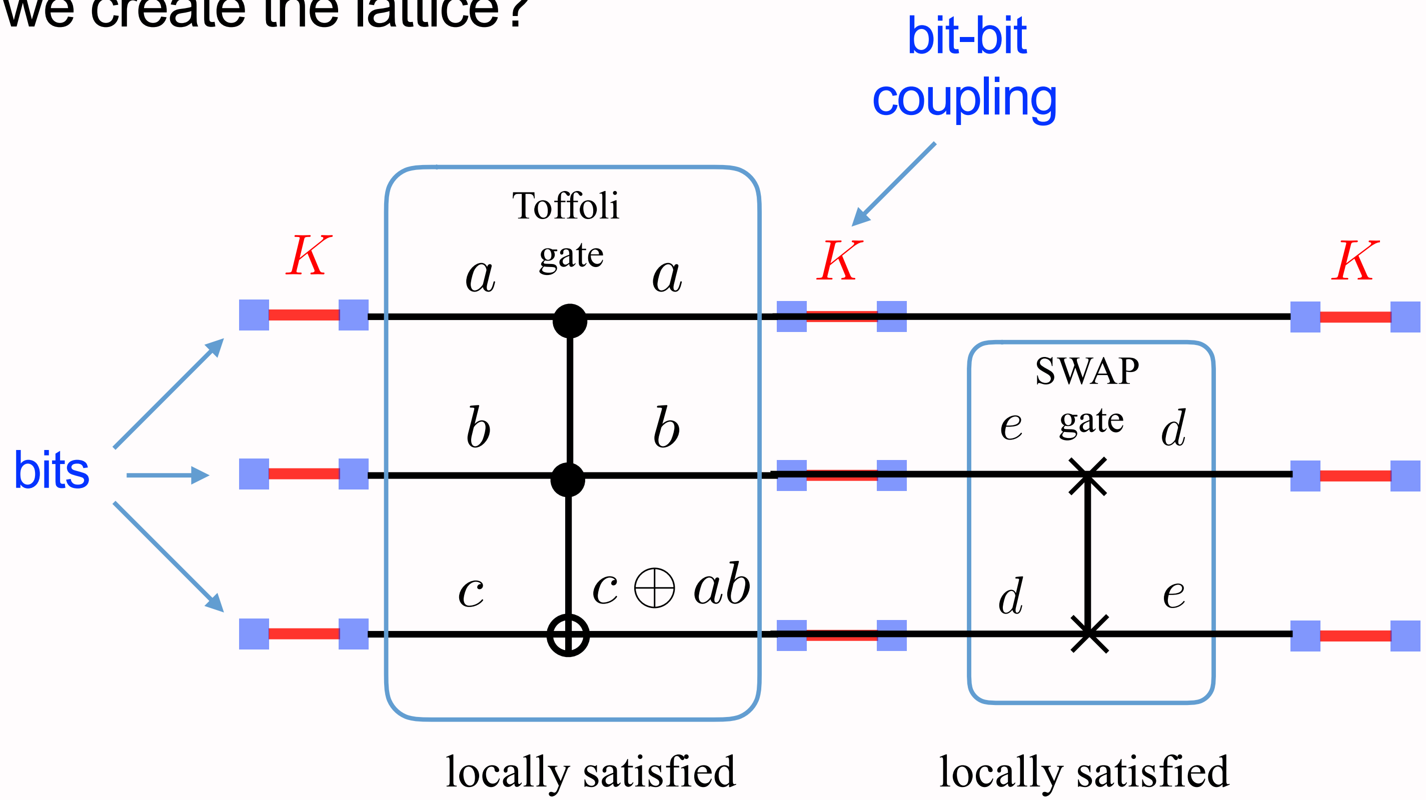
(A novel way to do ground-state computing)

- Create a two-dimensional lattice representation of a circuit; the gates are the vertices.
- One direction of the lattice represents "time".



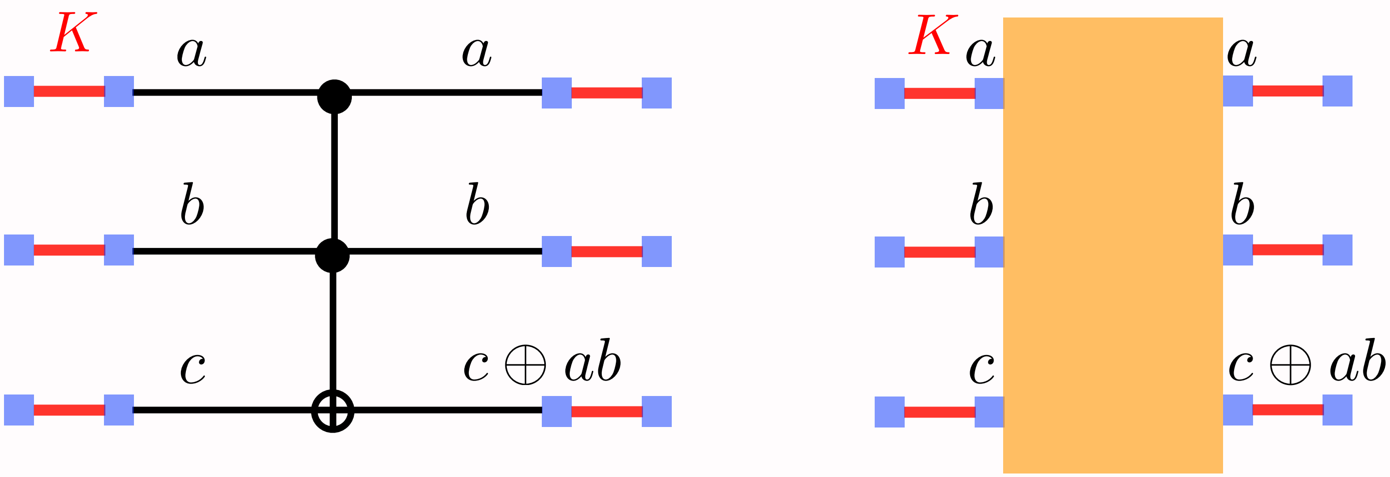
- The left and right boundaries contain the input and output states of the bits; can be fixed or free.
- Not limited to forward computations; can solve mixed-boundary problems.

How do we create the lattice?

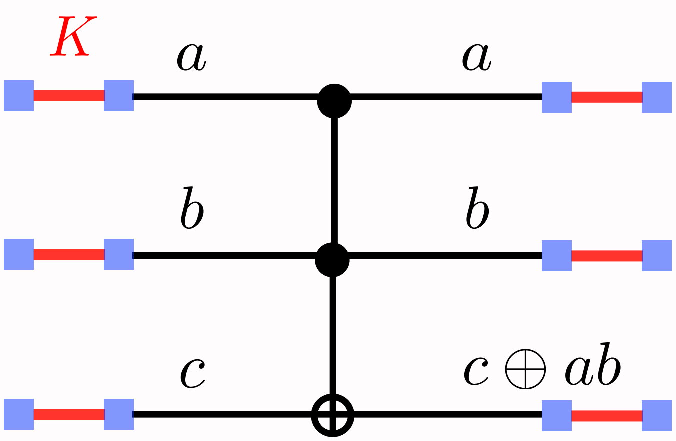


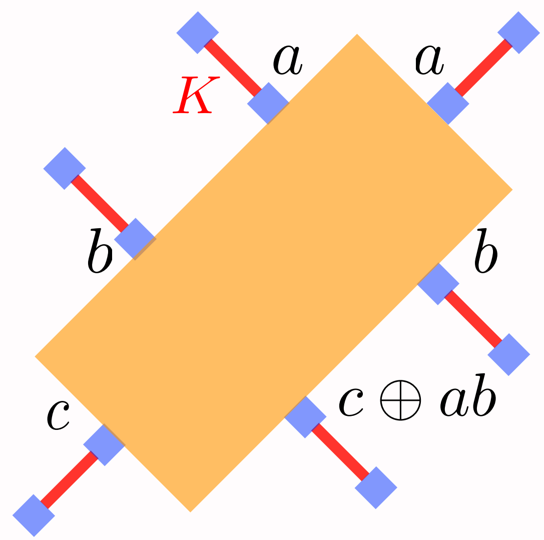
circuit building blocks: *reversible gates*

From gate to tile



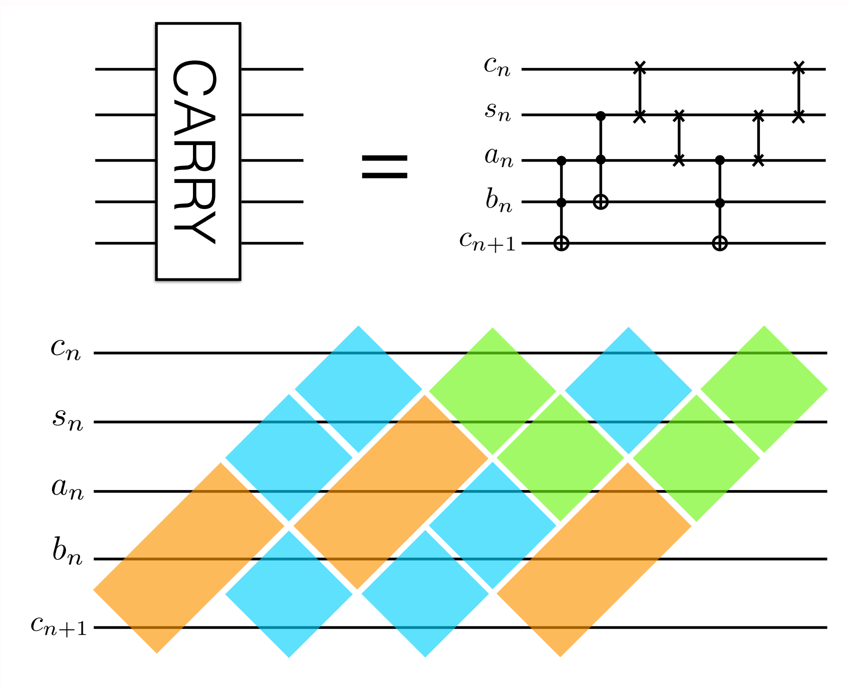
From gate to tile



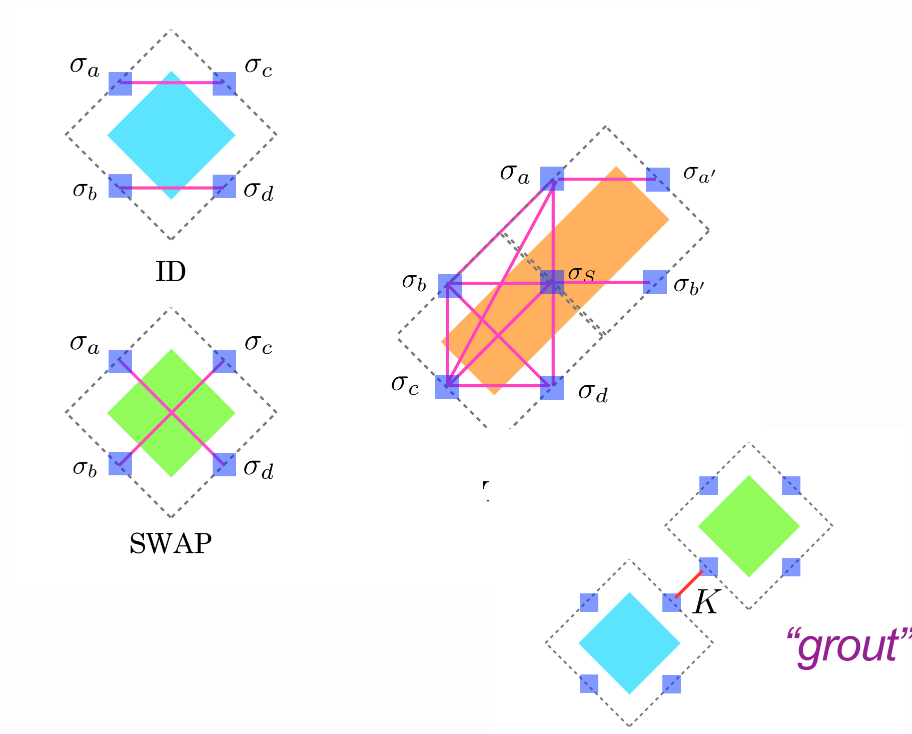


tilted for convenience

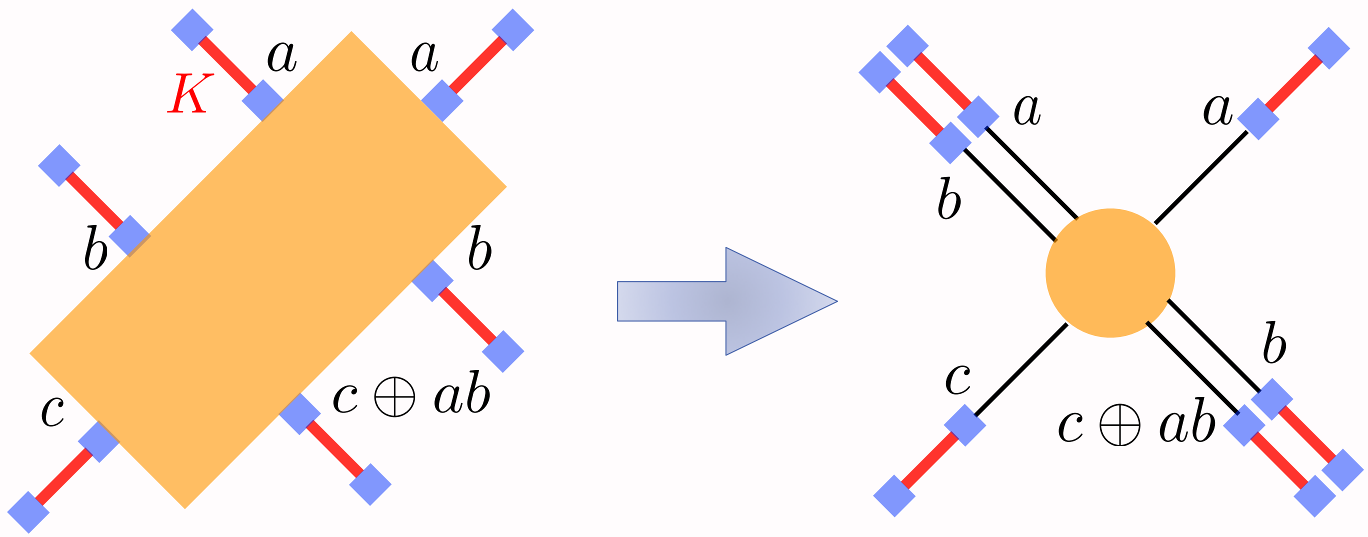
From circuits to tiled walls



All logic gates can be written using only **1- and 2-body** interactions

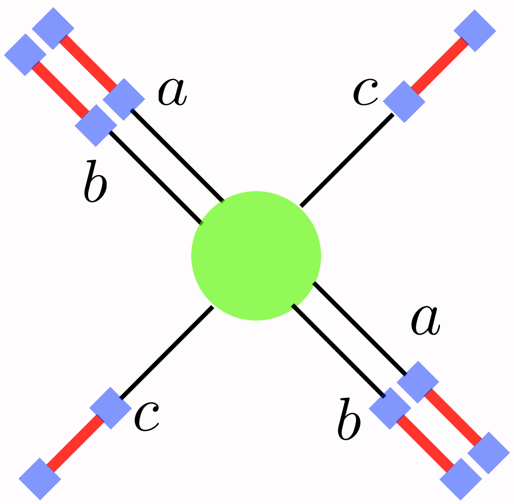


From tile to vertex

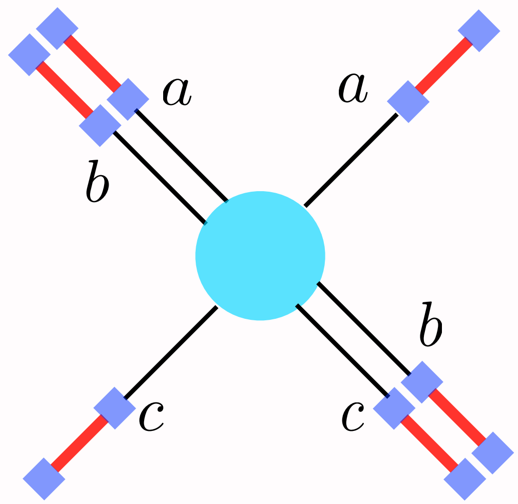


Mapping reversible classical circuits to a vertex model

Other necessary gates: ID-ID, ID-SWAP, SWAP-ID, SWAP-SWAP



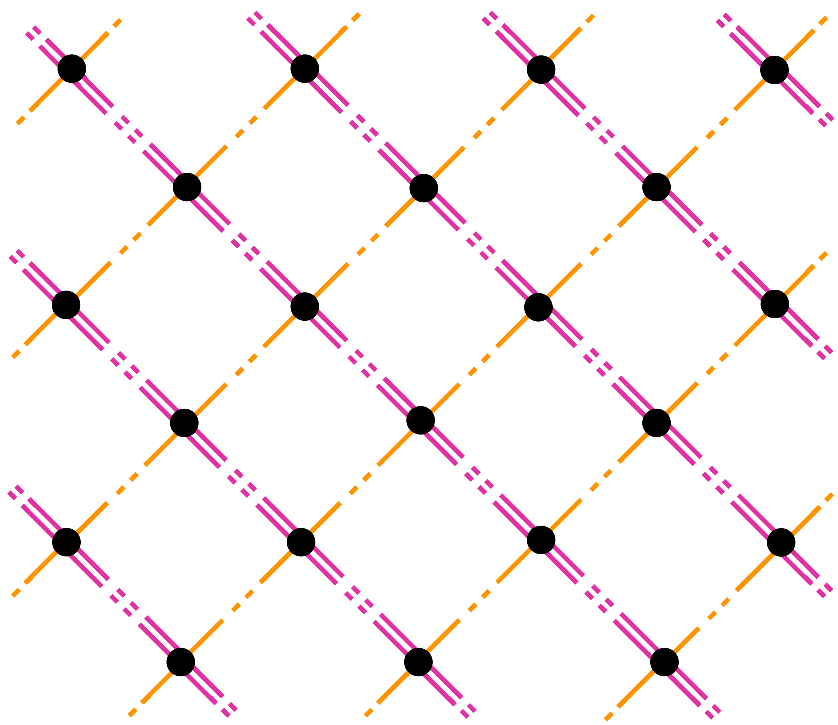
SWAP-SWAP



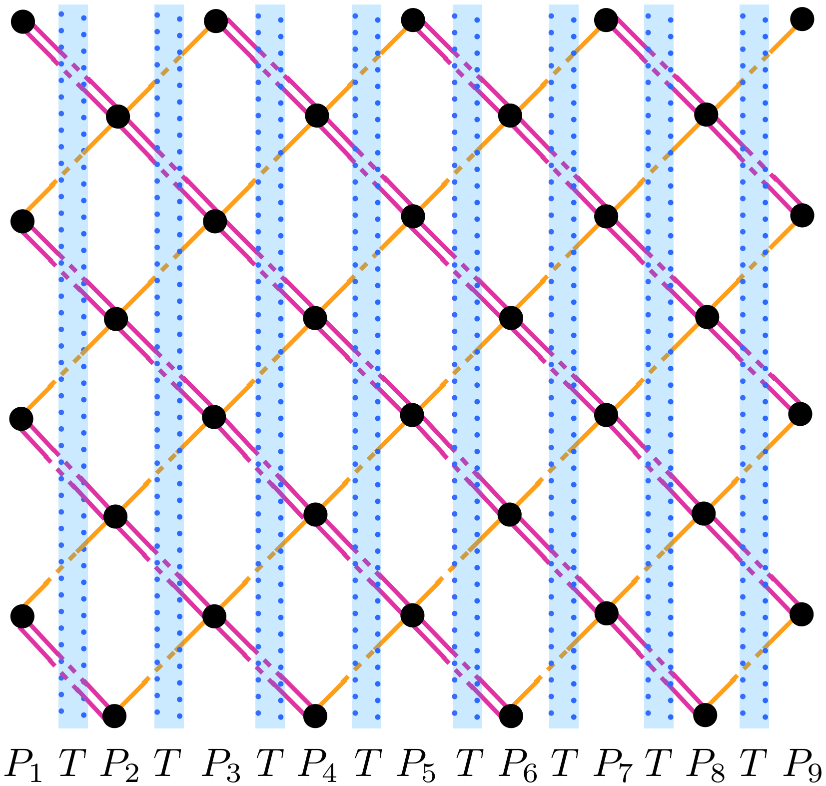
ID-ID

Mapping reversible classical circuits to a vertex model

Combining all gates (vertices) and couplings: a regular square lattice



Thermodynamics of the vertex model



P_j : *j*-th slice of reversible gates (permutation)

T_j : *j*-th slice of bit constraints (projector)

The exact partition function is computable!

<u>Result</u>: Paramagnet!

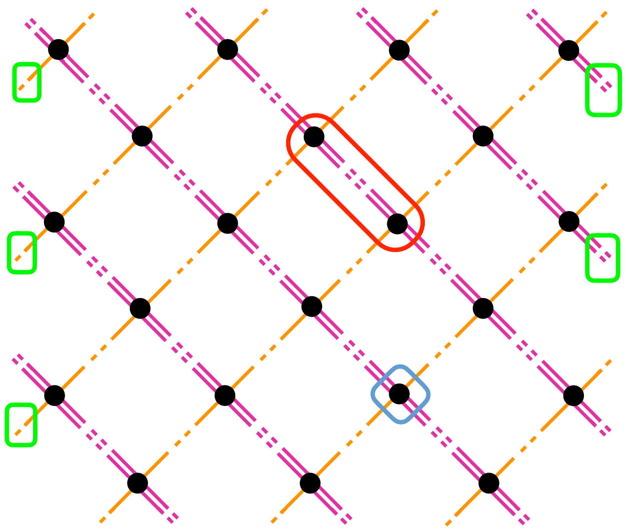
$$\boxed{Z = (2\cosh \beta K)^{3LW}}$$

No finite-temperature phase transition!

Quantum vertex model: adding a transverse field

$2^3 = 8$ states at each vertex: $q_s = 0, 1, \ldots, 7$

bits $\longrightarrow$ qubits



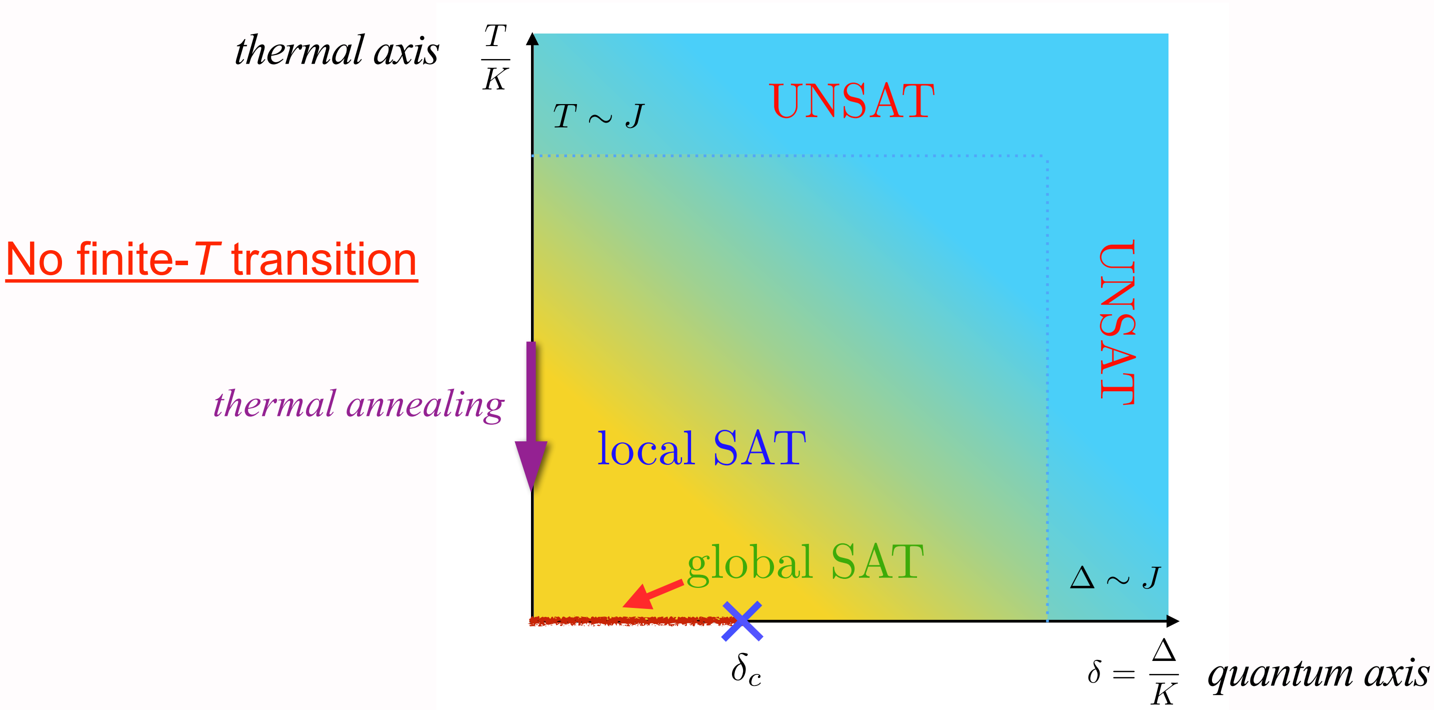
$$\hat{H} = \sum_{\langle ss' \rangle} \sum_{q_s, q_{s'}} \boxed{K^{g_s g_{s'}}_{q_s, q_{s'}}} |q_s q_{s'}\rangle\langle q_s q_{s'}| + \sum_{s \in \mathrm{boundary}} \sum_{q_s} \boxed{h_{q_s}} |q_s\rangle\langle q_s| + \sum_s \sum_{q_s, q'_s} \boxed{\Delta_{q_s, q'_s}} |q_s\rangle\langle q'_s| \,,$$

quantum tunneling term

$$J, h \gg K \gg \Delta$$

The mapping onto the vertex model removes the finite-temperature glass transition

Proposed phase diagram:



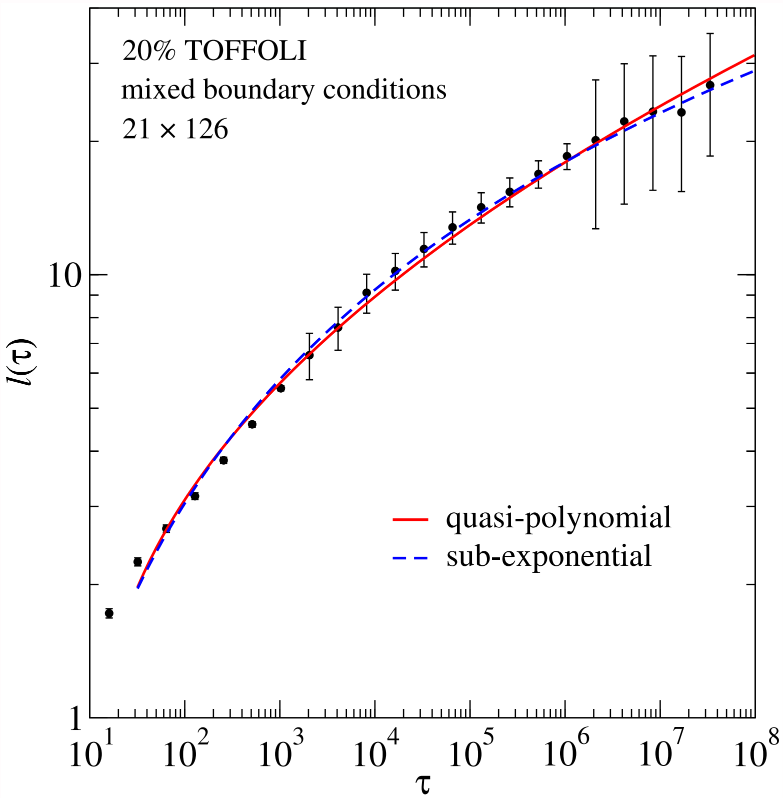
A solution can be reached… but how fast?

Dynamics is what matters!

The question to ask is:

How long does it take to thermalize?

Numerical investigation of thermal annealing dynamics



1) quasi-polynomial relax. times:

$$\ell(\tau) = \ell_0 \, \exp\{[\ln(\tau/\tau_0)]^\gamma\}$$

$\gamma \approx 0.475 \rightarrow \boxed{\tau_{\rm sol} \sim e^{(\#)\,(\ln L)^{2.1}}}$

2) sub-exponential relax. times:

$$\ell(\tau) = \ell_0 \, [\ln(\tau/\tau_0)]^\eta$$

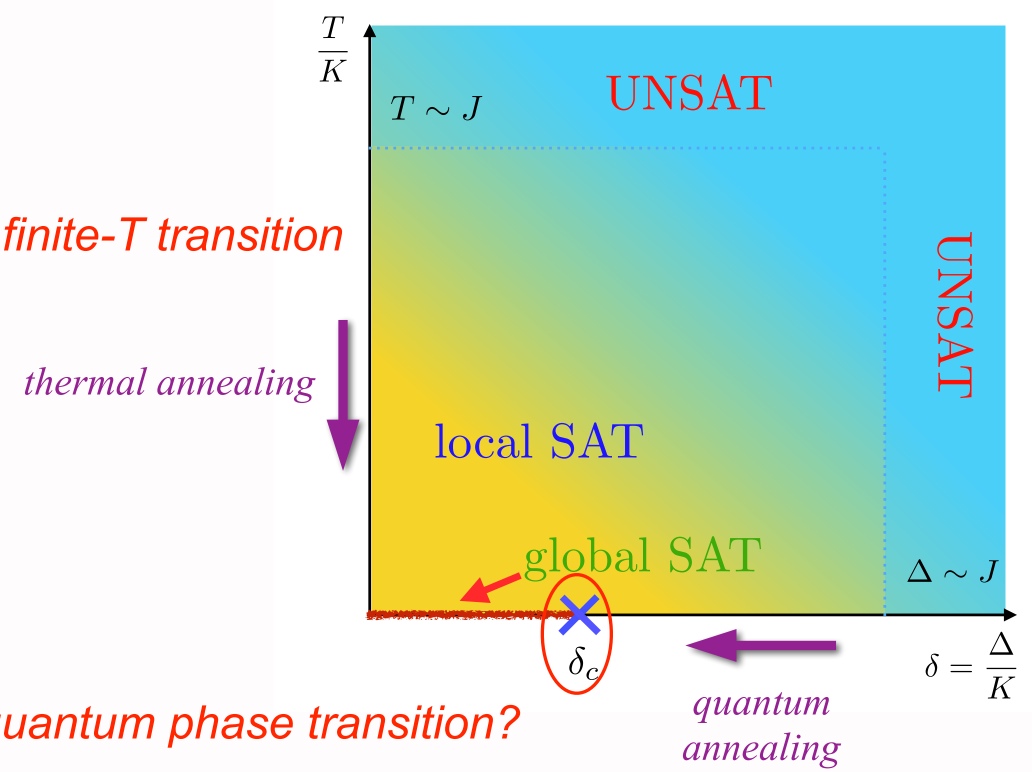
$\eta \approx 1.69 \rightarrow \boxed{\tau_{\rm sol} \sim e^{(\#)\,L^{0.6\theta}\ln L}}$

$(0.6\theta < 1)$

We cannot tell yet which one is the correct behavior!

Quantum annealing of the vertex model

No finite-T transition



Is there a quantum phase transition?

Quantum annealing of the vertex model

- When no Toffoli gates are presented: equivalent to 1D Ising chains + transverse field

Only a 2nd order quantum phase transition

↓

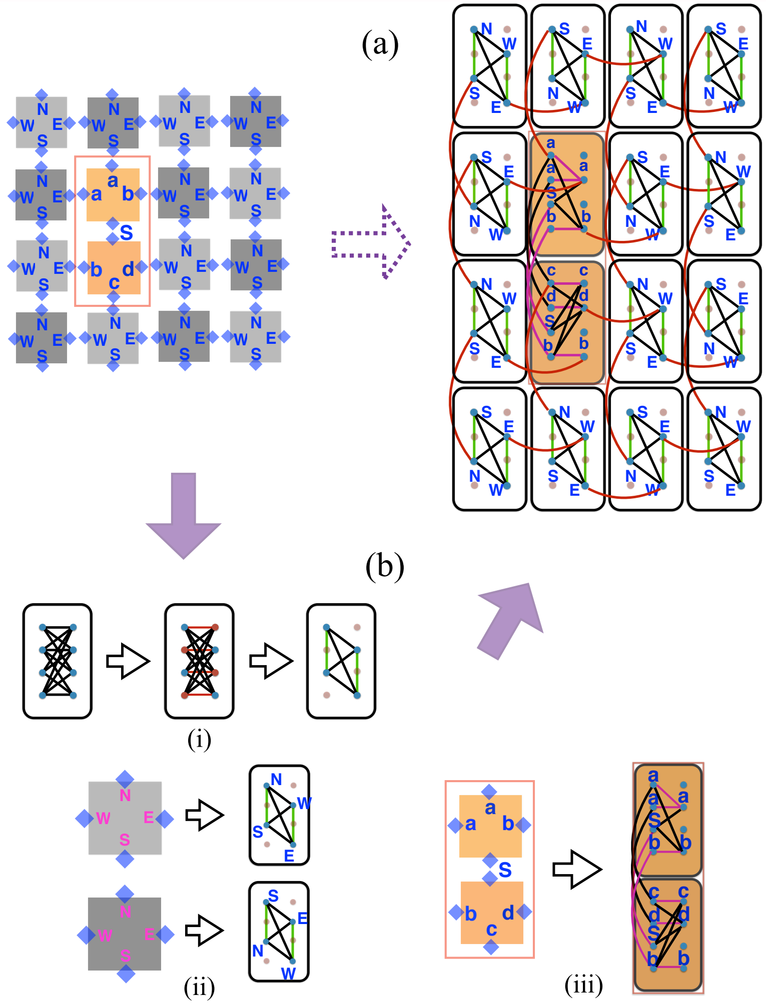
annealing in polynomial time!

- When a finite density of Toffoli gates are presented: the same scenario is likely. ***(conjecture)***

- Ongoing Quantum Monte Carlo studies to check it.

- Plans to verify it experimentally using a quantum annealer: **D-Wave machine**

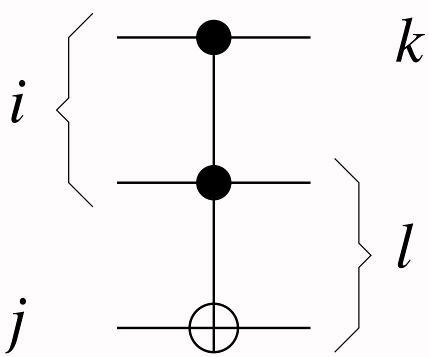
Embedding into the D-Wave Chimera Architecture

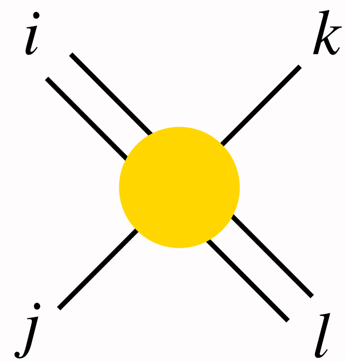


The quantum vertex model can be implemented in the D-Wave machine

Tensor Network Approach to Vertex Models

gates $\rightarrow$ tensors (vertices)



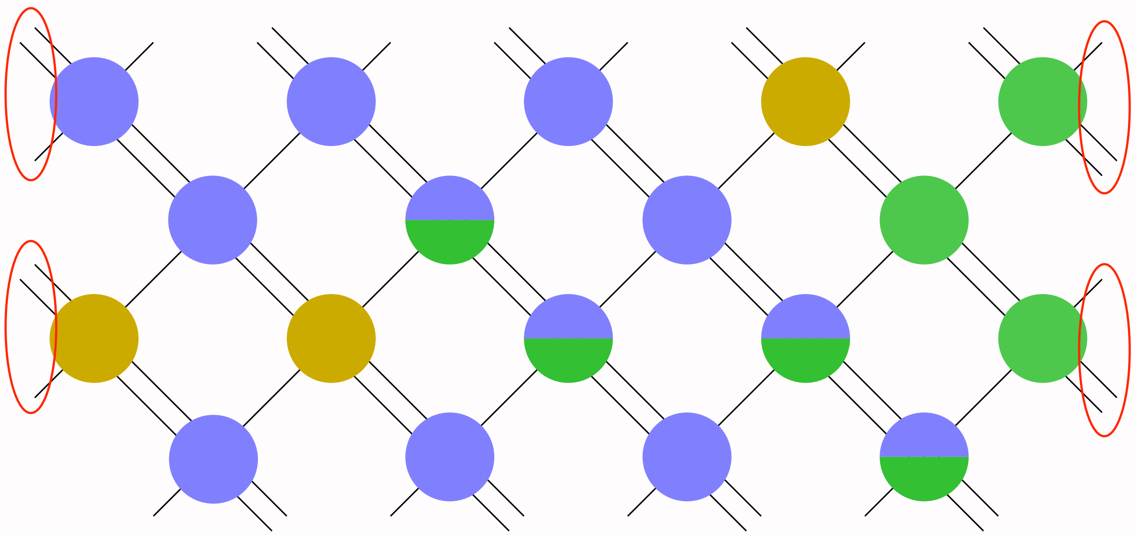


tensors enforce
gate truth tables

$$\boxed{\begin{aligned} k &= F_1(i,j) \\ l &= F_2(i,j) \end{aligned}}$$

$$T_{i,j,k,l} = \begin{cases} 1, & \text{if } k = F_1(i,j) \text{ and } l = F_2(i,j), \\ 0, & \text{otherwise.} \end{cases}$$

tensors → network



boundary indices: fixed or free, depending on the problem to be solved

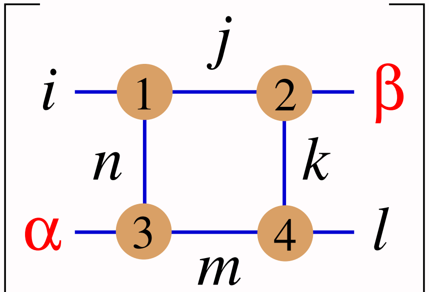
Instead of looking for ground states, we take a different approach:

$$Z = \mathrm{Tr} \prod_{n} T[n]_{i,j,k,l}$$

full contraction of the tensor network

<u>Example</u>:

$Z(\alpha, \beta) = \mathrm{Tr}$



$$= \sum_{i,j,k,l,m,n} T[1]_{i,j,n}\, T[2]_{j,\beta,l}\, T[3]_{\alpha,n,m}\, T[4]_{k,l,m}$$

fixed values

$Z(\alpha, \beta) =$ number of solutions to the problem encoded by the circuit for fixed α, β.

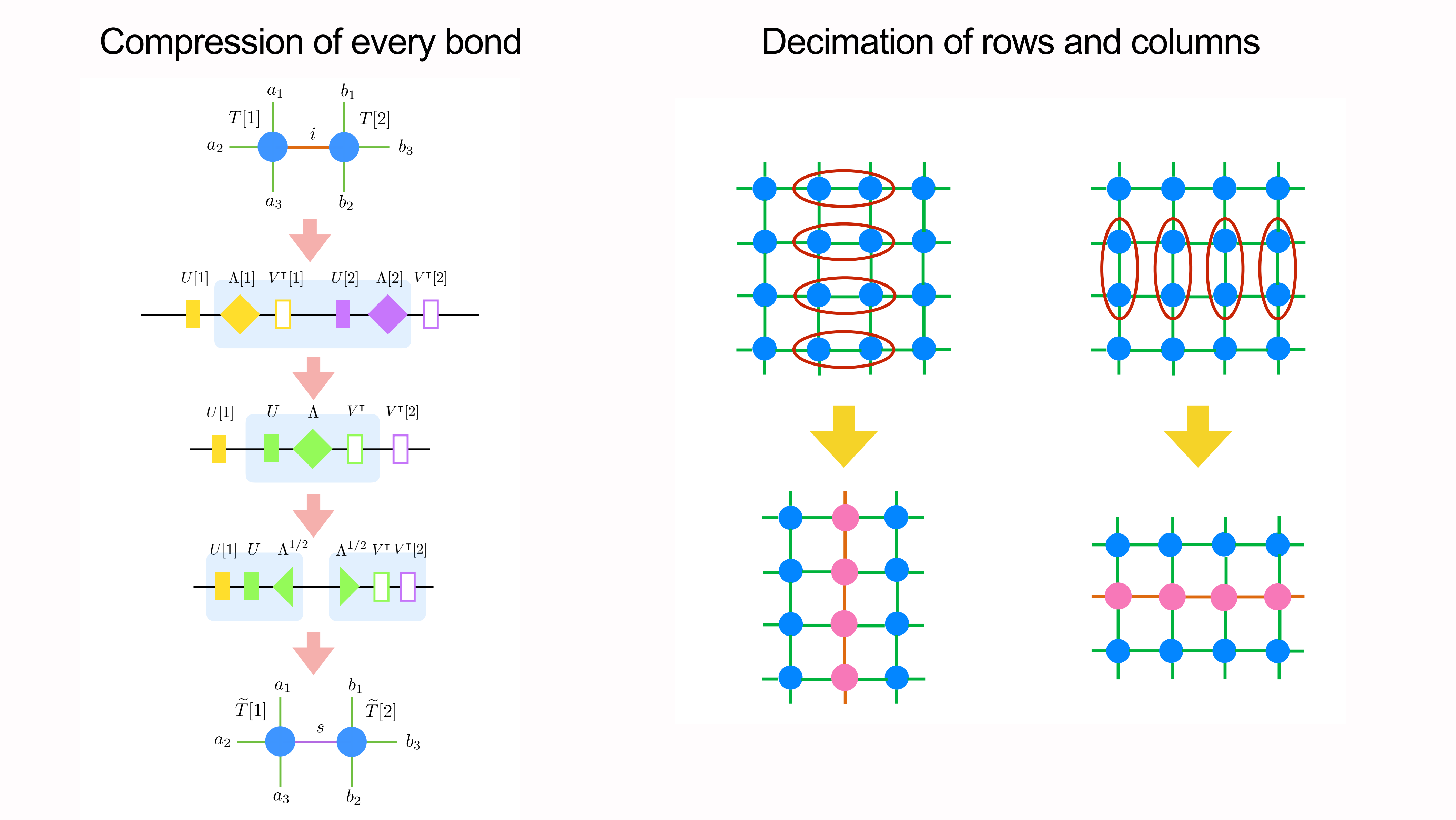
By varying boundary variables, one at a time, and monitoring Z, we can determine solutions to the problem.

<u>The catch</u>: it is exponentially hard to compute Z !! #P complexity class

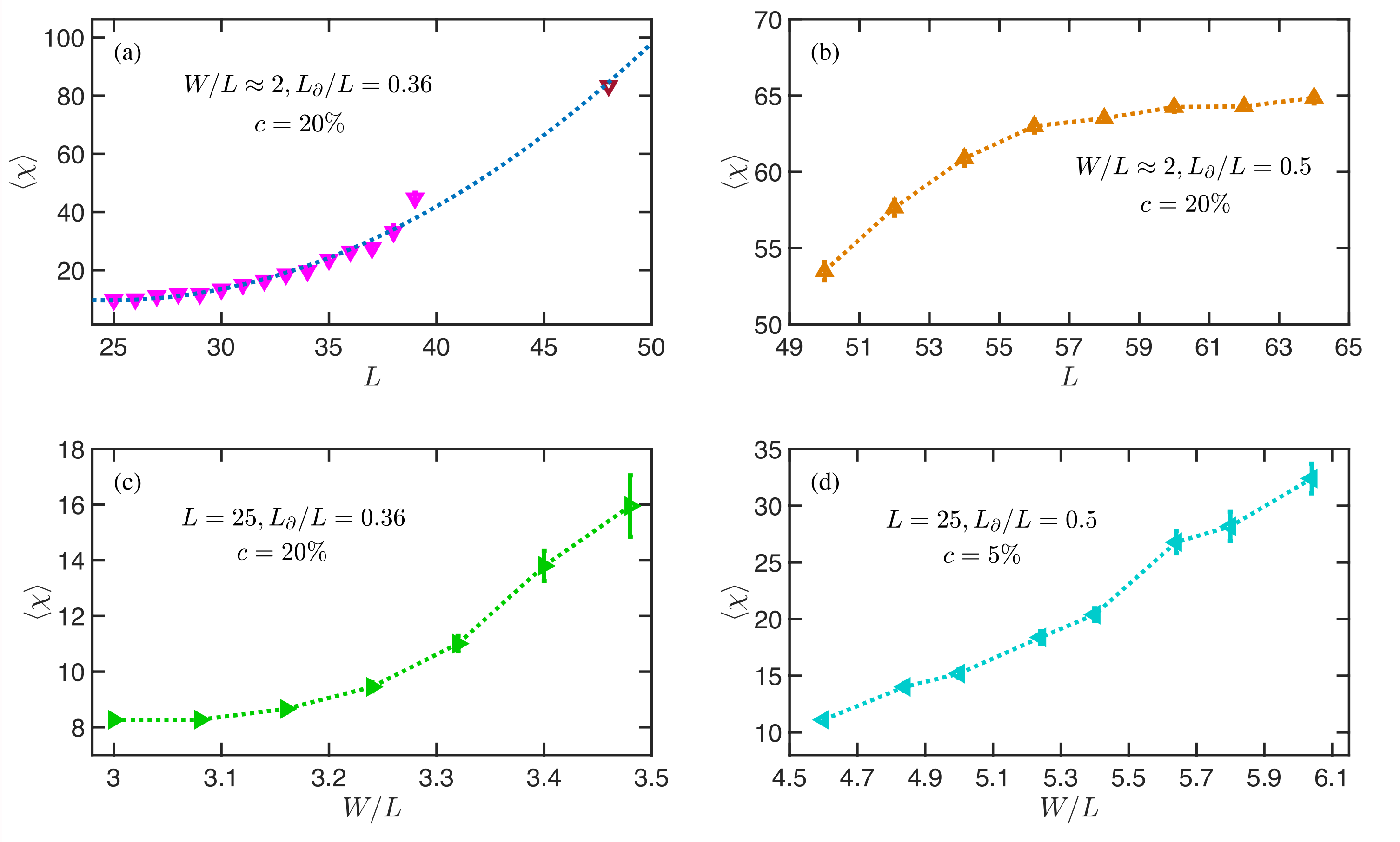
$$\text{computational cost} \sim O\left(\underset{\substack{\uparrow \\ \text{bond dimension}}}{\chi}^{\#\text{ of network links}}\right)$$

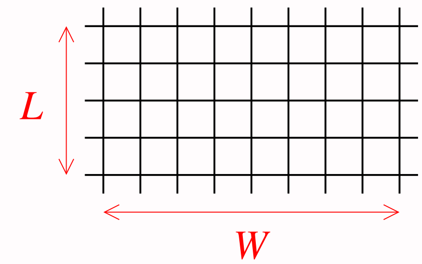
We have developed a scheme that attenuates the difficult:

Iterative Compression Decimation (ICD)


Compression of every bond
Decimation of rows and columns
a_1 b_1 $T[1]$ $T[2]$ i a_2 b_3 a_3 b_2
$U[1]$ $\Lambda[1]$ $V^\intercal[1]$ $U[2]$ $\Lambda[2]$ $V^\intercal[2]$
$U[1]$ U Λ $V^\intercal$ $V^\intercal[2]$
$U[1]$ U $\Lambda^{1/2}$ $\Lambda^{1/2}$ $V^\intercal$ $V^\intercal[2]$
a_1 b_1 $\widetilde{T}[1]$ $\widetilde{T}[2]$ s a_2 b_3 a_3 b_2

Some recent numerical results for the random Toffoli circuit:





We were able to reach $L = 96$.

A brute-force enumeration would require $8^{48} \sim 10^{43}$ iterations!!

SUMMARY:

- Close connections between Computer Science & Physics

- Physics constraints computations, but also inspires new methods and concepts

- Entanglement spectrum fluctuations reveal the difficult to reverse circuits

- Vertex models: a novel way to do ground-state computing (classical or quantum)

- ICD: A new scheme to solve vertex-model problems using tensor networks

Collaborators:

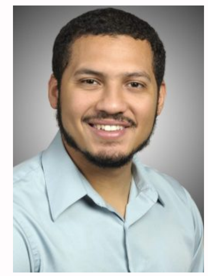
Claudio Chamon

Andrei Ruckenstein

Zhicheng Yang

Alioscia Hamma

Sabine Pelton



Justin Reyes

Stefanos Kourtis

Daniel Shaffer
(now at U Minnesota)

Lei Zhang

Dan Marinescu

Pawel Wocjan

Partial Funding:

NSF

THE END