Computational Complexity of the Local Hamiltonian Problem

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UC Irvine

The Local Hamiltonain Problem

Input:

$H_1, \ldots, H_r$:

Hermetian positive semi-definite matrices
operating on k qudits of dimension d
with bounded norm $\|H_i\| \leq 1$.
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Two real numbers E and $\Delta \geq 1/\text{poly}(n)$

Output:

Is the smallest eigenvalue of $H = H_1 + \cdots + H_r \leq E$
or are all eigenvalues $\geq E + \Delta$?

The class QMA (Quantum Merlin Arthur)

NP

A problem is in NP if there is a polynomial time Turing Machine M such that on input x, where $|x| = n$:

If $x \in L$, then there is a witness y such that $M(x, y)$ accepts.

If $x \notin L$, then for every y, $M(x, y)$ rejects.

$|y| \leq \text{poly}(x)$

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Guarantee:

There exists $|\Phi\rangle$ such that $\langle \Phi | H | \Phi \rangle \leq E$

OR

For all $|\Phi\rangle$, $\langle \Phi | H | \Phi \rangle \geq E + \Delta$

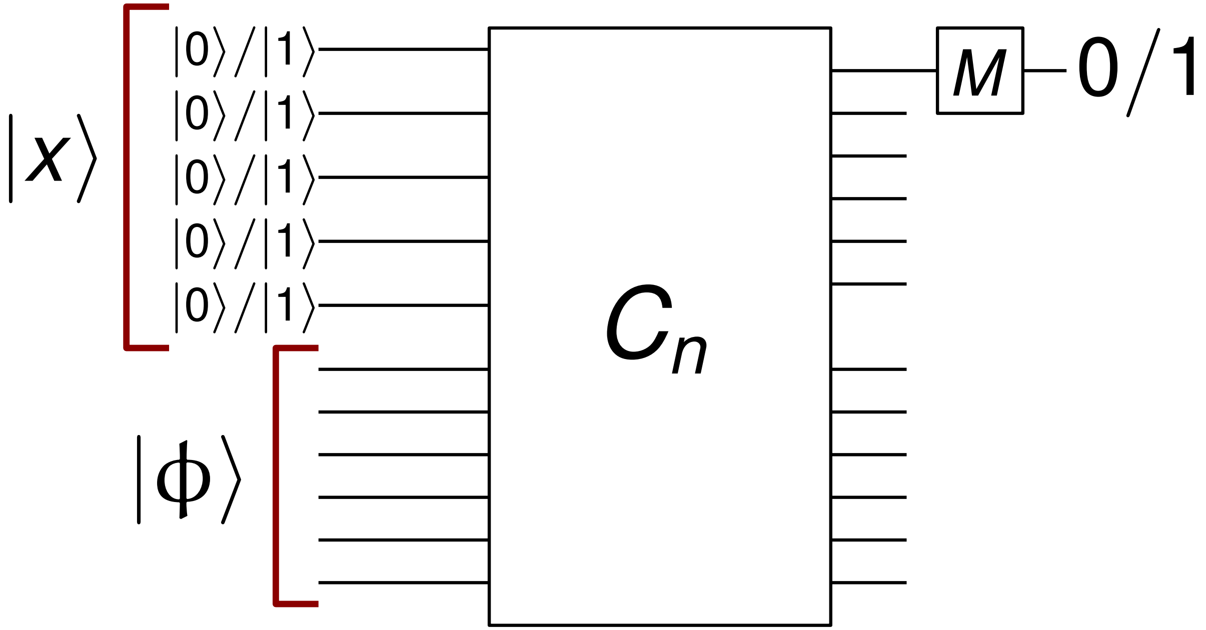
$\Longrightarrow$

Showed a measurement whose outcome = 1 with probability $\langle \Phi | H | \Phi \rangle / r$.

Local Hamiltonian is QMA-hard

Start with a generic language L in QMA

Is $x \in L$?



Is there a quantum state $\phi\rangle$
that causes this quantum circuit
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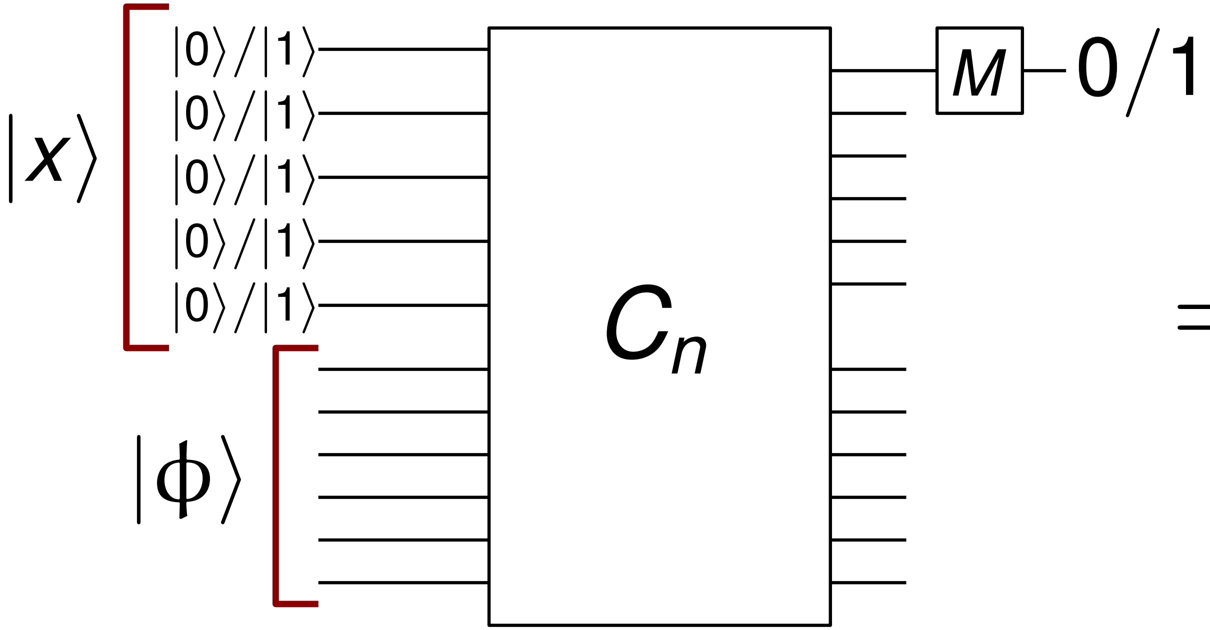

$\Rightarrow$ k-Local Hamiltonian: (H_x, E, Δ)

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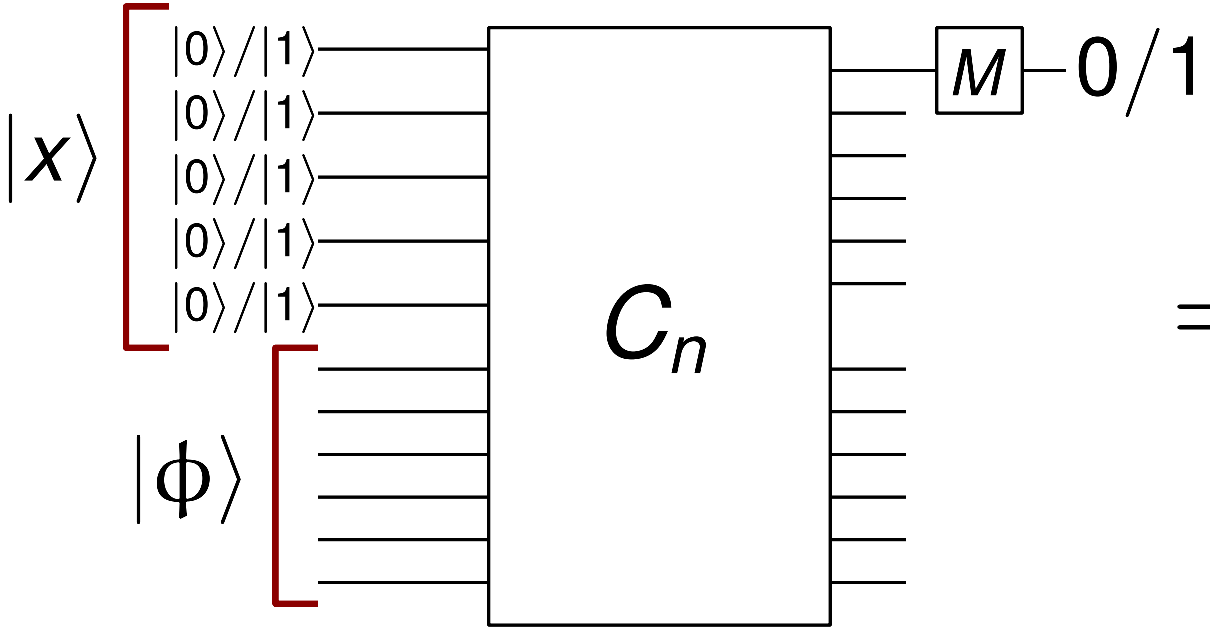

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$$H_t = \frac{1}{2}\left[I \otimes |t\rangle\langle t| + I \otimes |t-1\rangle\langle t-1| + U_t \otimes |t\rangle\langle t-1| - U_t^{\dagger} \otimes |t-1\rangle\langle t| \right]$$

$$H_{prop} = \sum_{t=1}^{T} H_t$$

Ground State:

$$\frac{1}{\sqrt{T+1}} \sum_{t=0}^{T} U_t U_{t-1} \cdots U_2 U_1 |x\rangle|\xi\rangle \otimes |t\rangle$$

Spectral Gap:

$$\geq \frac{1}{2(T+1)^2}$$

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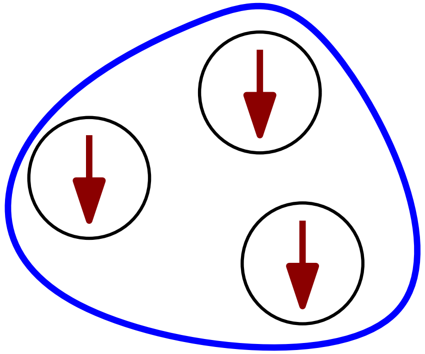
$$H = H_{prop} + H_{init} + H_{out}$$

Local Hamiltonian Variations



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$H = \sum_a H_a$

where each H_a acts on at most k qudits

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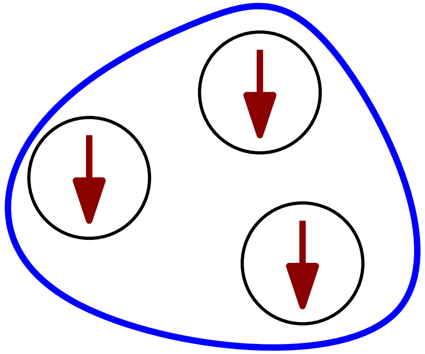

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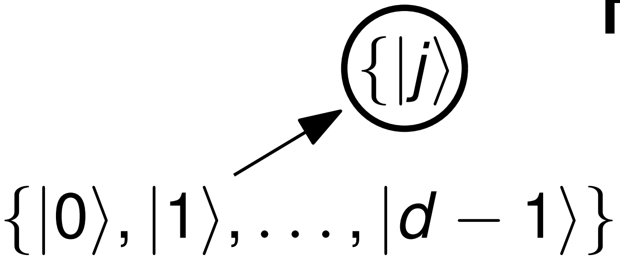

Particle Dimension

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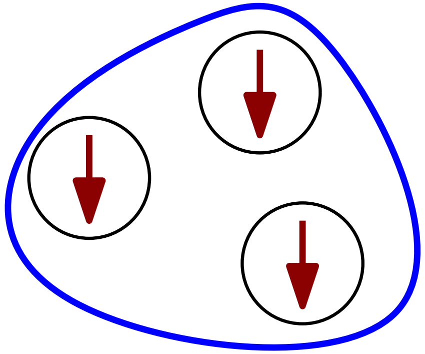

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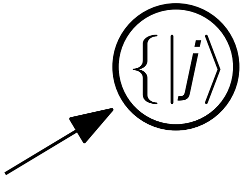
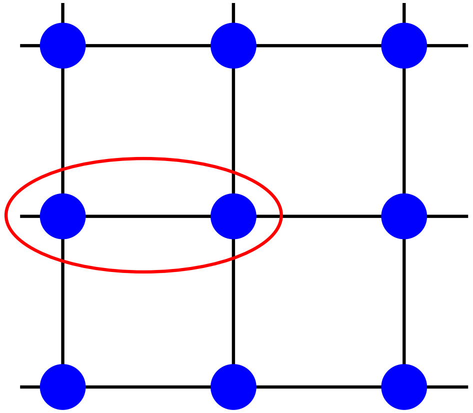


$\{|0\rangle, |1\rangle, \ldots, |d-1\rangle\}$

Geometry



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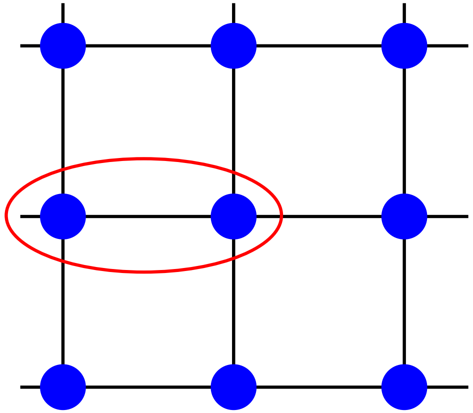

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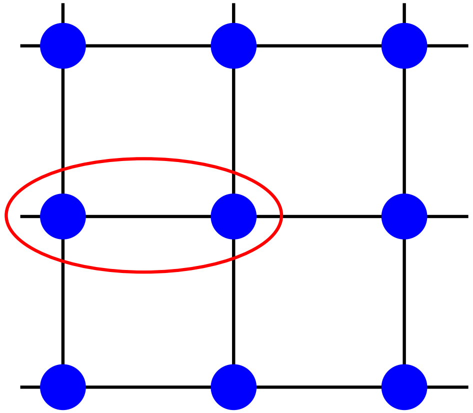

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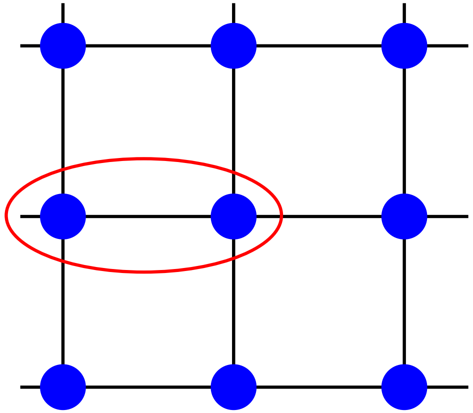

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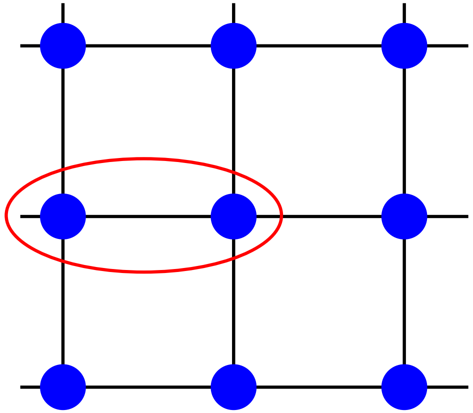

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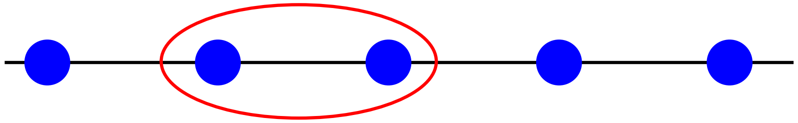

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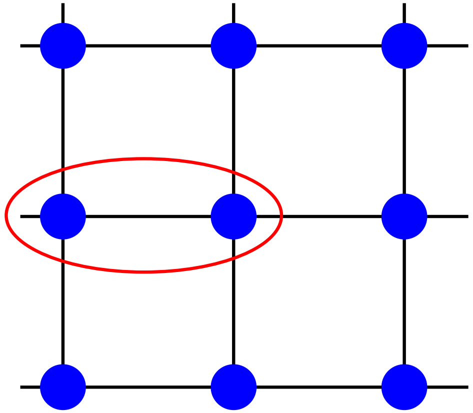

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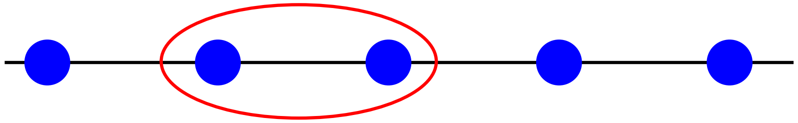

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Spectral gap of $H(t)$

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Originally suggested in the context of solving NP-hard problems
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  Yes - [van Dam, Mosca, Vazirani]

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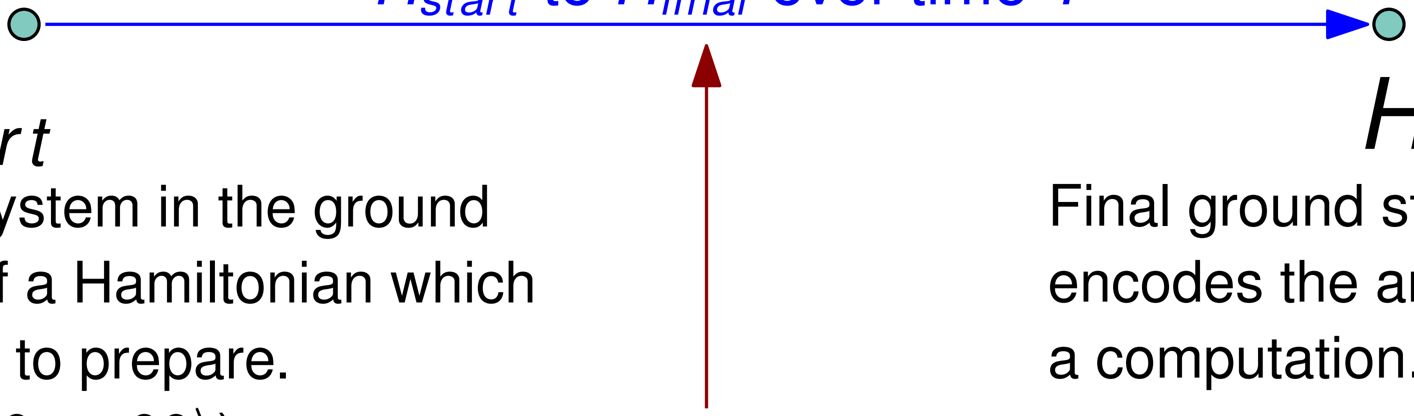

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$H_{final} = H_{prop}$

Hamiltonian whose ground state is the computation state for Quantum Circuit C with input x. (No witness)

[Aharonov, van Dam, Kempe, Landau, Lloyd, Regev 2004]

Circuit to Adiabatic Computation

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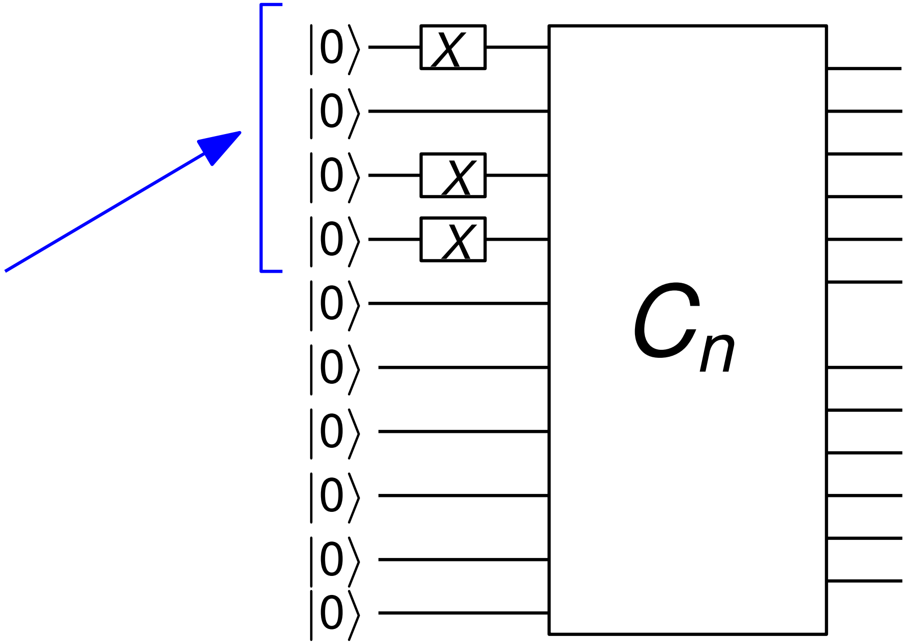
Initial X gates set the input bits according to input x



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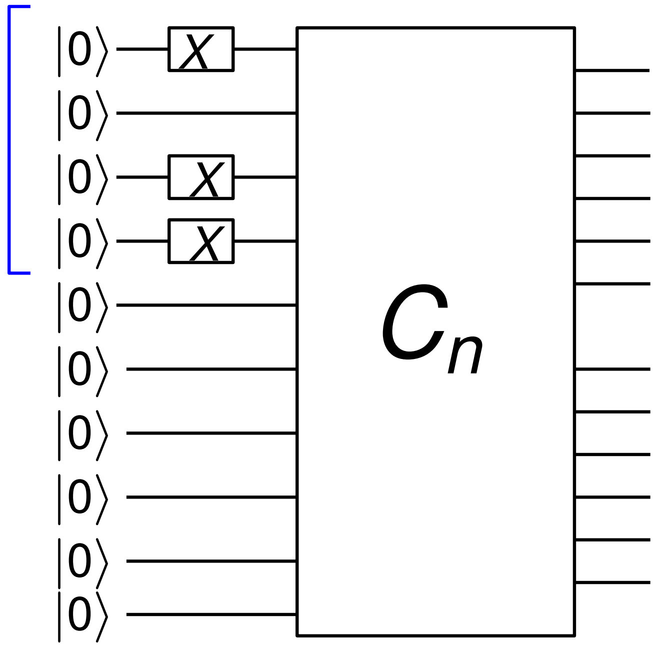

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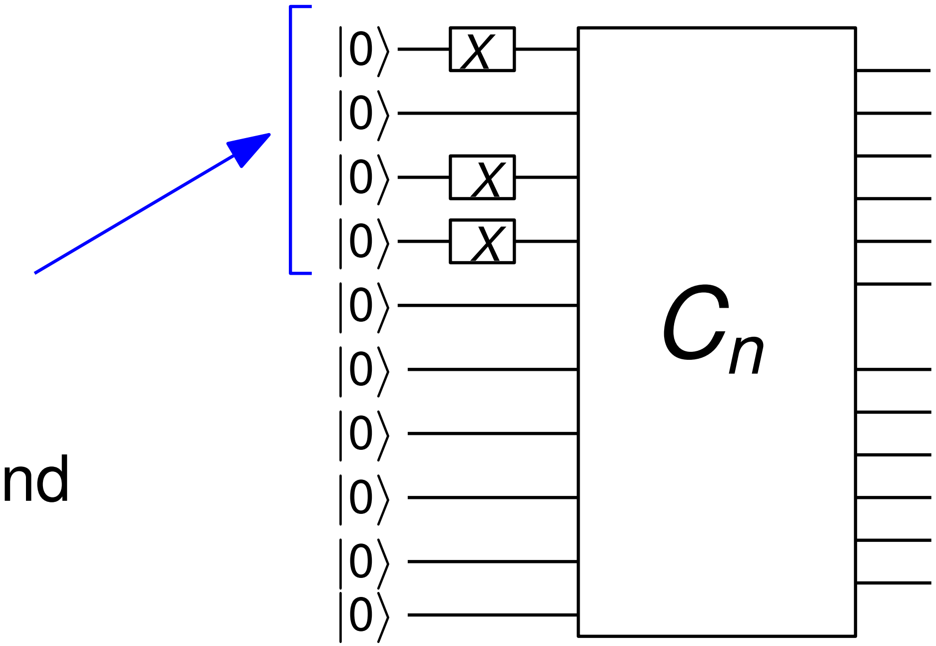

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Measure:

$$|T\rangle\langle T|_{clock} \quad \text{then} \quad |1\rangle\langle 1|_{out}$$

Probability to measure the clock in state T is $\frac{1}{T+1}$

Lower Bound Spectral Gap

$$H_{start} = \begin{bmatrix} 0 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & \ddots & & \\ & & & & 1 & \\ & & & & & 1 \end{bmatrix} \qquad H_{final} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & & & & & & \\ -\frac{1}{2} & 1 & -\frac{1}{2} & & & & & \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & & & & \\ & & & \cdot & & & & \\ & & & & \cdot & & & \\ & & & & & \cdot & & \\ & & & & -\frac{1}{2} & 1 & -\frac{1}{2} & 0 \\ & & & & & -\frac{1}{2} & 1 & -\frac{1}{2} \\ & & & & & & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

Spectral gap of:

$$(1 - s)H_{start} + sH_{final} \text{ for } s \in [0, 1] \text{ is } \geq \frac{1}{2(T + 1)^2}$$

QMA-complete Problems

5-local 2-state Hamiltonian is QMA-Complete [Kitaev 1995]

2-dimensional 2-local 6-state Hamiltoanian is QMA-complete
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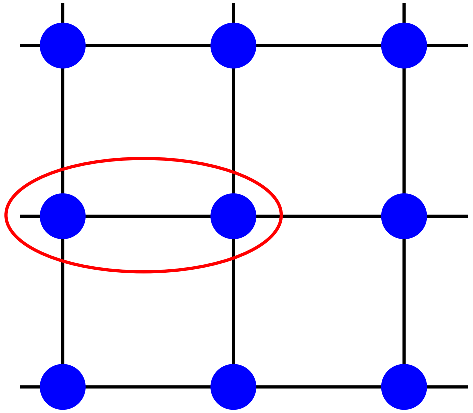

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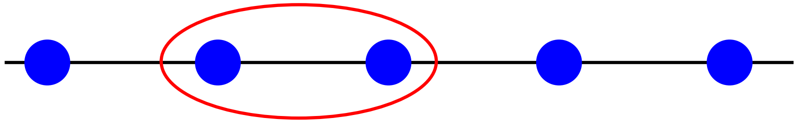

2D Local Hamiltonian Reduction

Kitaev Construction:

$$\frac{1}{\sqrt{T+1}}\sum_{t=0}^{T}\underbrace{|\psi_t\rangle}_{\text{Computation Qubits}}\underbrace{|1^{t+1}0^{T-t}\rangle}_{\text{Clock Qubits}}$$

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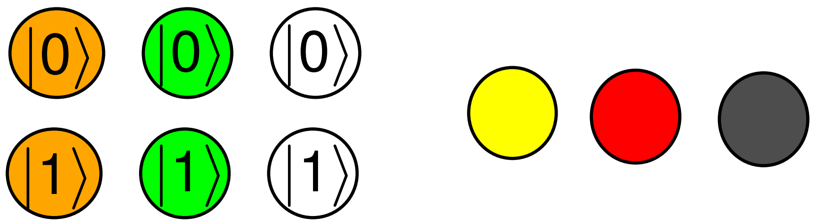
The "Clock" is distributed throughout the entire quantum system:

State space for a particle:

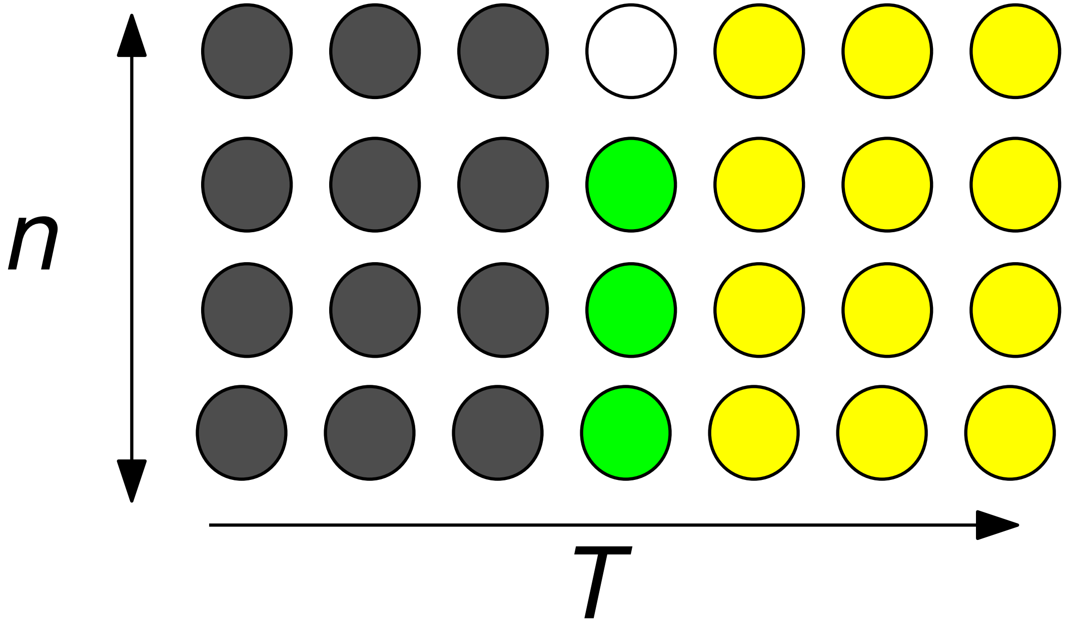
$\{|0\rangle, |1\rangle\} \otimes \{|$🟠$\rangle, |$🟢$\rangle, |$○$\rangle\}$

$\cup \ \{|$🔴$\rangle, |$⚫$\rangle, |$🟡$\rangle\}$



2D Local Hamiltonian Reduction, cont.

Clock state is a pattern of colors on the 2D grid of particles:



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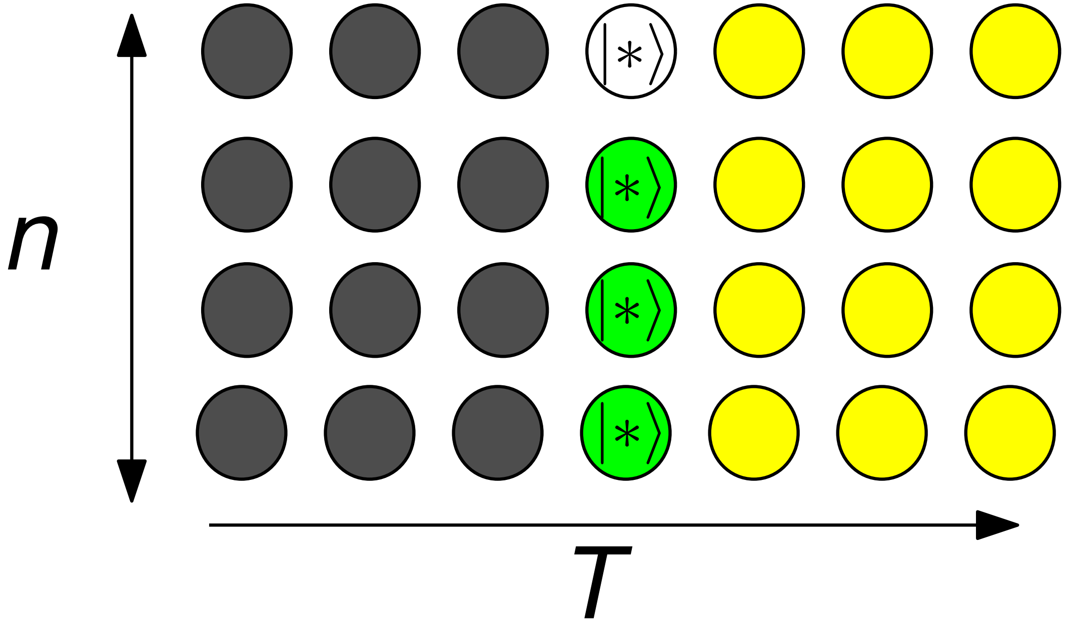

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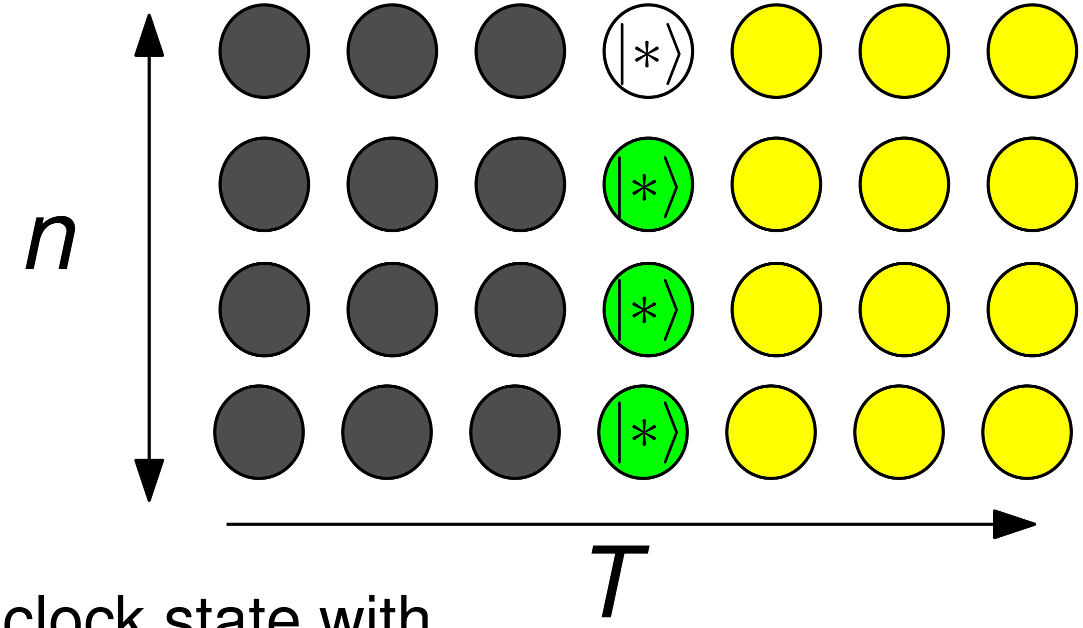
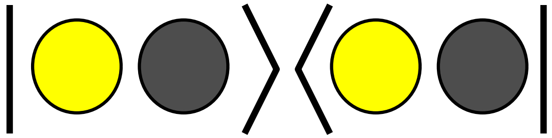


Enforce valid clock state with
”forbidden”
local configurations:



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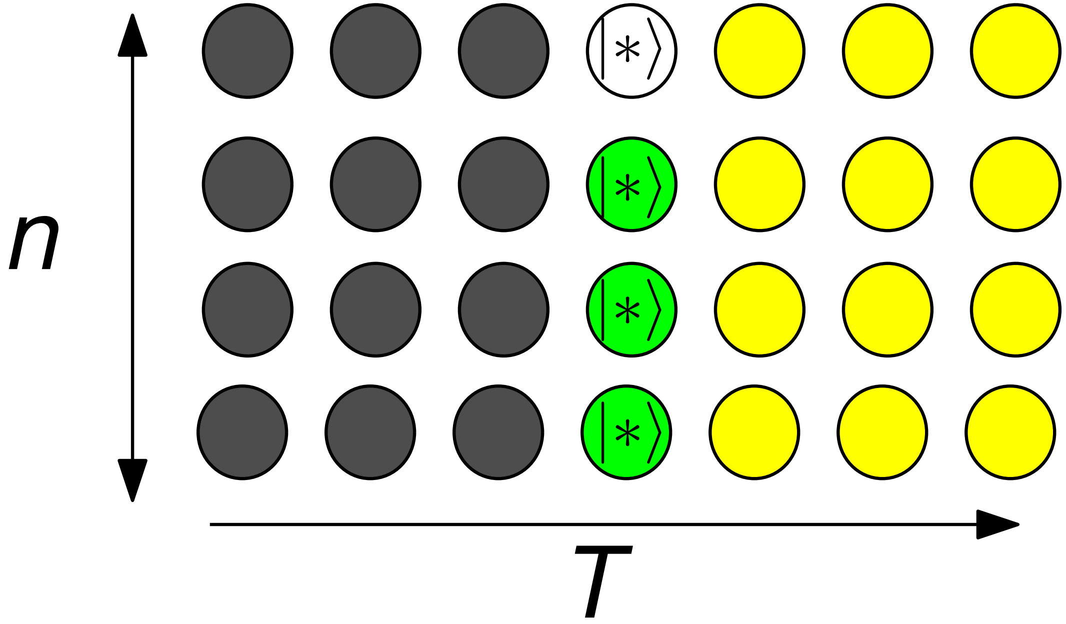

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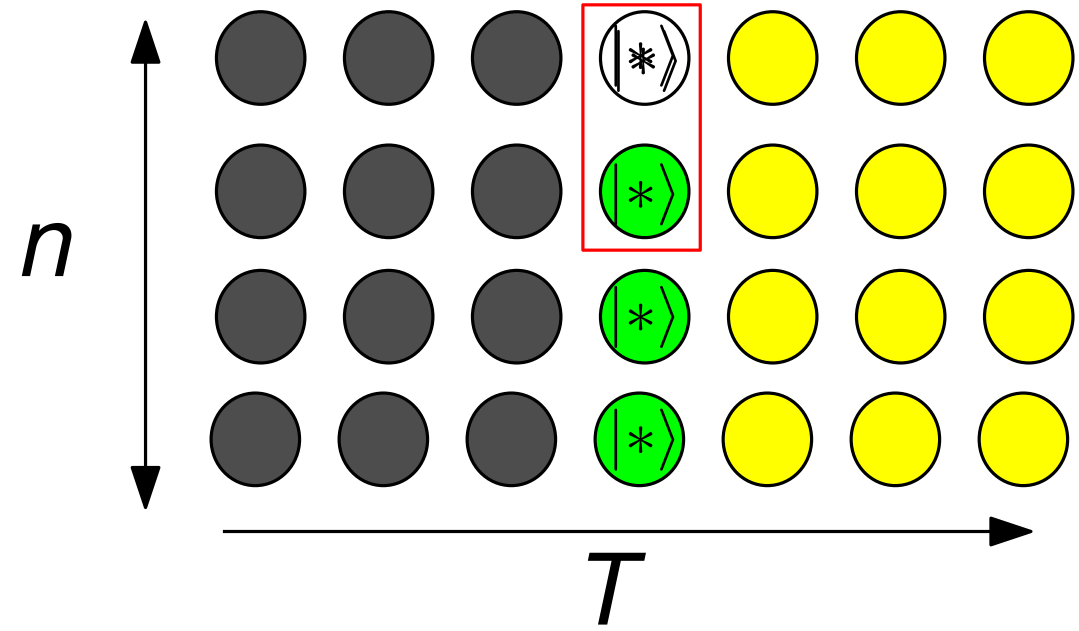

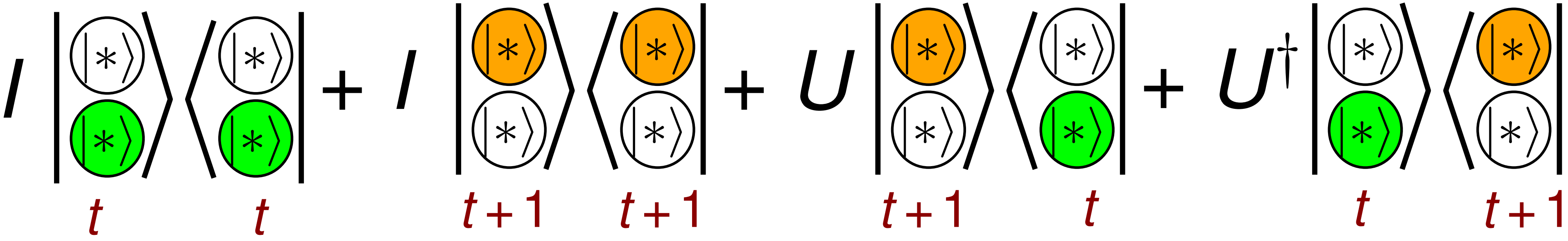

Applied to two particles in ☐

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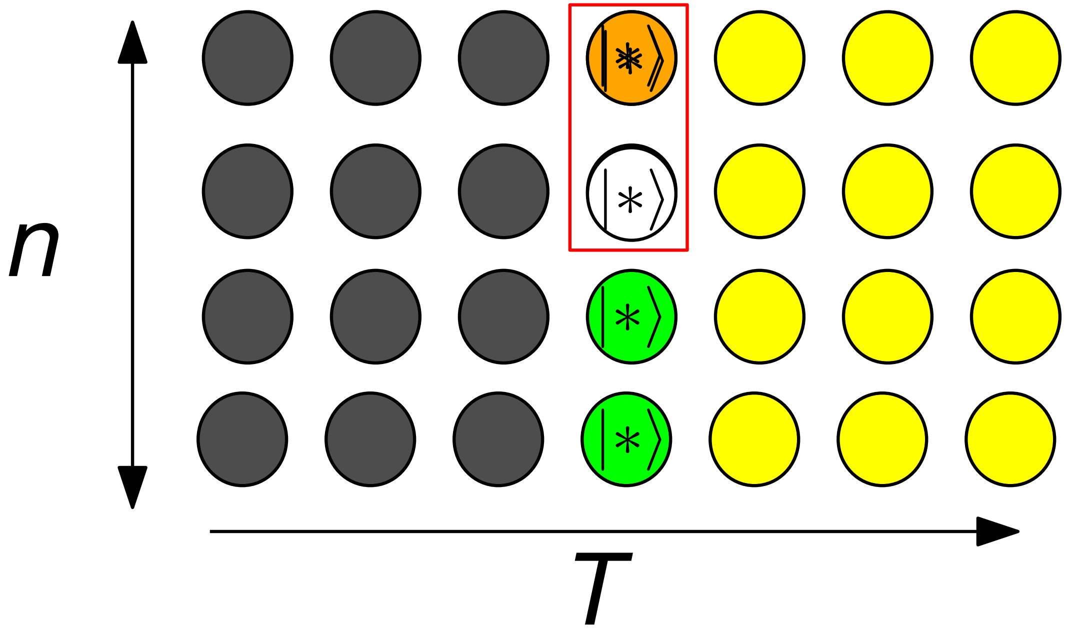

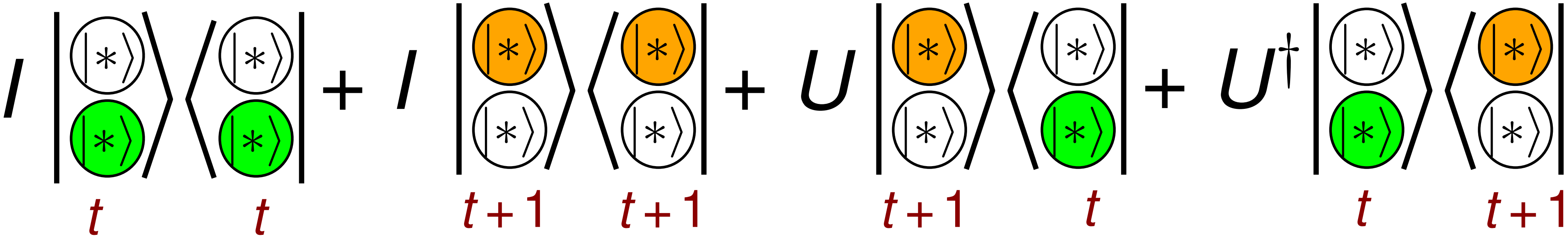

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Clock Configuration Graph

Need to ensure at most one propogation term applied to each valid clock state.

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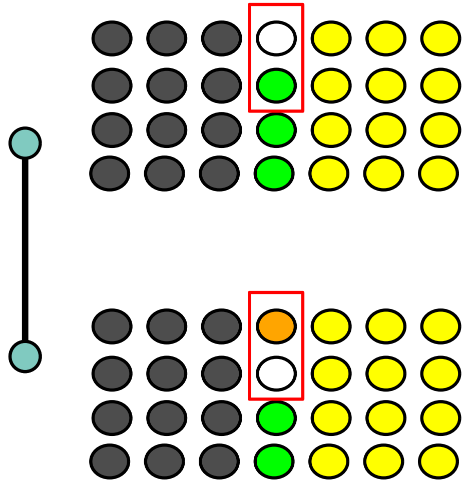

Vertices: Standard basis of clock states

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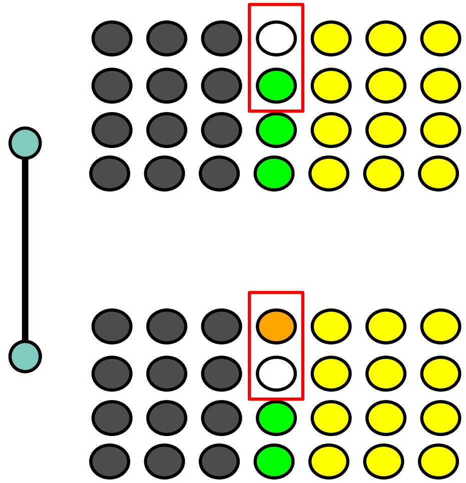

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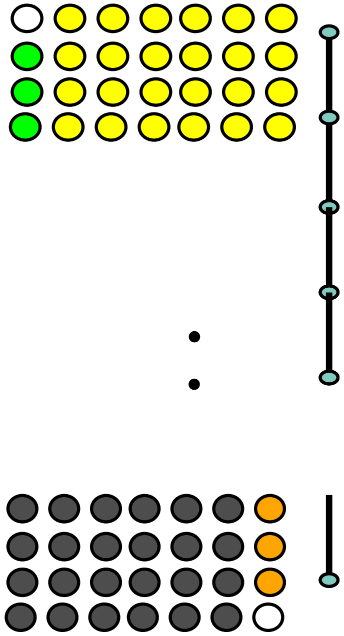

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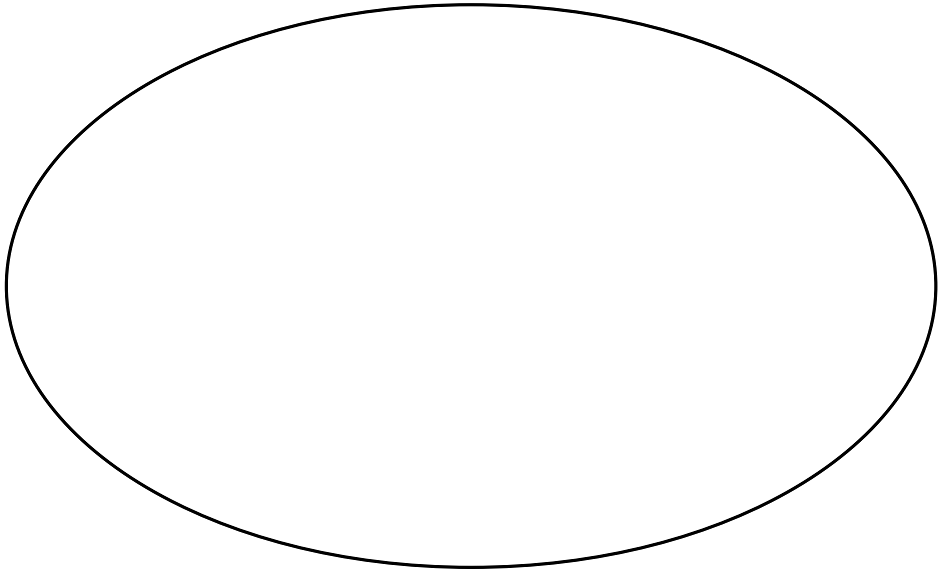

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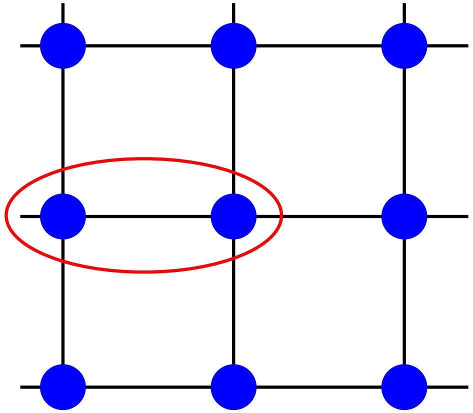

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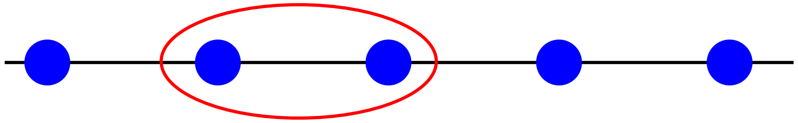

1-Dimensional Local Hamiltonian

Classical Methods:

DMRG (Density Matrix Renormalization Group) [White 1992]

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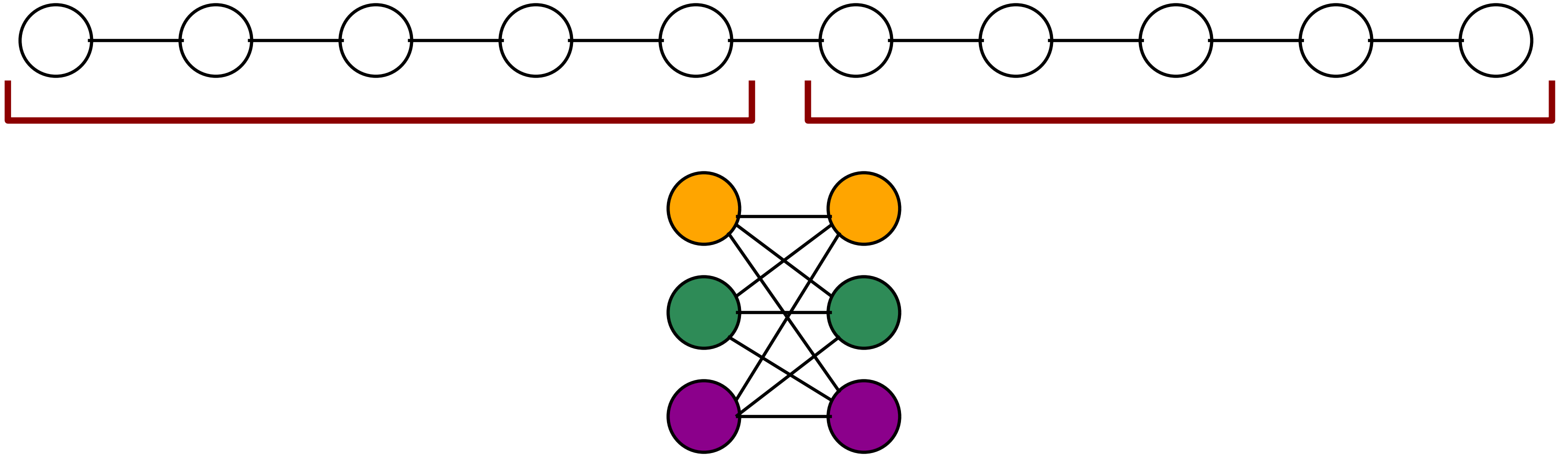

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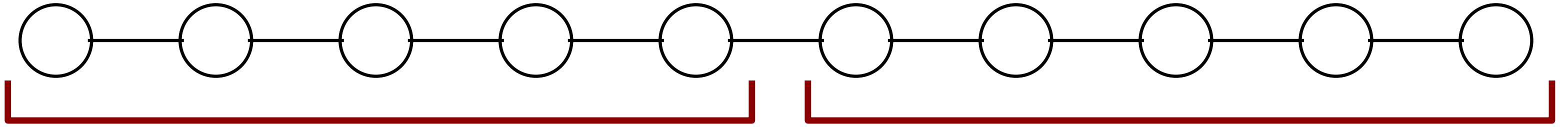

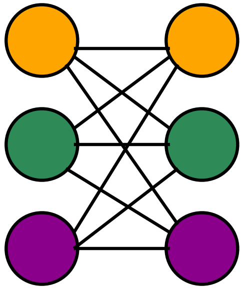

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$$\Rightarrow$$

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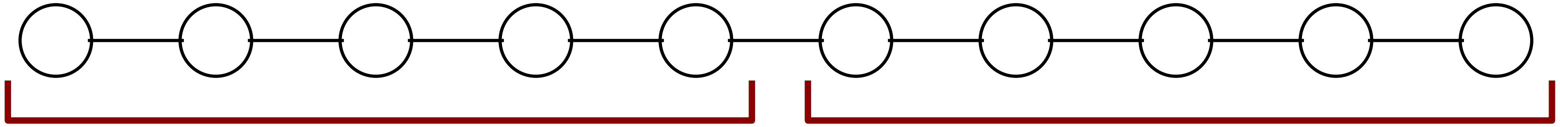

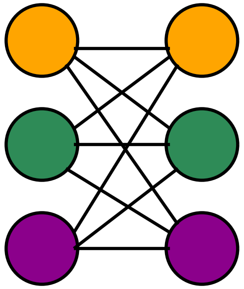

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Why the difference?

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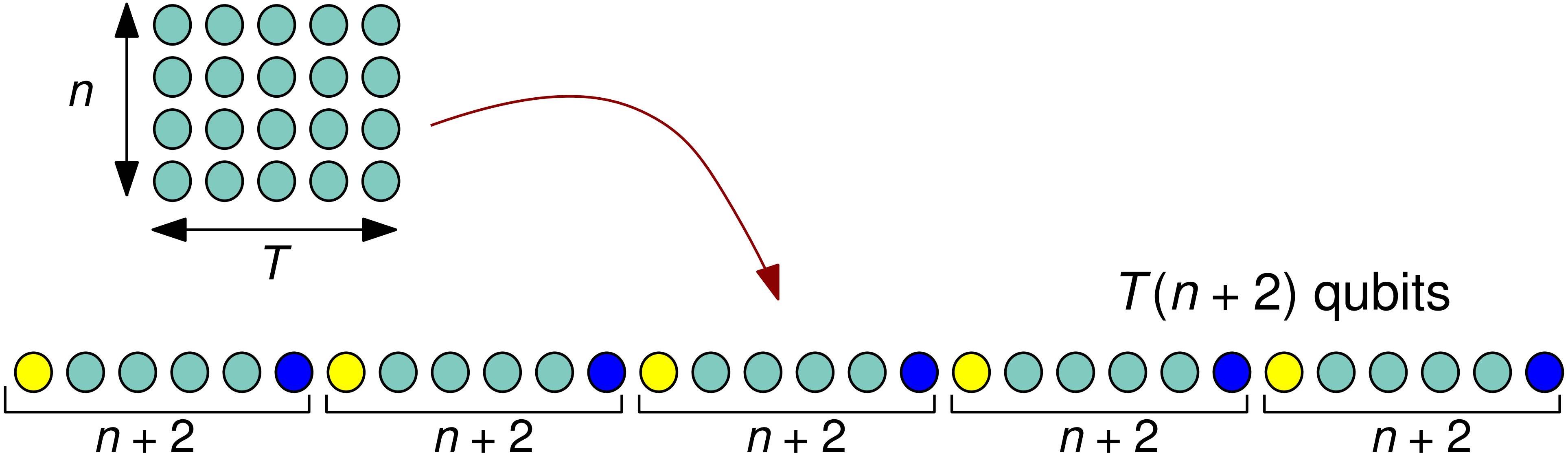
1D Local Hamiltonian



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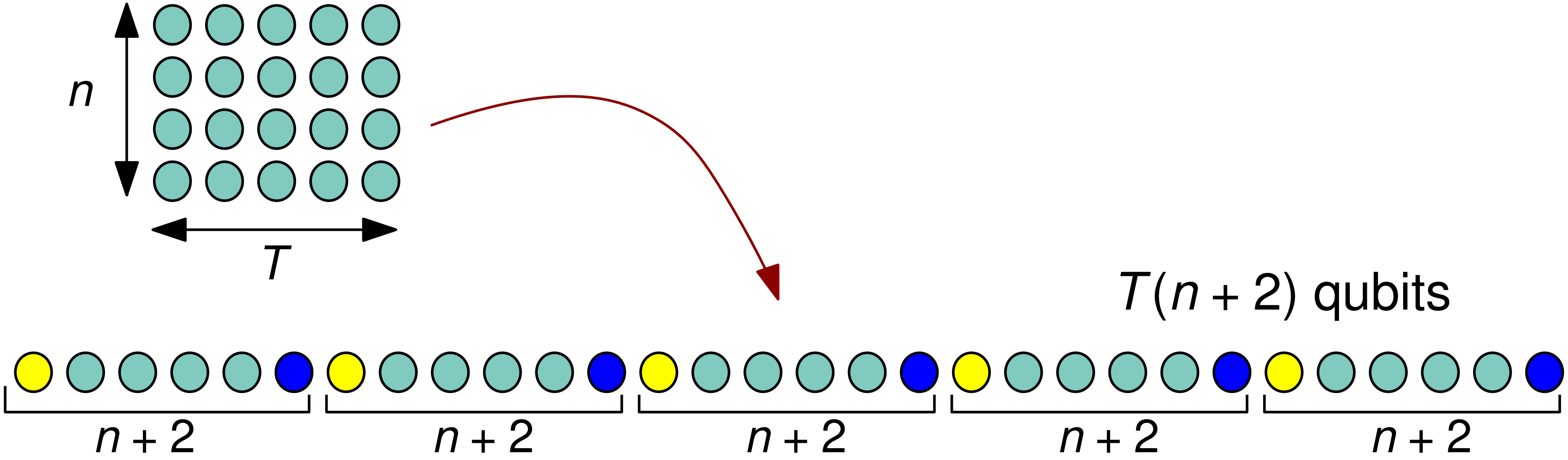

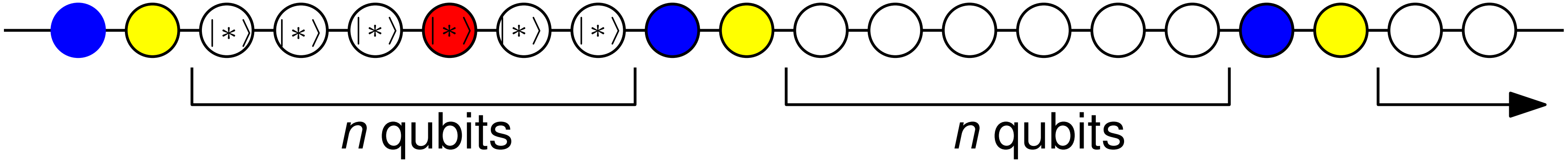

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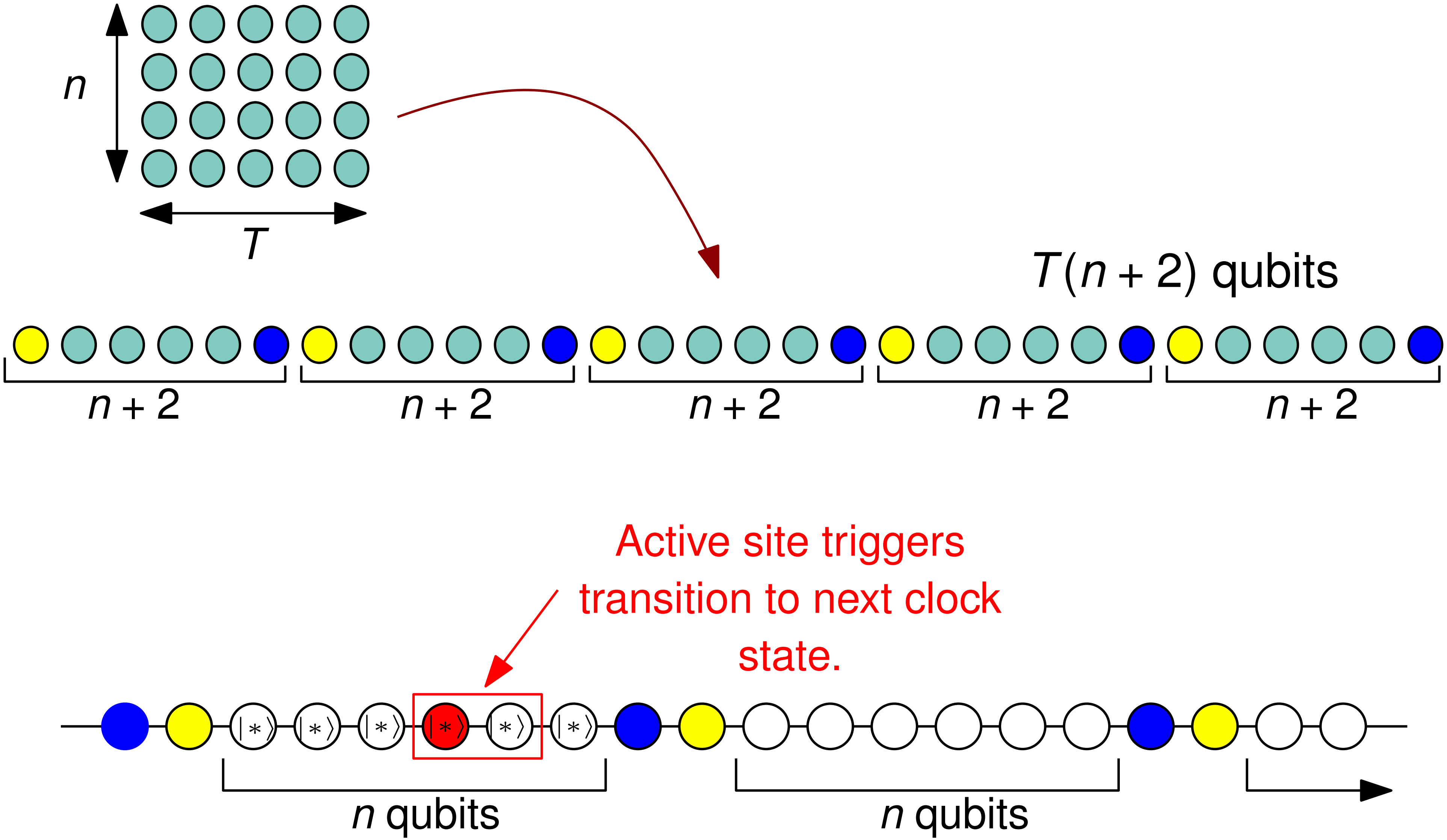
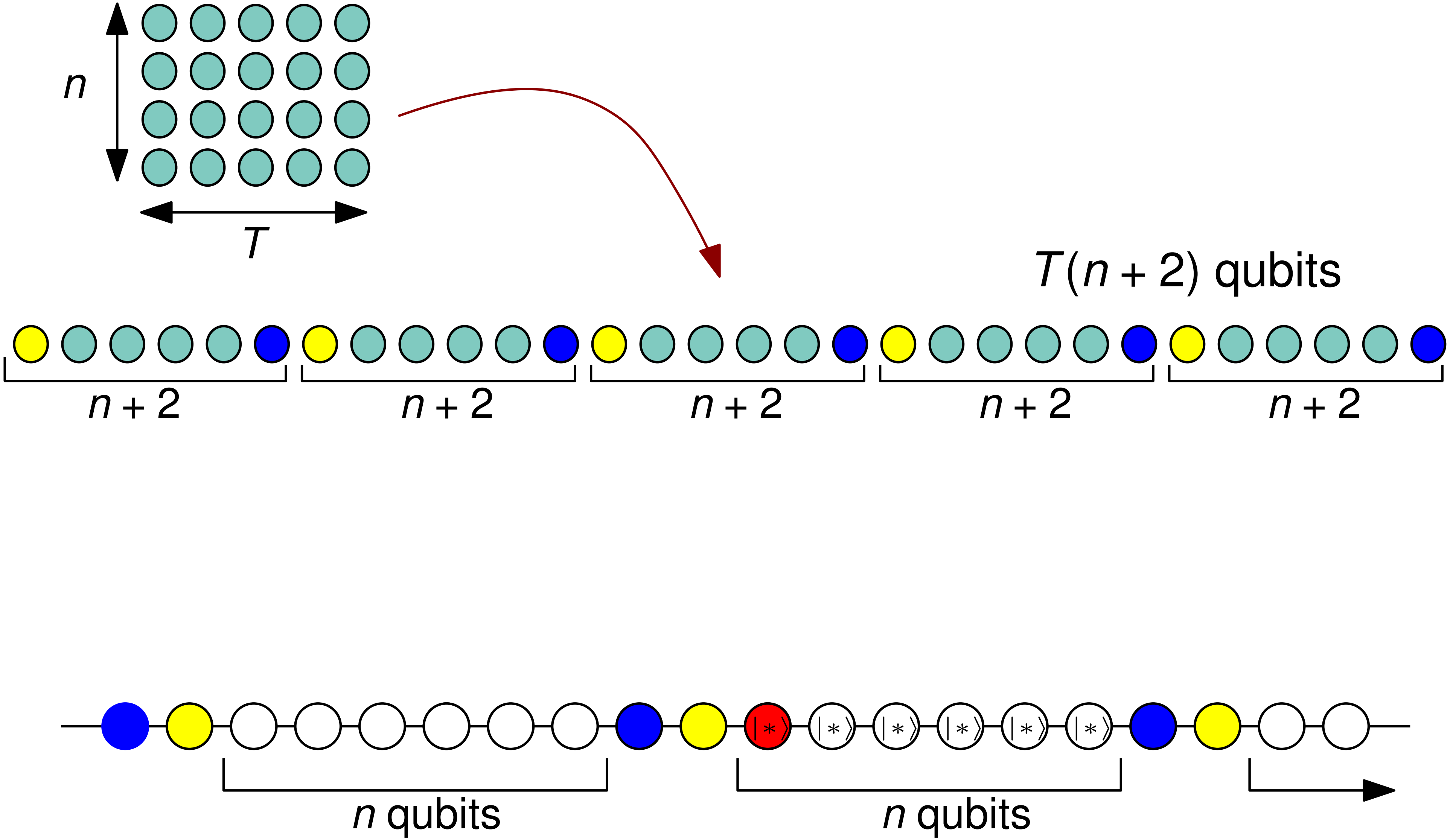


Active site triggers transition to next clock state.

1D Local Hamiltonian



Clairvoyance Lemma

1D clock: can’t eliminate all invalid clock states with a local term

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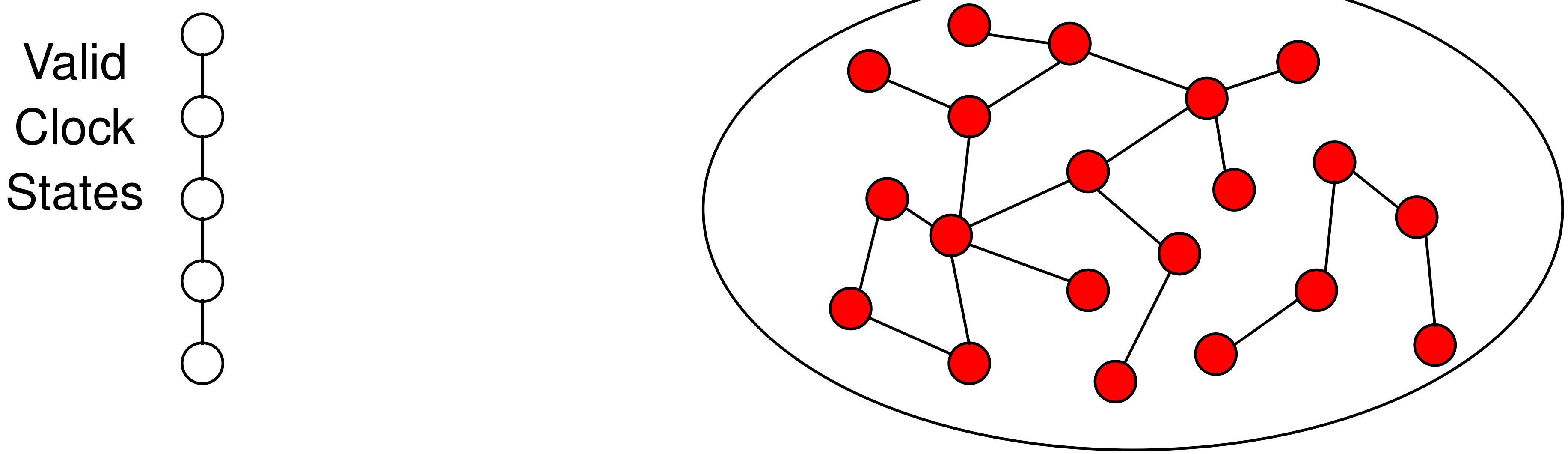

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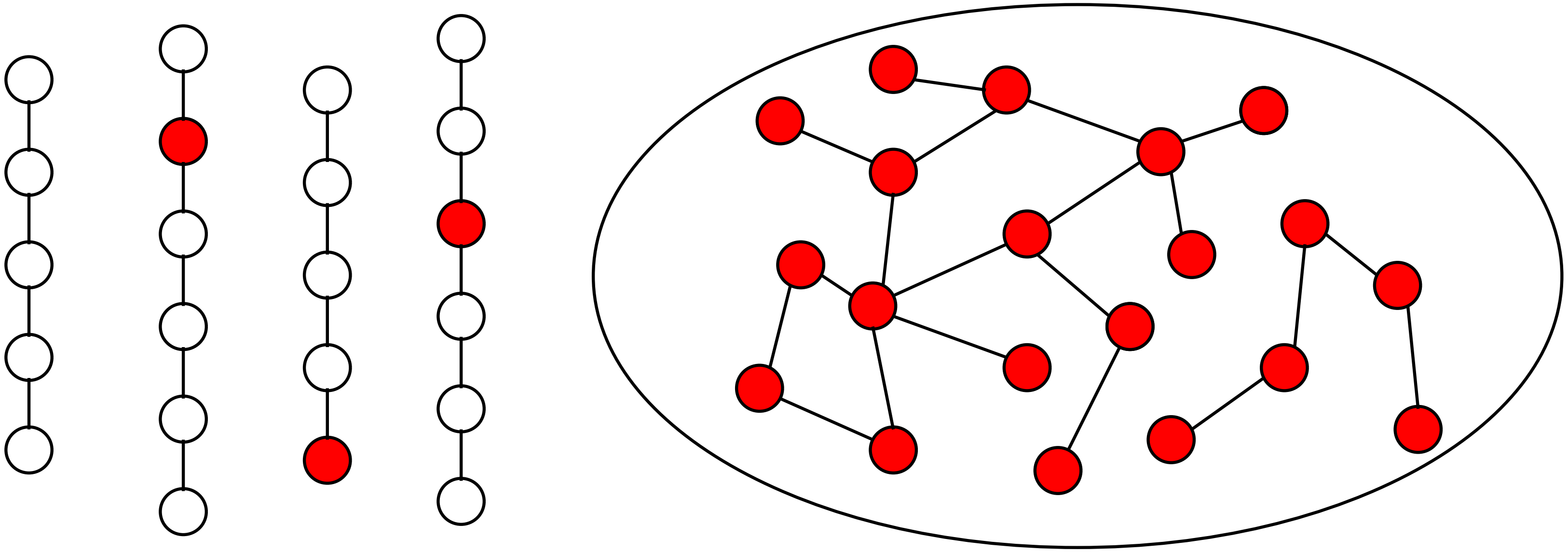

Valid Clock States

Clairvoyance Lemma

Need to lower bound lowest eigenvalue of:

$$\begin{bmatrix} 0 & & & & & \\ & 0 & & & & \\ & & 1 & & & \\ & & & \ddots & & \\ & & & & 0 & \\ & & & & & 0 \end{bmatrix} + \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & & & & & & \\ -\frac{1}{2} & 1 & -\frac{1}{2} & & & & & \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & & & & \\ & & & \cdot & & & & \\ & & & & \cdot & & & \\ & & & & & \cdot & & \\ & & & & -\frac{1}{2} & 1 & -\frac{1}{2} & 0 \\ & & & & & -\frac{1}{2} & 1 & -\frac{1}{2} \\ & & & & & & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

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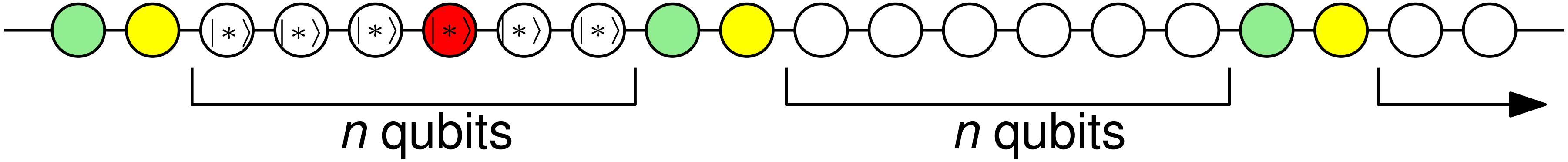
$\Omega(1/K^3)$, where K is the length of the chain

Need to upper bound the length of the ”invalid” chains

1D Local Hamiltonian



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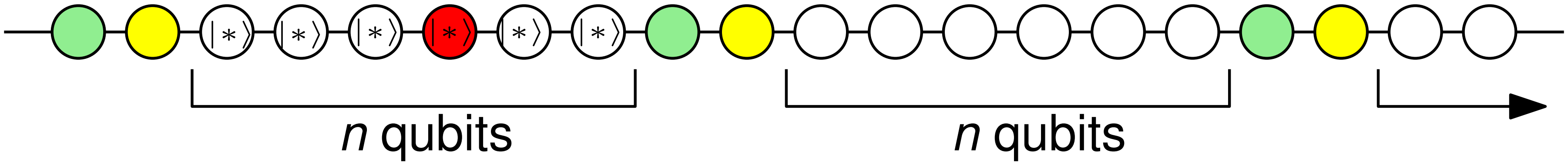

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Terms are position-dependent. (Very non-physical!)

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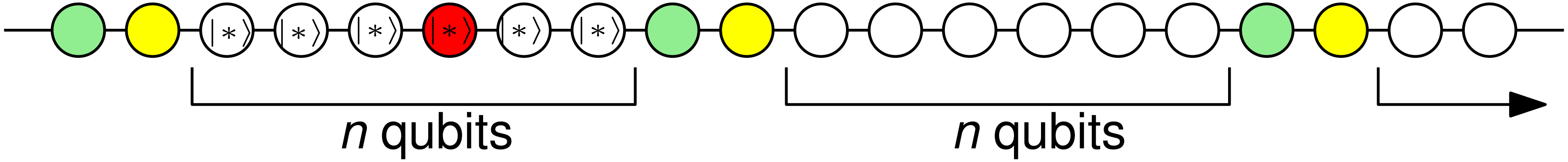

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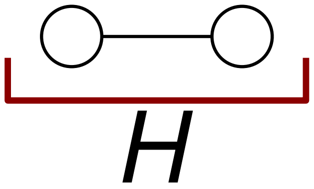
Translational Invariance

How hard is it to find ground states of translationally invariant quantum systems?

Problem parameters:



Hamiltonian term H on two d-dimensional particles

Fixed $2^d \times 2^d$ matrix.

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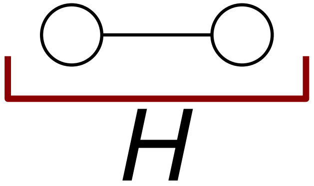

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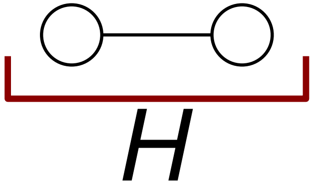

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When H is applied to every pair of neighboring particles in a line of n particles, is the ground energy

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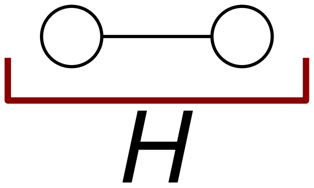

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$\log N$ bits

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$L \in$ QMA if there is a
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If $x \in L \Rightarrow \exists \, |\phi\rangle$
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EXP-time quantum
Turing Machine V

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$$\boxed{\begin{array}{c}\exists|\psi\rangle \text{ such that prob} \\ V(x,|\psi\rangle) \text{ accepts} \geq 2/3\end{array}} \Rightarrow \boxed{\begin{array}{c}H \text{ on } N\text{-particle chain has} \\ \text{ground energy} \leq p(N)\end{array}}$$

Translationally Invariant Local Hamiltonian

1-Dimensional Translationally Invariant Local Hamiltonian is QMA_{EXP}-complete. [Gottesman, Irani, 2010]

To reduce a language L in QMA_{EXP} to **T.I.** Local Hamiltonian:

$L \Rightarrow$ finite term H.

Polynomials p and q
(depend on running time of V)

Description of L
(i.e. the verifier)
needs to be encoded in a
constant-sized H.

Instance $x \Rightarrow N$ size of the system

$\exists|\psi\rangle$ such that prob $V(x, |\psi\rangle)$ accepts $\geq 2/3$ $\Rightarrow$ H on N-particle chain has ground energy $\leq p(N)$

$\forall|\psi\rangle$: $V(x, |\psi\rangle)$ accepts $\leq 1/3$ $\Rightarrow$ H on N-particle chain has ground energy $\geq p(N) + 1/q(N)$

Translationally Invariant Local Hamiltonian

Ground State of H is ”computation state” encoding a *process*:

1) ”Count” the number of particles and write the number in binary on the tape.
2) Use the result of Step 1 as the input to Verifier V

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Contents of the tape are a binary counter.

Start with 0 and continually increment the couner.

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After N steps, $f(N)$ appears on the tape.

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M_{BC} can be made quantum. [Bernstein-Vazirani]

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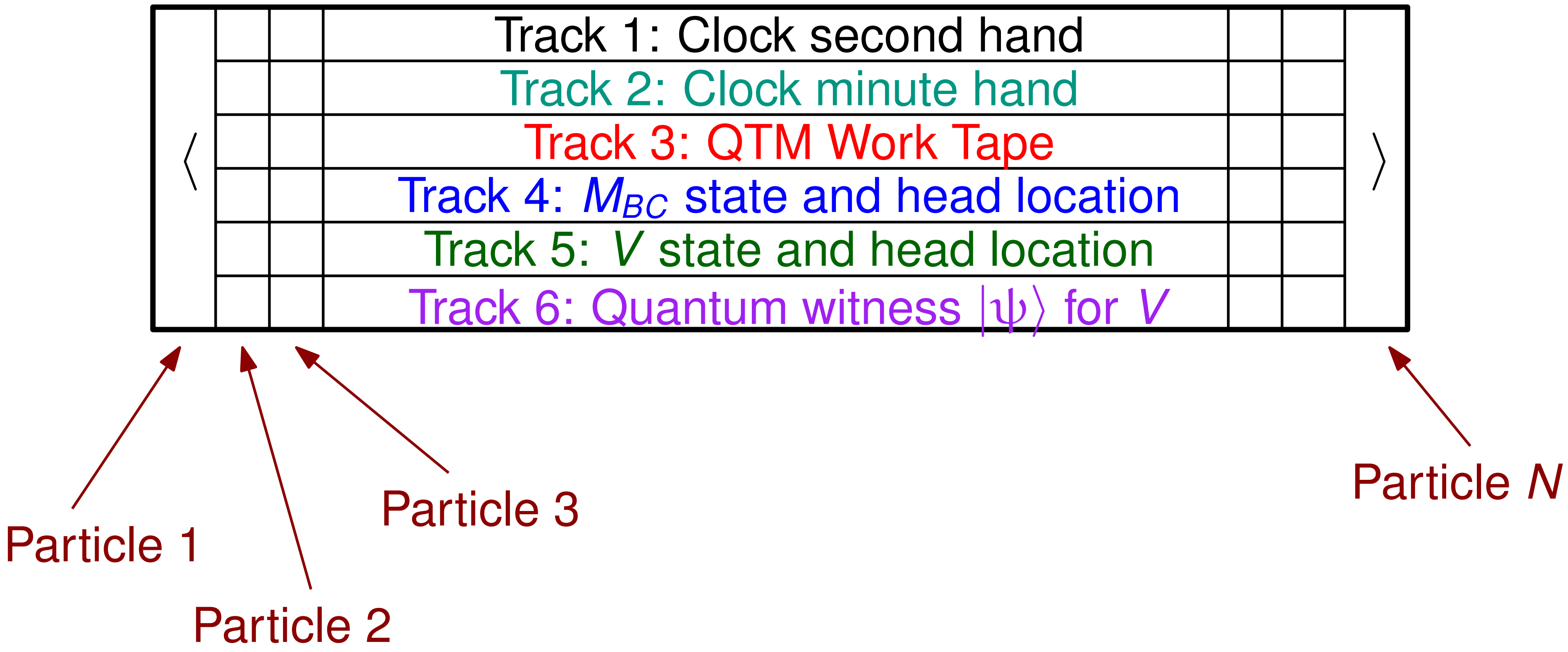
Need a clock that counts the number of particles in the chain twice.

Each ”tick” of the clock triggers a step of a QTM.

Translationally Invariant Local Hamiltonian



$\langle$

Track 1: Clock second hand

Track 2: Clock minute hand

Track 3: QTM Work Tape

Track 4: M_{BC} state and head location

Track 5: V state and head location

Track 6: Quantum witness $|\psi\rangle$ for V

$\rangle$

Particle 1

Particle 2

Particle 3

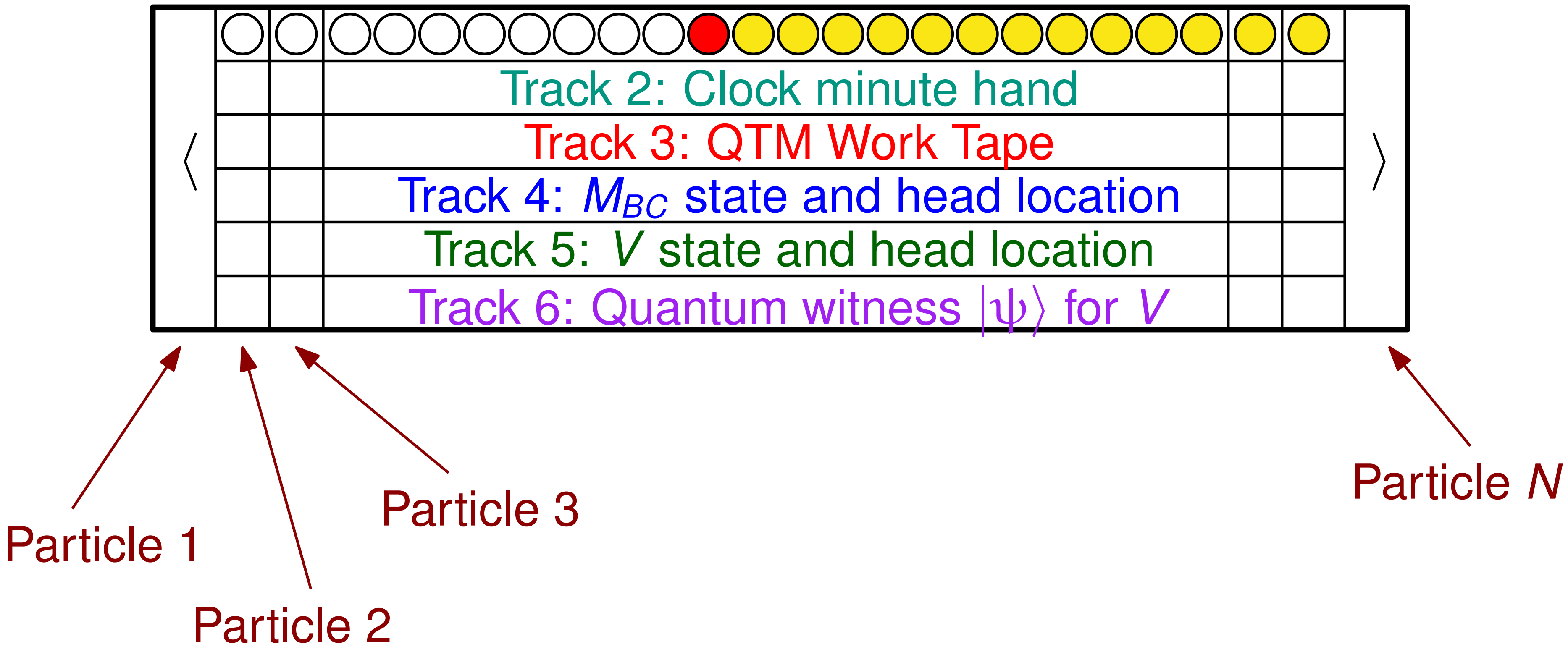
Particle N

Particle states:

6-tuple denoting the state for each track.

OR $\boxed{\langle}$ OR $\boxed{\rangle}$

Translationally Invariant Local Hamiltonian



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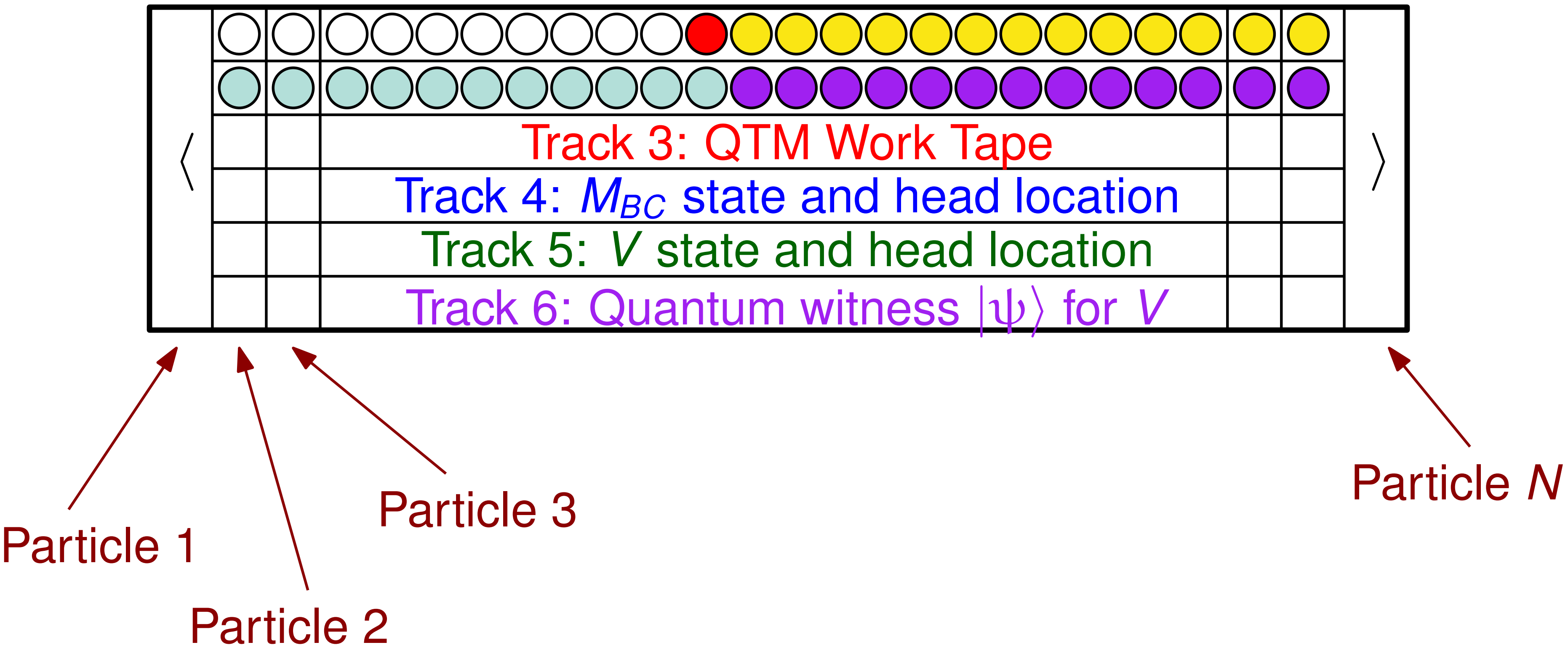

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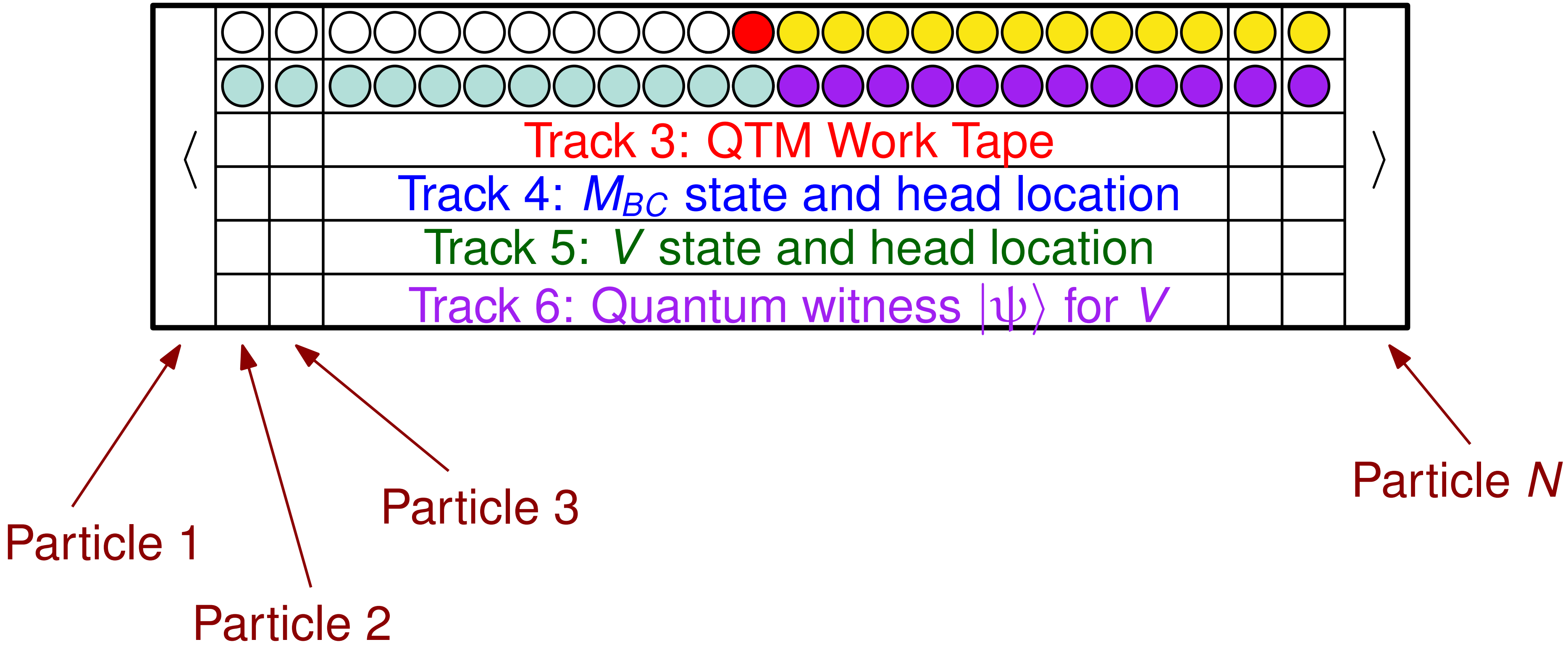

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The Thermodynamic Limit

What is the ground Energy Density (energy per particle) when H is applied to an infinite grid/line?

Input: Hamiltonian term H on two d-dimenaional particles. (n bits)

In 2D: $H = (H_{horiz}, H_{vert})$

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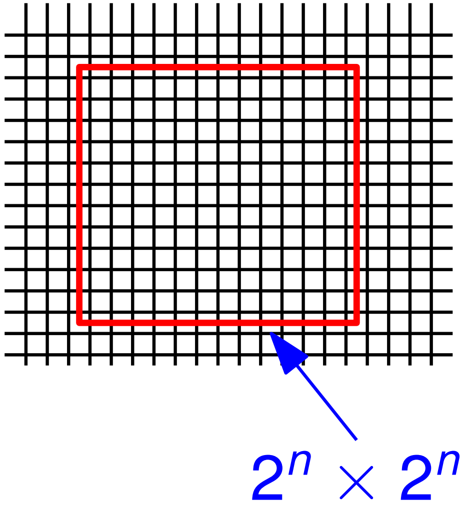

Determining the Energy Density to within the n^{th} bit of precision is QMA_{EXP}-complete.

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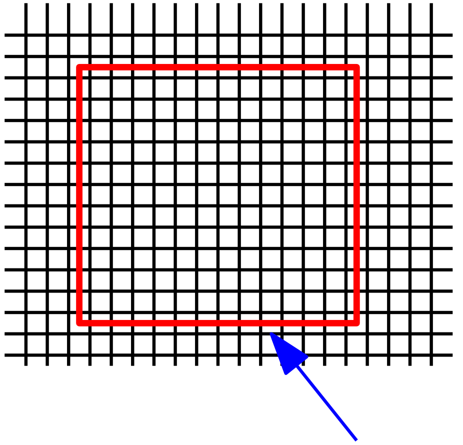

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[Gottesman, Irani, 2010]

Determining the Spectral Gap of H is undecidable.

Is $\Delta \geq 1$ or is H gapless?

[Cubitt, Perez-Garcia, Wolf *Nature*, 2015] ← 2D

[Bausch, Cubitt, Lucia, Perez-Garcia, 2018] ← 1D

Energy Density $\propto$ Spectral Gap

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H_L is the Hamiltonian H appied to an $L \times L$ grid.

Energy Density of H is: $$E(H) = \lim_{L \to \infty} \frac{\lambda_0(H_L)}{L^2}$$

Given H determine if:

$$E(H) \geq c > 0$$

OR if $E(H)$ approaches 0 from below.

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$$\left.\begin{array}{r} E(\hat{H}) = 0 \\ \lambda_0(\hat{H}_L) < 0 \end{array}\right] \quad \Rightarrow \quad H' \text{ is gapless}$$

Energy Density $\propto$ Spectral Gap

Let H_d be a gapless translationally invariant Hamiltonian.

$$\text{Spec(H')} = \{0\} \cup \underbrace{S}_{\geq 1} \cup \{\text{Spec}(\hat{H}) + \text{Spec}(H_d)\}$$

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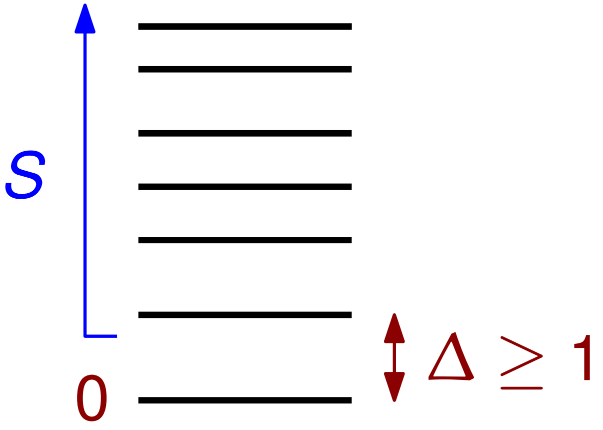

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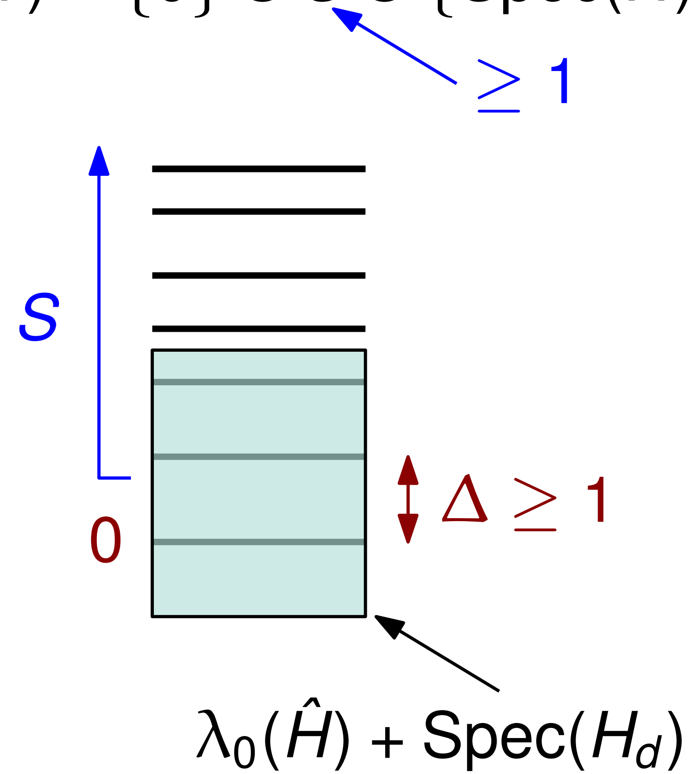

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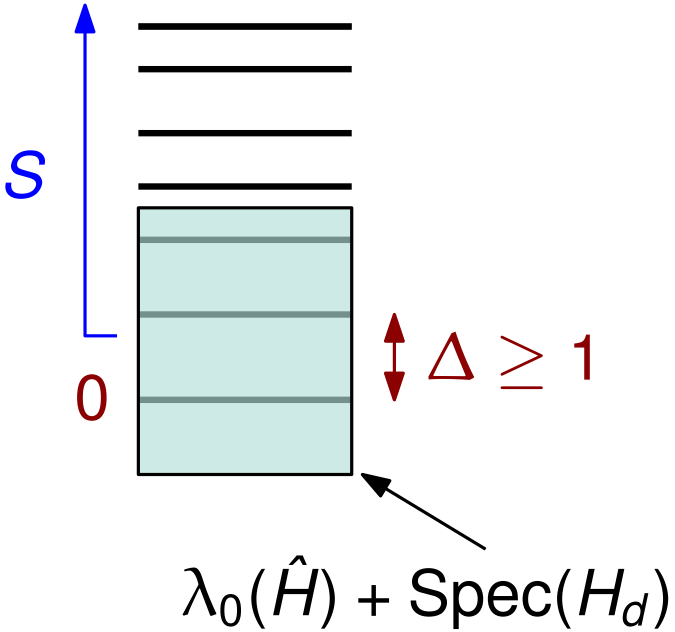

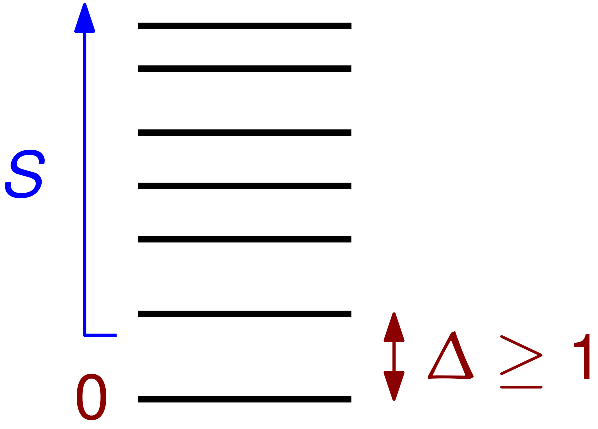

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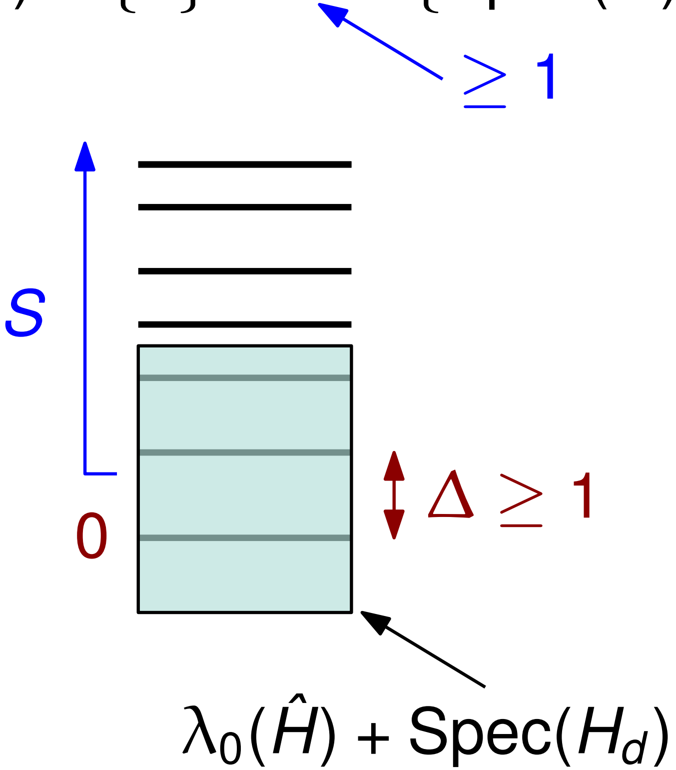

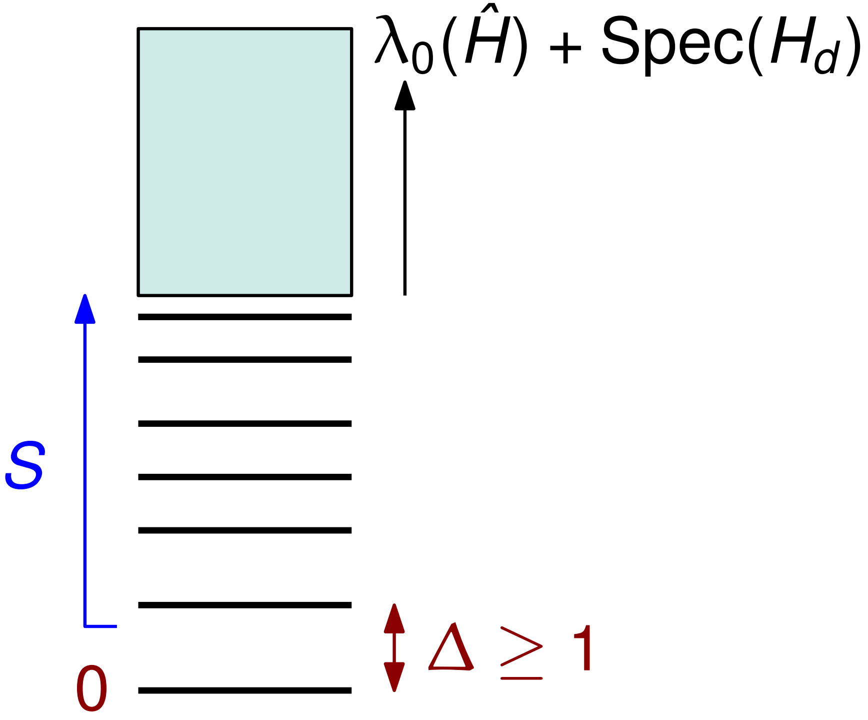

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$$\mathcal{H}' = |0\rangle \oplus (\mathcal{H}_d \otimes \hat{\mathcal{H}})$$

$$H = |0\rangle\langle 0| \otimes (I - |0\rangle\langle 0|) + (I - |0\rangle\langle 0|) \otimes |0\rangle\langle 0|$$
$$+ \; H_d \otimes I \; + \; I \otimes \hat{H}$$

Particle 1

Particle 2

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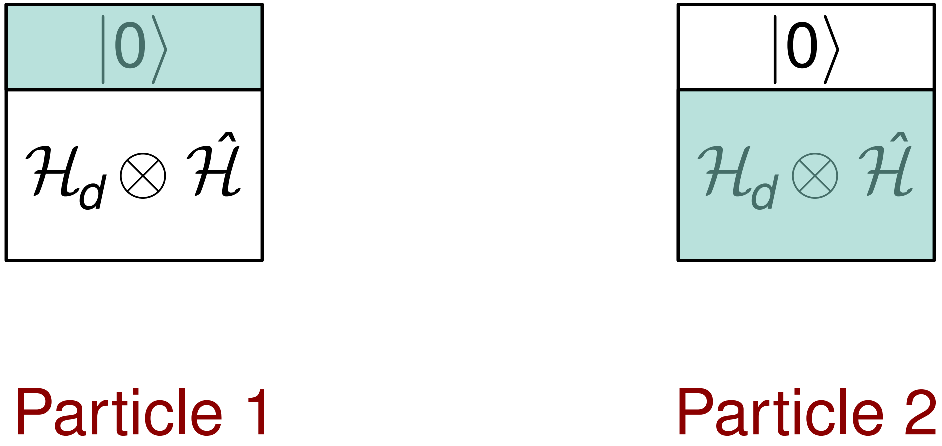

Spectrum $S \geq 1$

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$|0\rangle$ | $\mathcal{H}_d \otimes \hat{\mathcal{H}}$

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$|00\rangle$ is a 0 energy state.

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$$\{\mathrm{Spec}(\hat{H}) + \mathrm{Spec}(H_d)\}$$

Energy Density is Undecidable

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2D Wang Tiles

Set of tiles: $T = \{$🟥 🟩 🟧 🟪 $\ldots\}$

2D Wang Tiles

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Two cost functions:

$C_{horiz}($ 🟪 , 🟧 $) = d_1$

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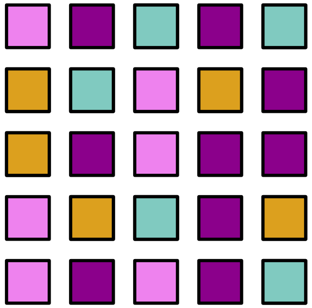
What's the minimum cost tiling of an $N \times N$ grid?



Or average cost per square of the infinite grid? [Wang 1961]

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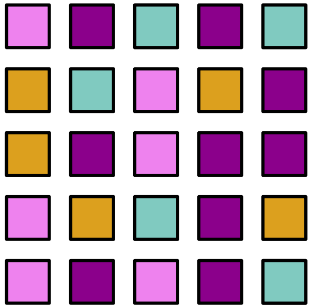

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Tiling is a (classical) special case of Local Hamiltonian:

$d_1 \left|\text{🟥🟧}\right\rangle\left\langle\text{🟥🟧}\right|$

$d_2 \left|\begin{matrix}\text{🟦}\\\text{🟥}\end{matrix}\right\rangle\left\langle\begin{matrix}\text{🟦}\\\text{🟥}\end{matrix}\right|$

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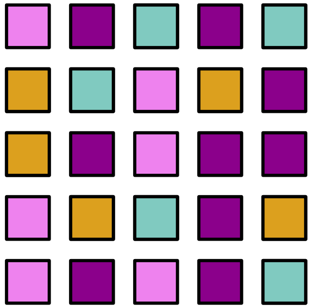

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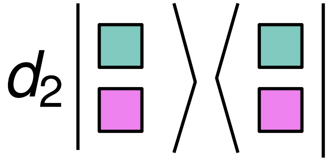

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Robinson Tiling:

Minimum cost tiling of the infinite grid is aperiodic.

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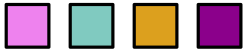
Set of tiles: $T = \{$  $\ldots\}$

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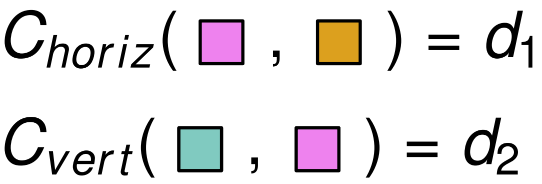

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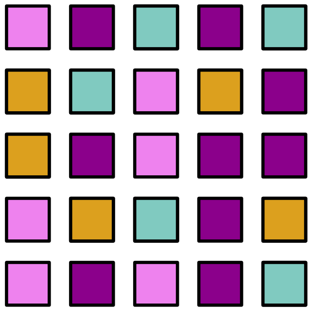

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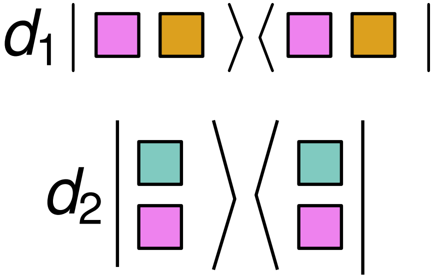


Robinson Tiling:

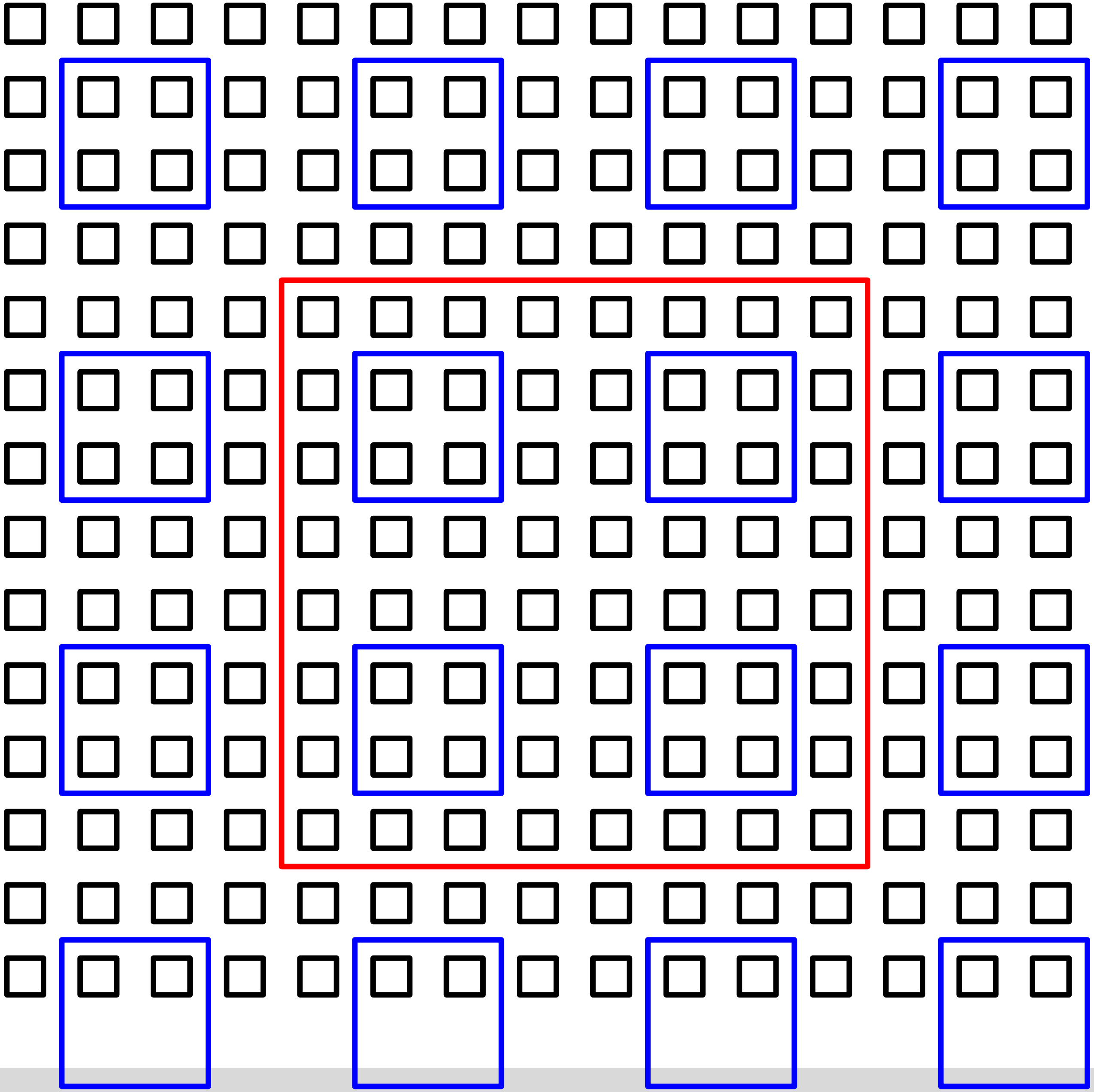
Minimum cost tiling of the infinite grid is aperiodic.

For every k:

- squares of size $4^k \times 4^k$
- frequency $\sim 1/4^k$

[Robinson 1971]

Robinson Tiling



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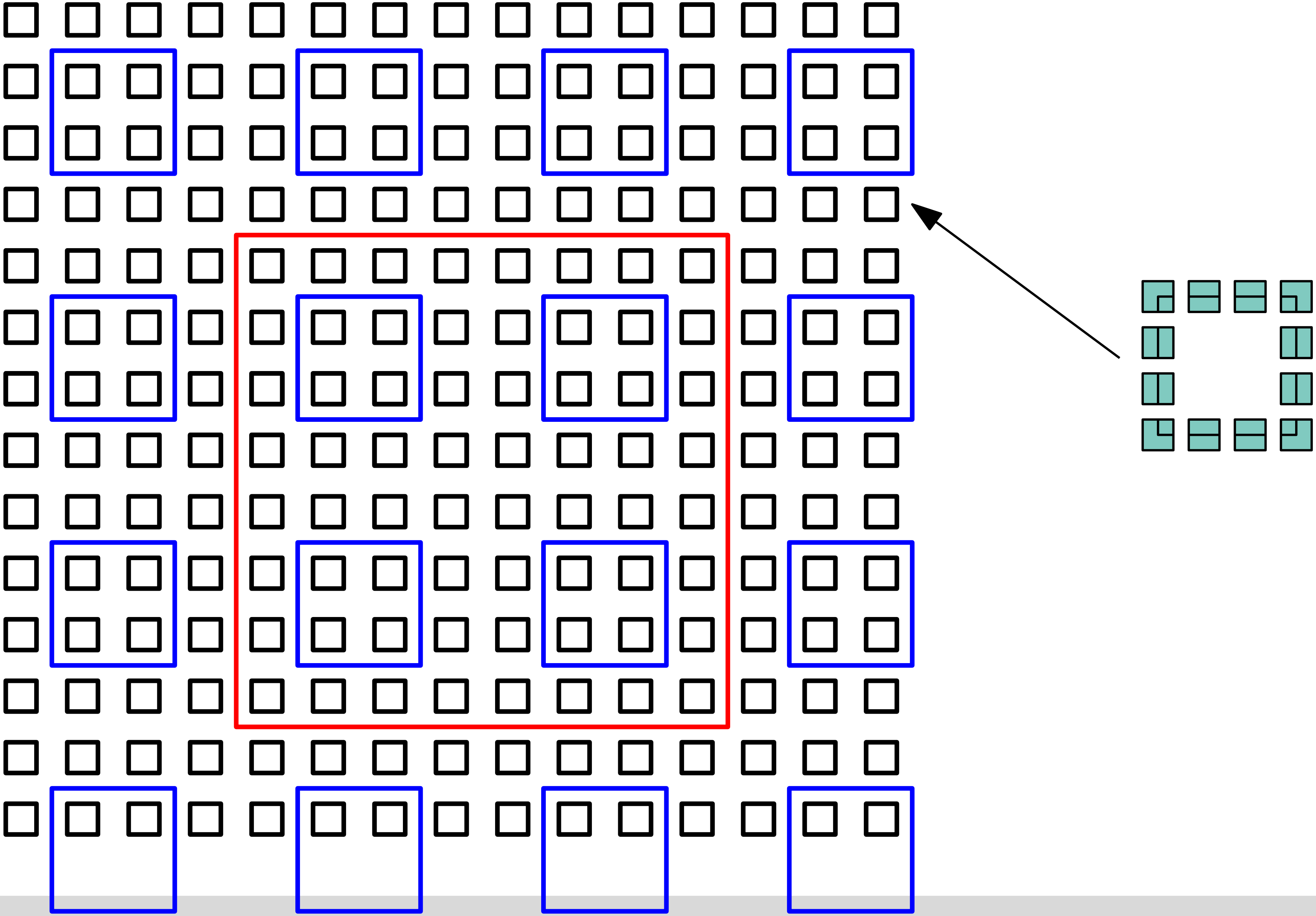
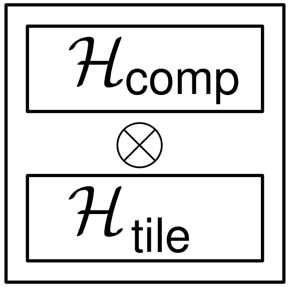


Two Layers of the Construction

Particle Space: $\mathcal{H}_{\text{comp}} \otimes \mathcal{H}_{\text{tile}}$



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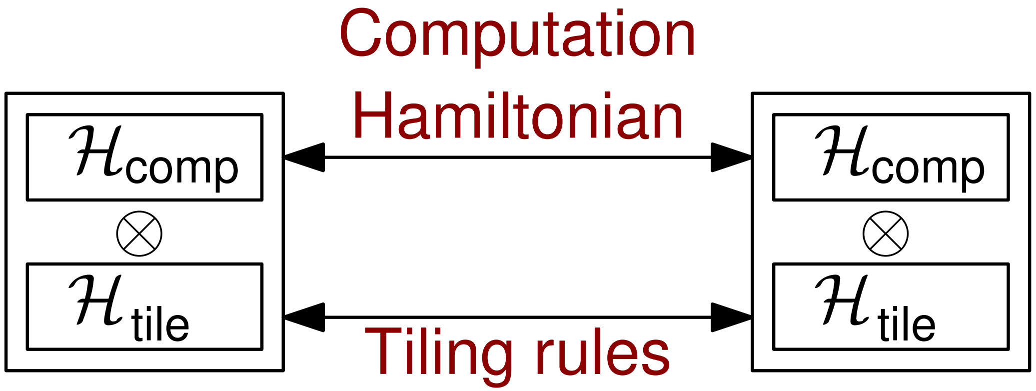

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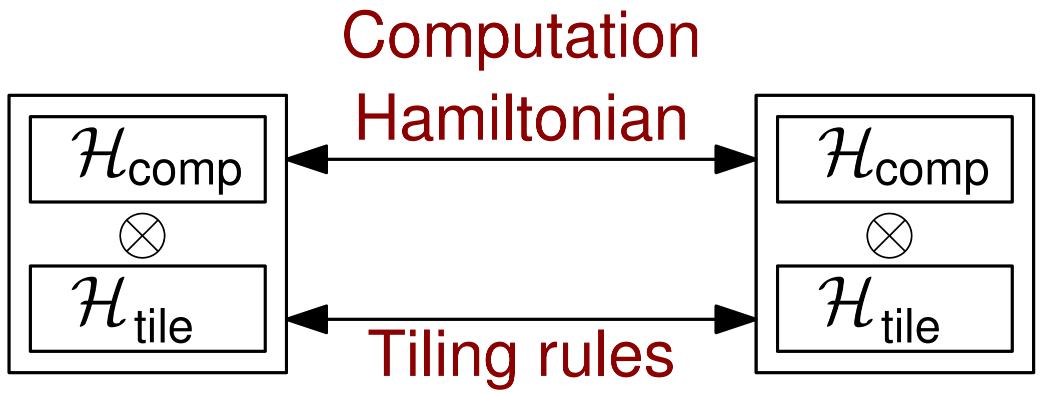

Computation Hamiltonian

$\mathcal{H}_{\text{comp}}$ $\otimes$ $\mathcal{H}_{\text{tile}}$

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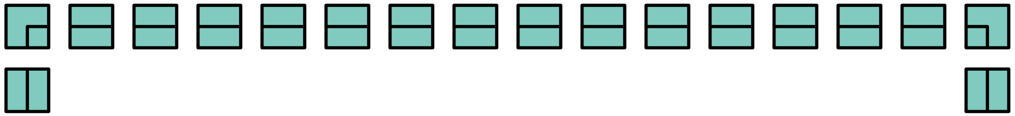
Tiling rules



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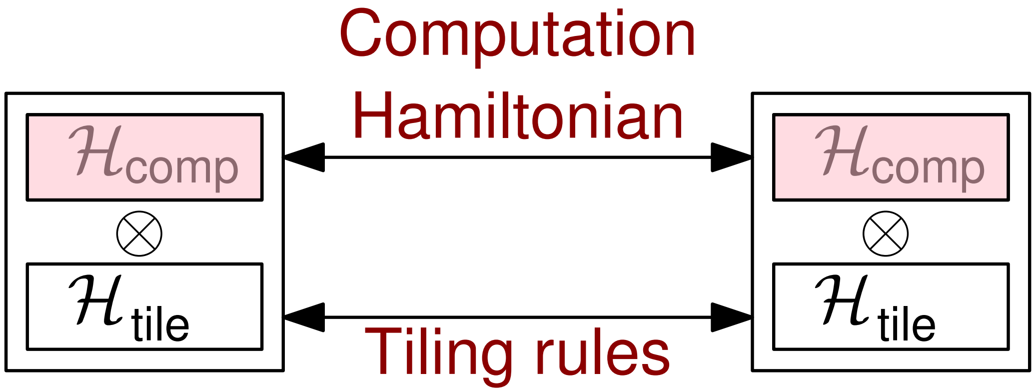

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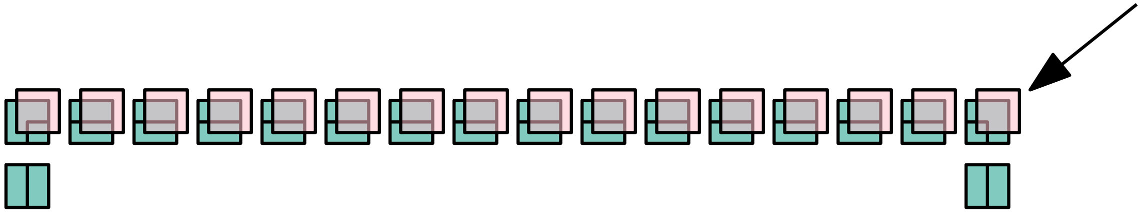

Computation Hamiltonian:

Ground state is a history state of a computational process.

The Computational Process Encoded in $H(n)$

Computation Hamiltonian: $H(n)$

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1) Write n in binary on the QTM tape

Phase estimation on the quantum gate: $\begin{bmatrix} 1 & 0 \\ 0 & e^{2\pi i \phi} \end{bmatrix}$

$\phi = n/2^{|n|}$ rational number whose binary expansion is n.

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4^k is the dimension of the square ”hosting” the computation.

Use the clock from Gottesman-I to count the number of steps.

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Use the clock from Gottesman-I to count the number of steps.

3) Add an energy charge for halting

$|q_{halt}\rangle\langle q_{halt}|$

The Computational Process Encoded in $H(n)$

Computation Hamiltonian: $H(n)$

1) Write n in binary on the QTM tape

Phase estimation on the quantum gate: $\begin{bmatrix} 1 & 0 \\ 0 & e^{2\pi i \phi} \end{bmatrix}$

$\phi = n/2^{|n|}$ rational number whose binary expansion is n.

2) Simulate Universal TM U on input n for 4^k steps.

4^k is the dimension of the square ”hosting” the computation.

Use the clock from Gottesman-I to count the number of steps.

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$|q_{halt}\rangle\langle q_{halt}|$

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The Computational Process Encoded in $H(n)$

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If the computation halts...

Number of step of H_{prop}

$T = \text{poly}(n, 4^k)$

Energy per square $\Omega(1/T^3)$

Energy density $\Omega(1/(4^k T^3))$

Energy Density is Undecidable

Reduction: $n \Rightarrow H(n)$

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Complexity in the thermodynamic limit:?

How stable are hard Translationally Invariant instances with respect to some measure on the Hamiltonian terms?

More ”natural” Hamiltonians?

Bose-Hubbard Model is QMA-Complete [Childs, Gosset Webb 2013]

Input: interaction graph $G = (V, E)$

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Equivalent to:

$$\sum_{(i,j)\in E, i\neq j} \frac{\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j}{2} + \sum_{(i,i)\in E} \frac{1 - \sigma_z^i}{2}$$

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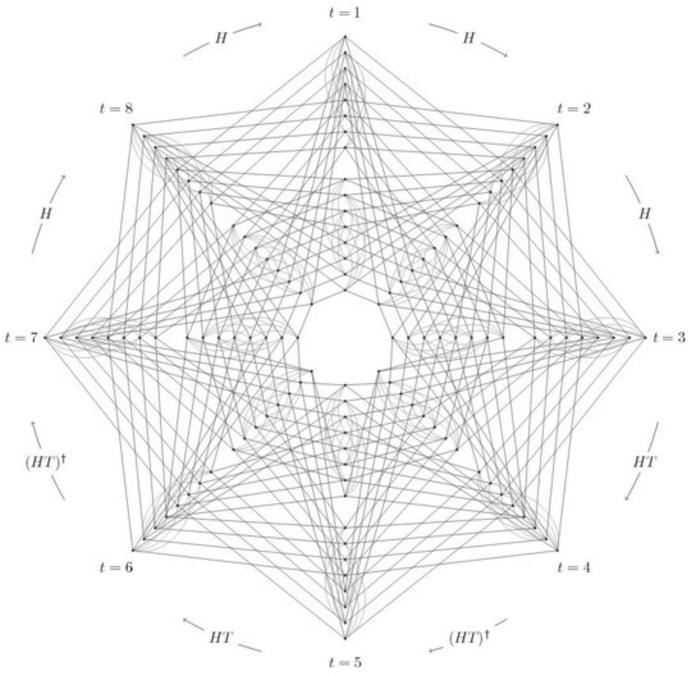
Self-loops

Input graph has no self-loops [Childs, Gosset Webb 2015]

Bose-Hubbard and X-Y Model

Input graph encodes the computation of a quantum circuit.



(Graph image from CGW)

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New directions:

Variations on Bose-Hubbard

$t_{hop} < 0$ and/or $J < 0$.

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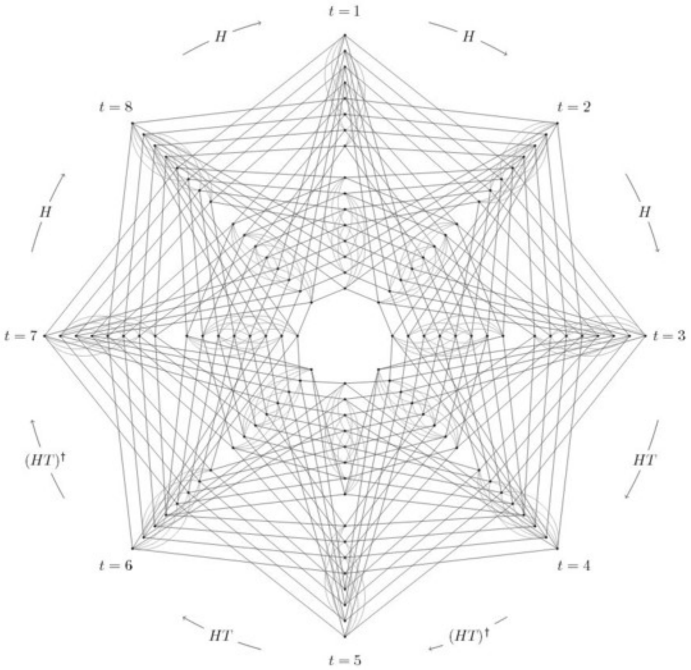
[Bravyi, DiVincenzo, Oliveira, Terhal 2007]



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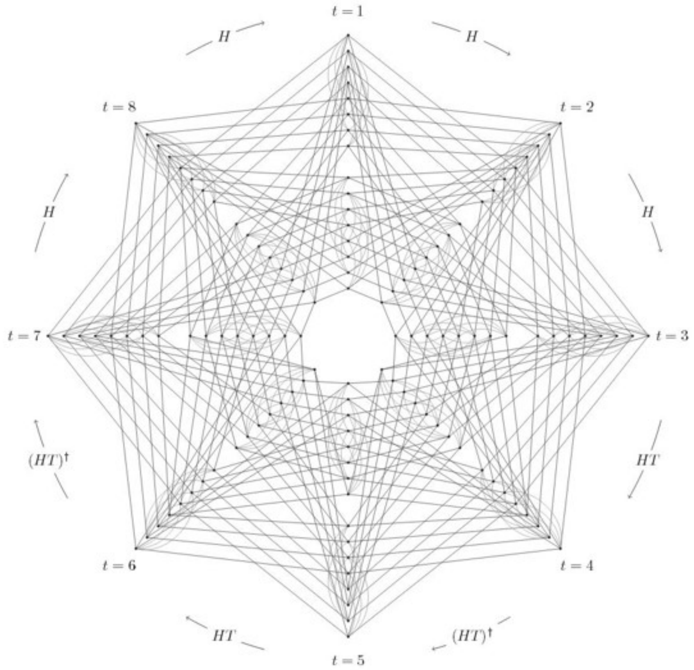

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Simpler Graphs

Planar?

Subset of a grid?

$N \times N$ grid?

Classifying 2-Qubit Terms [Cubitt, Montanaro 2016]

When is a *k*-qubit Hamiltonian term useful for building gadets?

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If U is a 1-qudit unitary
Then U *locally diaginalizes* S if

$$U^{\otimes k} H (U^{\dagger})^{\otimes k}$$

is diagonal for every $H \in S$

Perturbation Gadgets

[Kempe Kitaev Regev 05] 2-local Hamiltonian is QMA complete

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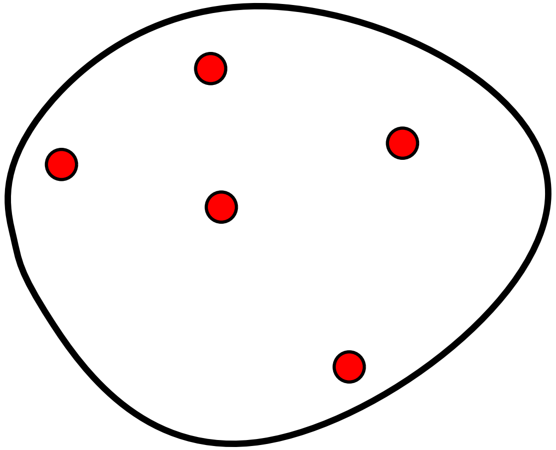

5-local term *H*

Perturbation Gadgets

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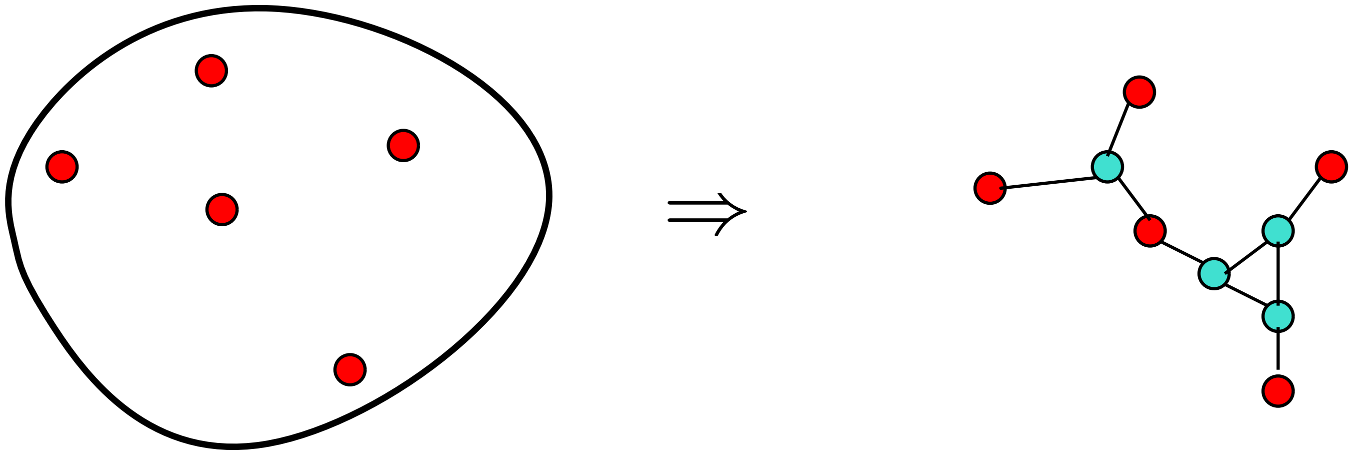

5-local term H $\Rightarrow$ Sum of 2-local terms H'

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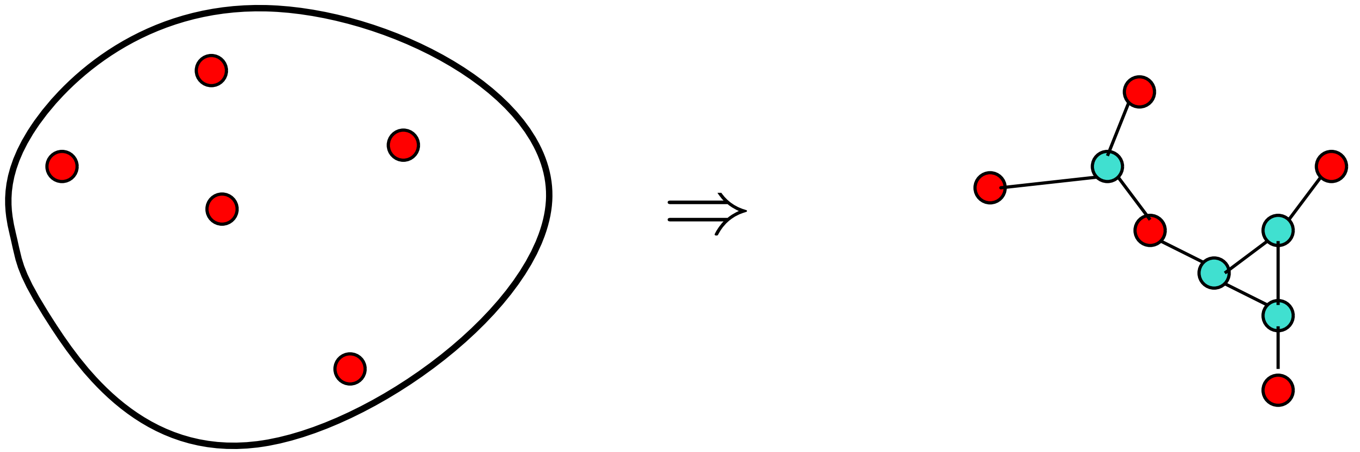

5-local term H

Sum of
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$$H \quad \approx \quad H'\big|_{\leq \Delta}$$

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Un-physical aspects:

1) Negative and positive coefficients.

2) Arbitrary interaction graph.

3) Large (poly in system size) coefficients.

Classifying 2-Qubit Terms [Piddock, Montanaro 2015]

$H = \alpha XX + \beta YY + \gamma ZZ$

positive coeffients

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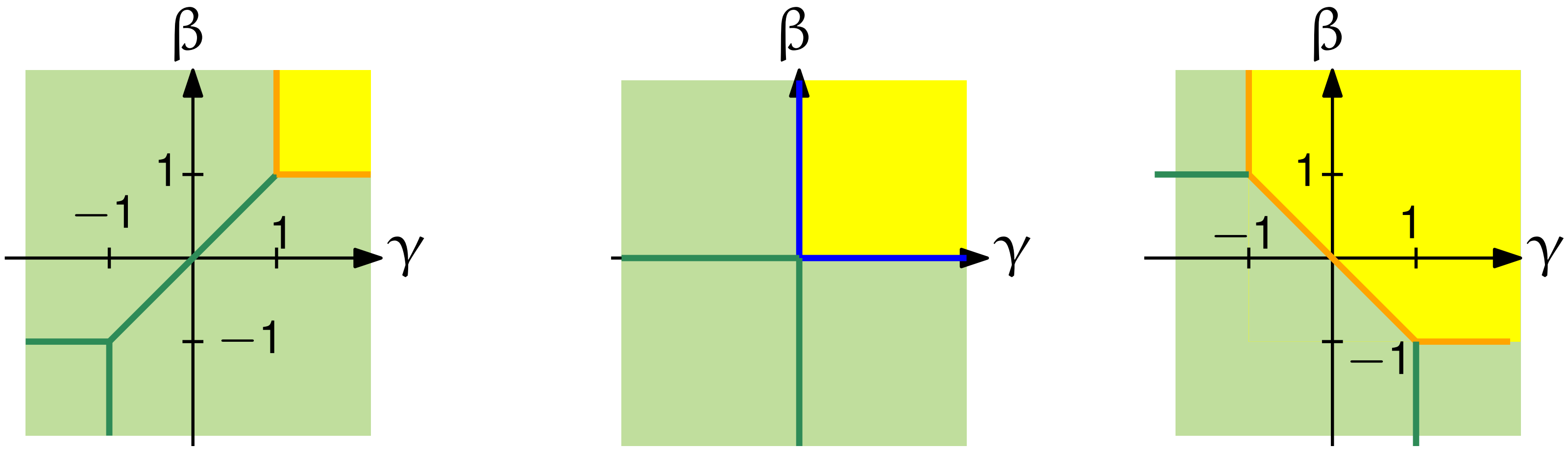

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NP-complete

P

🟩 StoqMA

StoqMA-complete

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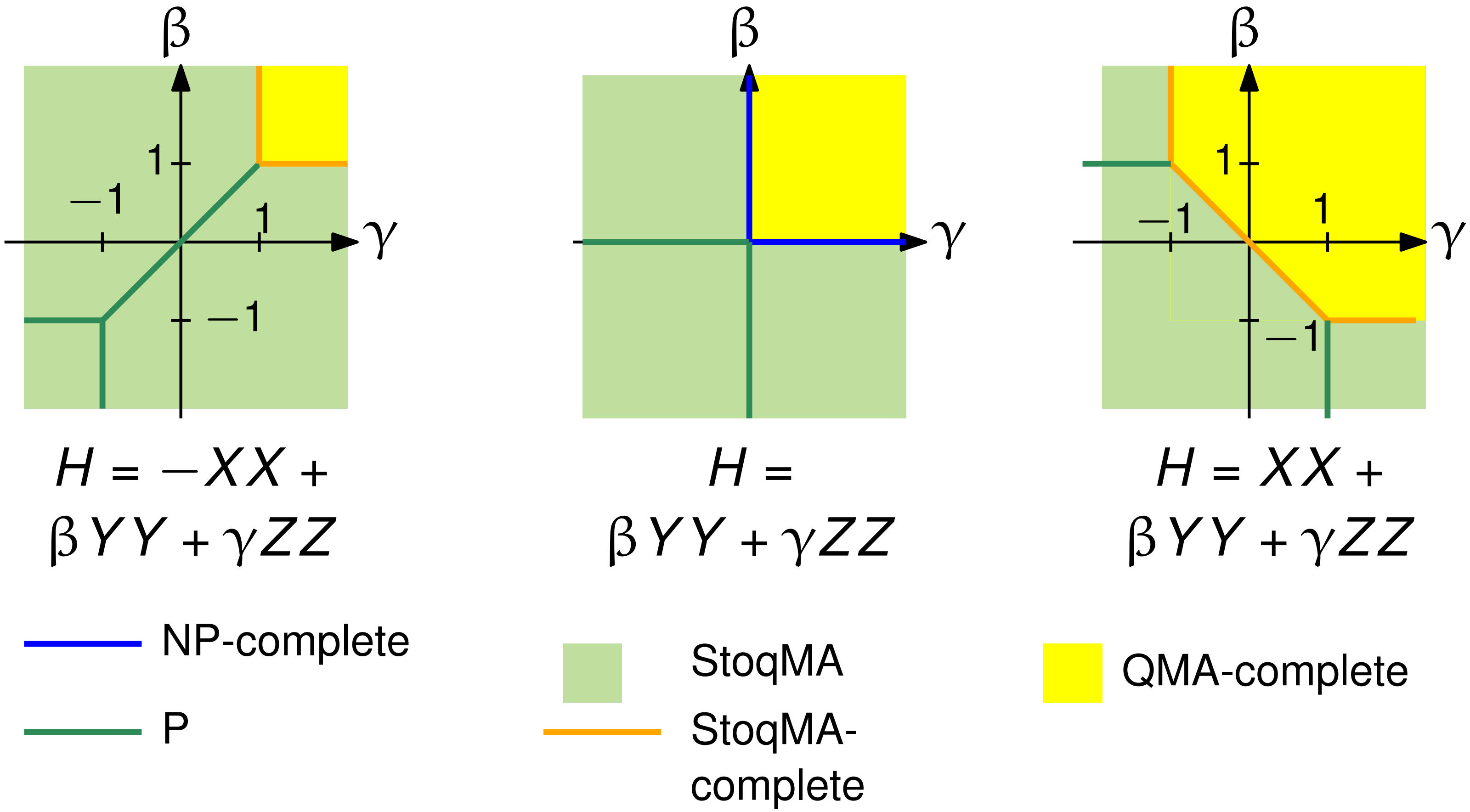

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Important special cases: $XX + YY + ZZ$ and $XX + YY$

Classifying 2-Qubit Terms

[Piddock, Montanaro 2015]

$H = \sum M_{ij} \sigma_i \otimes \sigma_j +$ 1-qubit terms.

Pauli rank of H = rank(M)

Theorem: If the Pauli rank of H is at least 2 and the 2-local part of H is not proportional to $XX + YY + ZZ$, then $\{H\}^+$-Hamiltonian is QMA-complete on the 2D grid.

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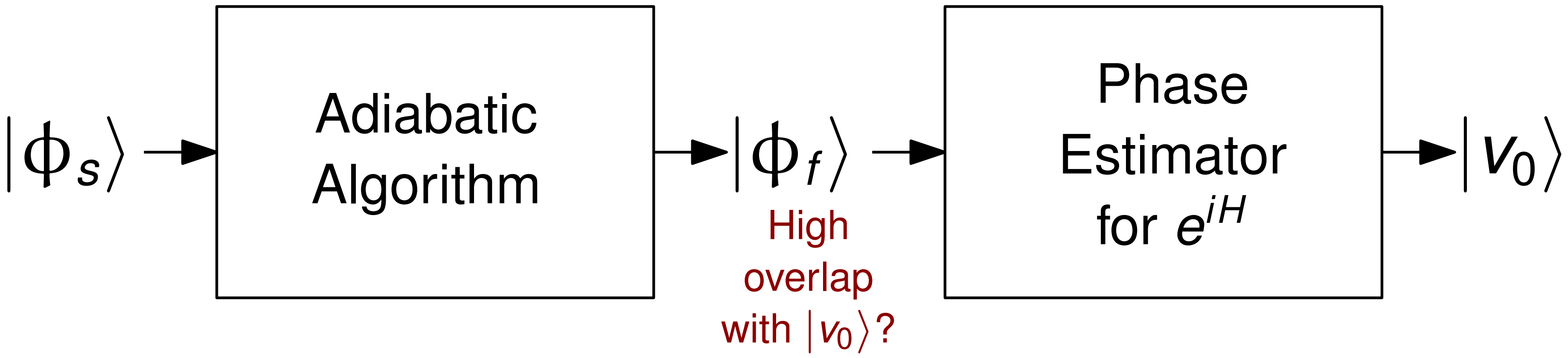
$$\text{P} \subseteq \text{NP} \subseteq \text{StoqMA} \subseteq \text{QMA}$$

Ground State Preparation (Hybrid)



$|\phi_s\rangle \rightarrow$ Adiabatic Algorithm $\rightarrow |\phi_f\rangle \rightarrow$ Phase Estimator for e^{iH} $\rightarrow |v_0\rangle$

High overlap with $|v_0\rangle$?

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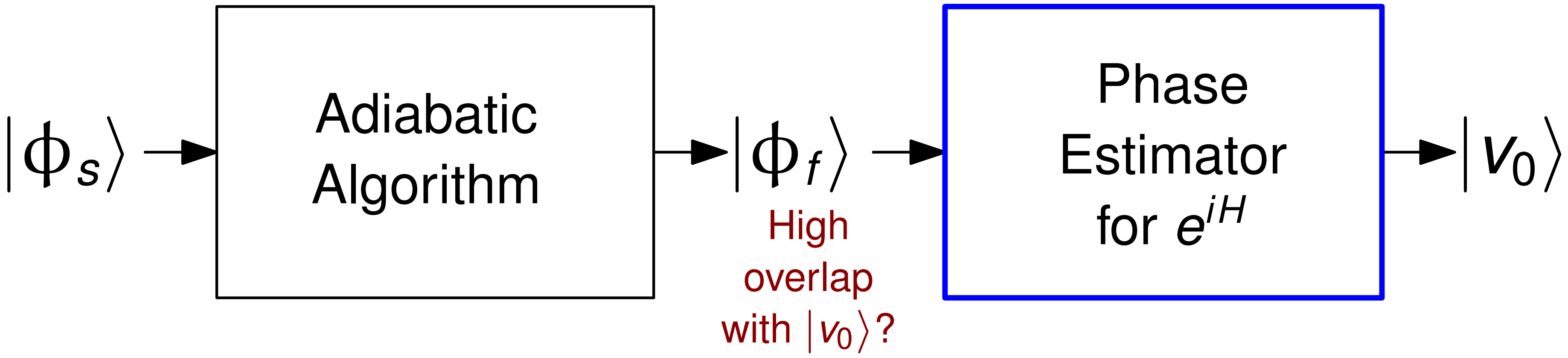

Can be combined with Amplitude Amplification [Grover 1996]

To improve dependence on $|\langle v_0|\phi_f\rangle|$ from $1/|\langle v_0|\phi_f\rangle|^2$ to $1/|\langle v_0|\phi_f\rangle|$.

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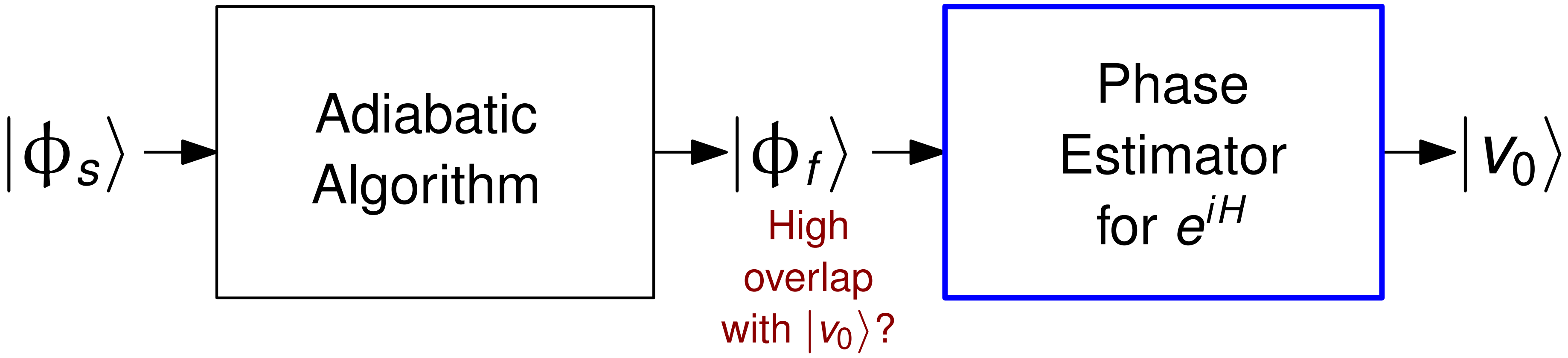

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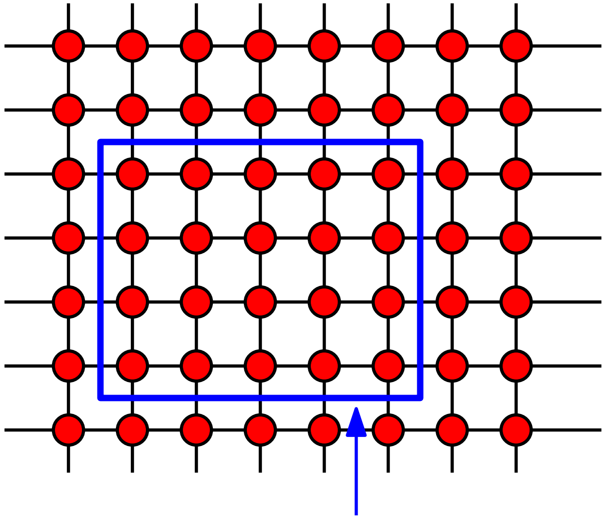
Also concerned about:
Number of qubits used
Dependence on spectral gap, required accuracy, etc.

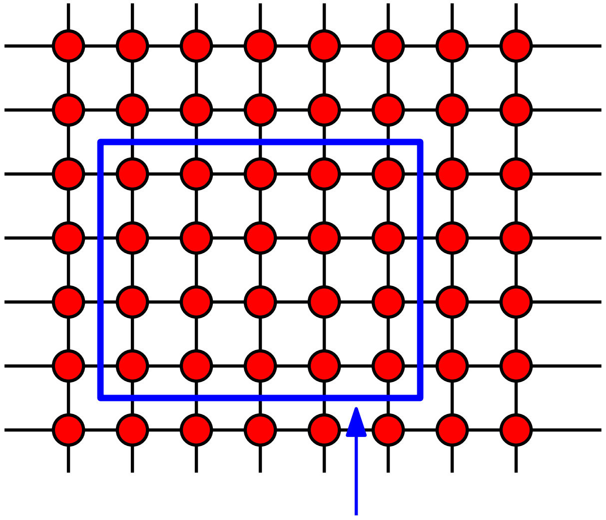
[Oh 2007] [Poulin,Wocjan 2009] [Ge, Tura, Cirac 2018]

Area Laws and Hamiltonian Complexity



Set *A* of qudits.

Area Laws and Hamiltonian Complexity



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$$|\Omega\rangle = \sum_j \lambda_j |a_j\rangle_A |b_j\rangle_B$$

Entropy of Entanglement:

$$S_A = -\sum_j (\lambda_j)^2 \log(\lambda_j)^2$$

$$S_A = -\mathrm{Tr}(\rho_A \log \rho_A)$$

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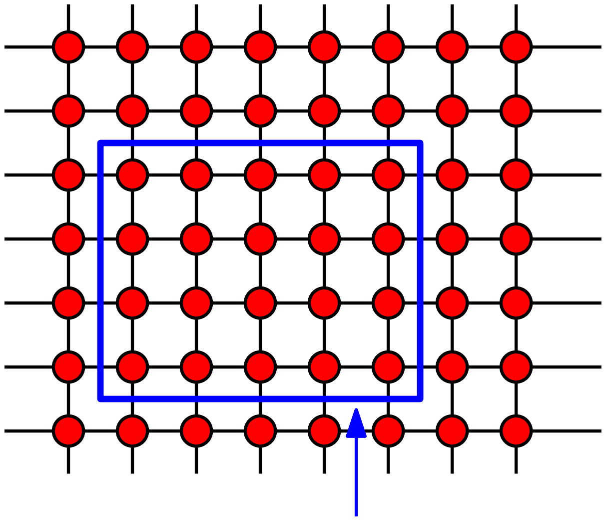

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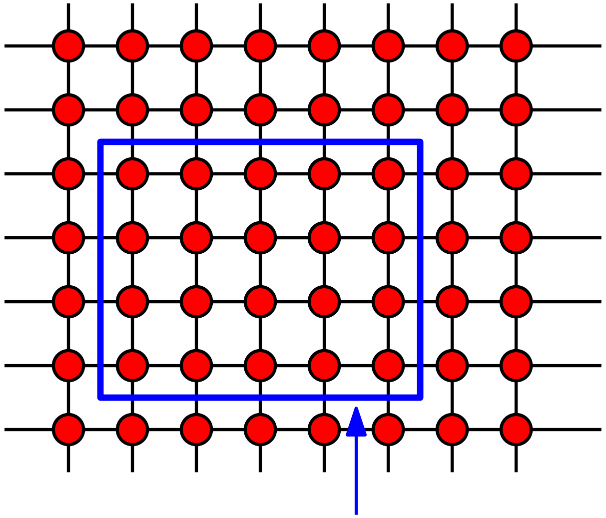
If $|\Omega\rangle$ is the ground state of a ”gapped” local Hamiltonian, then S_A is proportional to the size of the boundary of A.

Area Laws and Hamiltonian Complexity



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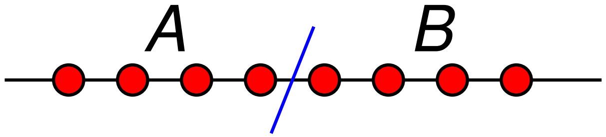
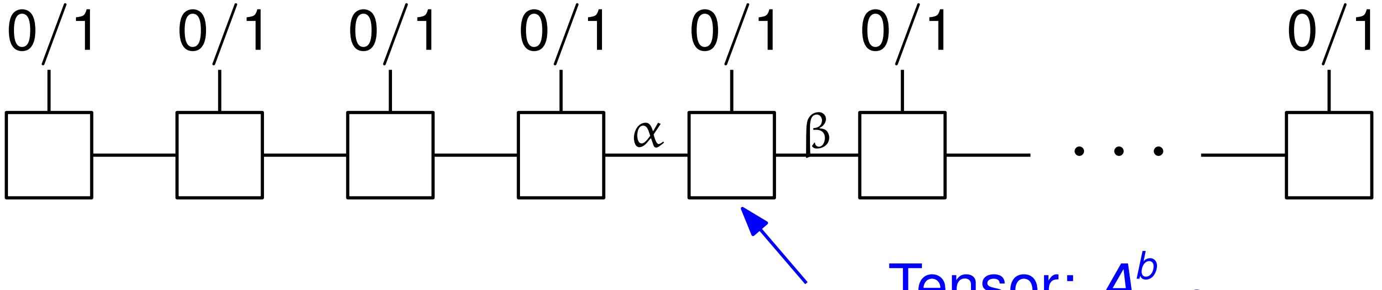


[Hastings 08] [Arad, Kitaev, Landau, Vazirani 13]

$$S_A = O\left(\frac{\log^3 d}{\epsilon}\right)$$

Area Laws and Tensor Networks

Area law in 1D implies that ground states of gapped Hamiltonians can be closely approximated by Matrix Product States.



Tensor: $A^{b}_{\alpha,\beta}$

$b = 0/1, \quad 1 \leq \alpha, \beta \leq B$

B = ”bond dimension”

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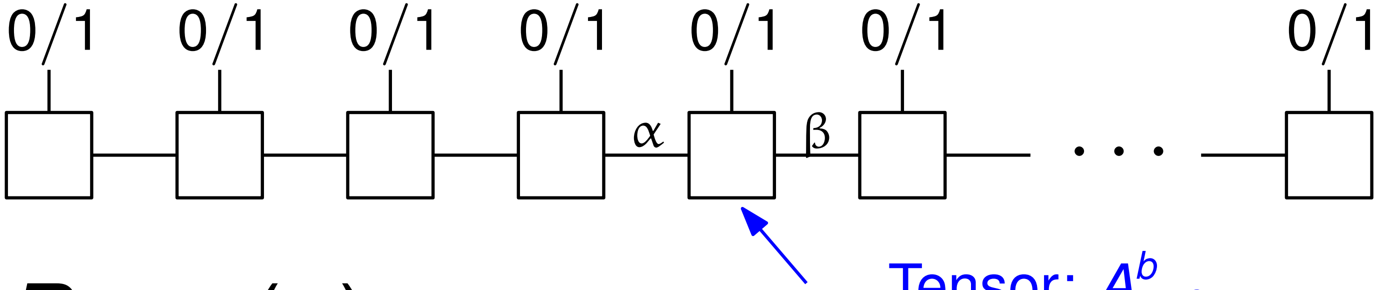

Tensor: $A^{b}_{\alpha,\beta}$

$b = 0/1, \quad 1 \leq \alpha, \beta \leq B$

B = "bond dimension"

$$B = o(n)$$

[Arad, Kitaev, Landau, Vazirani 13]

Area Laws and Tensor Networks

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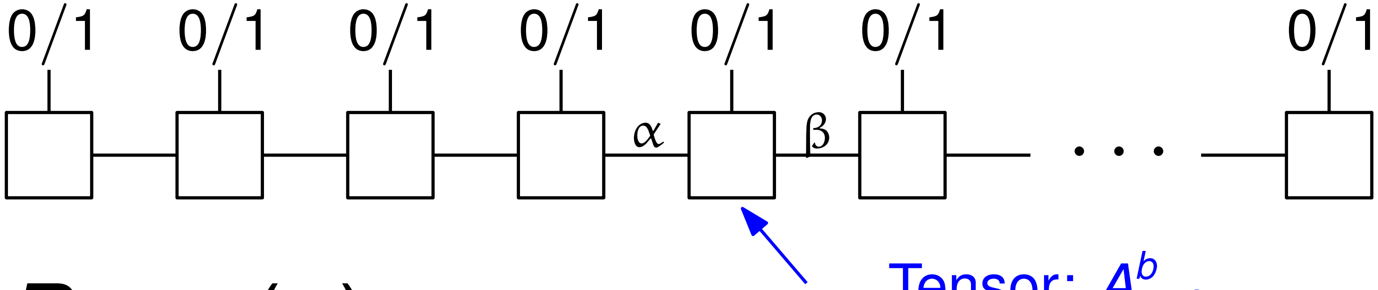

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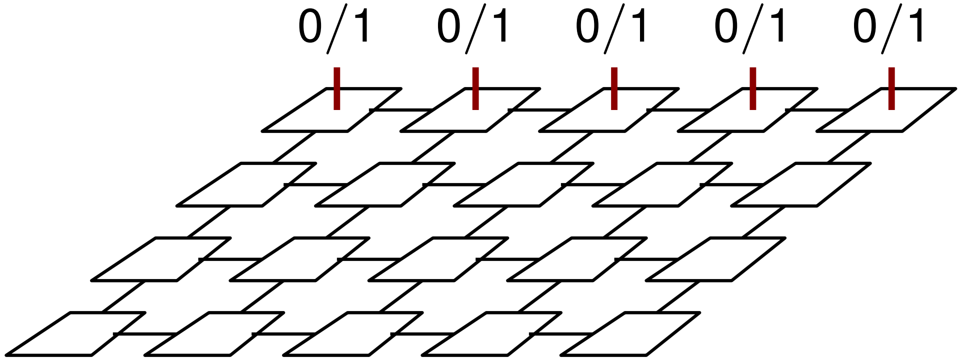
In 2D: PEPS (Projected Entangled Pair States)

[Verstraete, Cirac]



Critical Systems and the Log Correction

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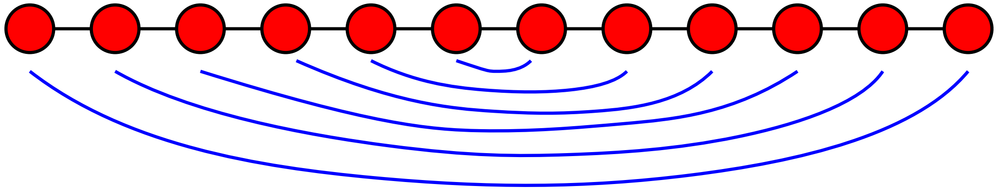
Not a universal rule:
Examples with $\Delta(H_n) = \Theta(1/poly(n))$ and ground state entropy $\Omega(n)$.



[Gottesman, Hastings]
[Irani]
[Movassagh, Shor]

Thank You!