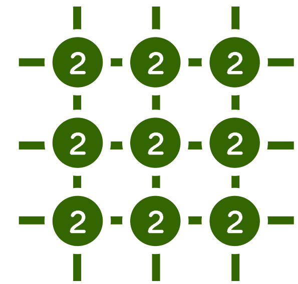
many-body physics & complexity 2

the problems & the tools

Daniel Nagaj
universität wien

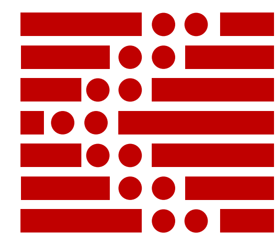
1 **local hamiltonian**

its simple & difficult variants



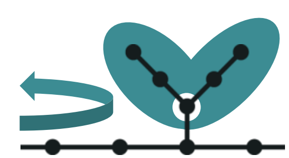
2 **the algorithms**

what works well & what we wish we had



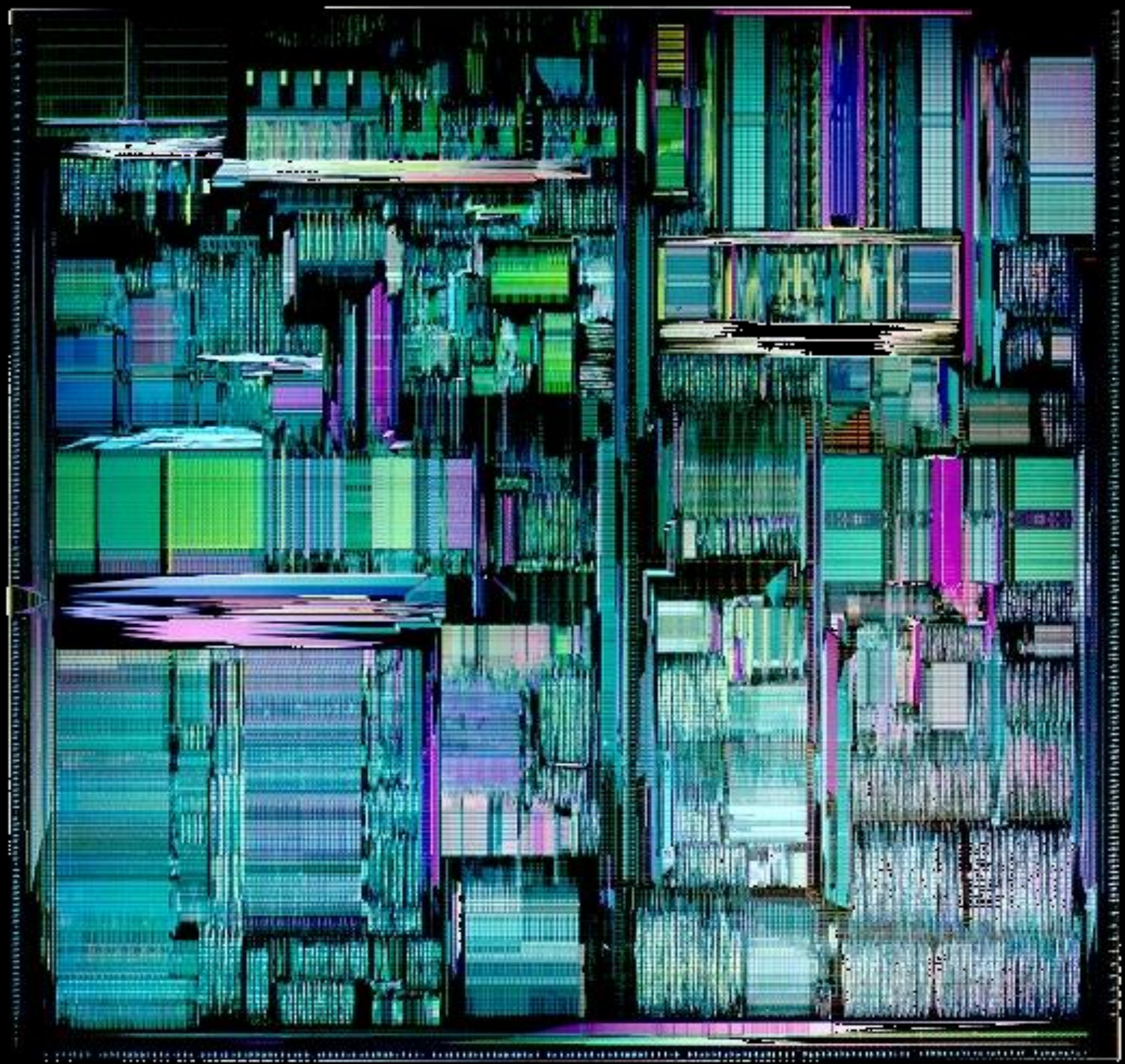
3 **let's make it work**

computers & simulators

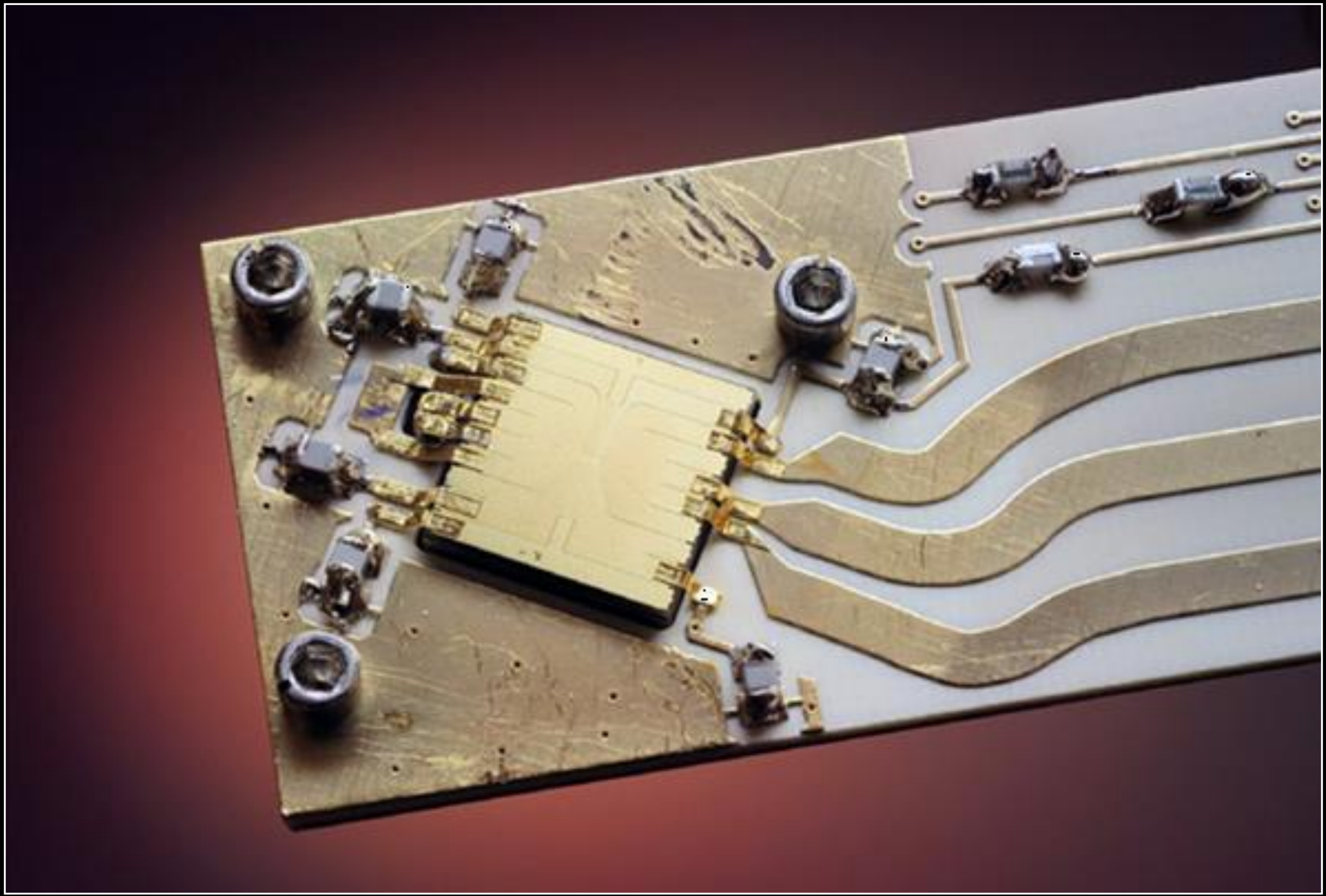


Is
the
ground
state
energy
of a

LH

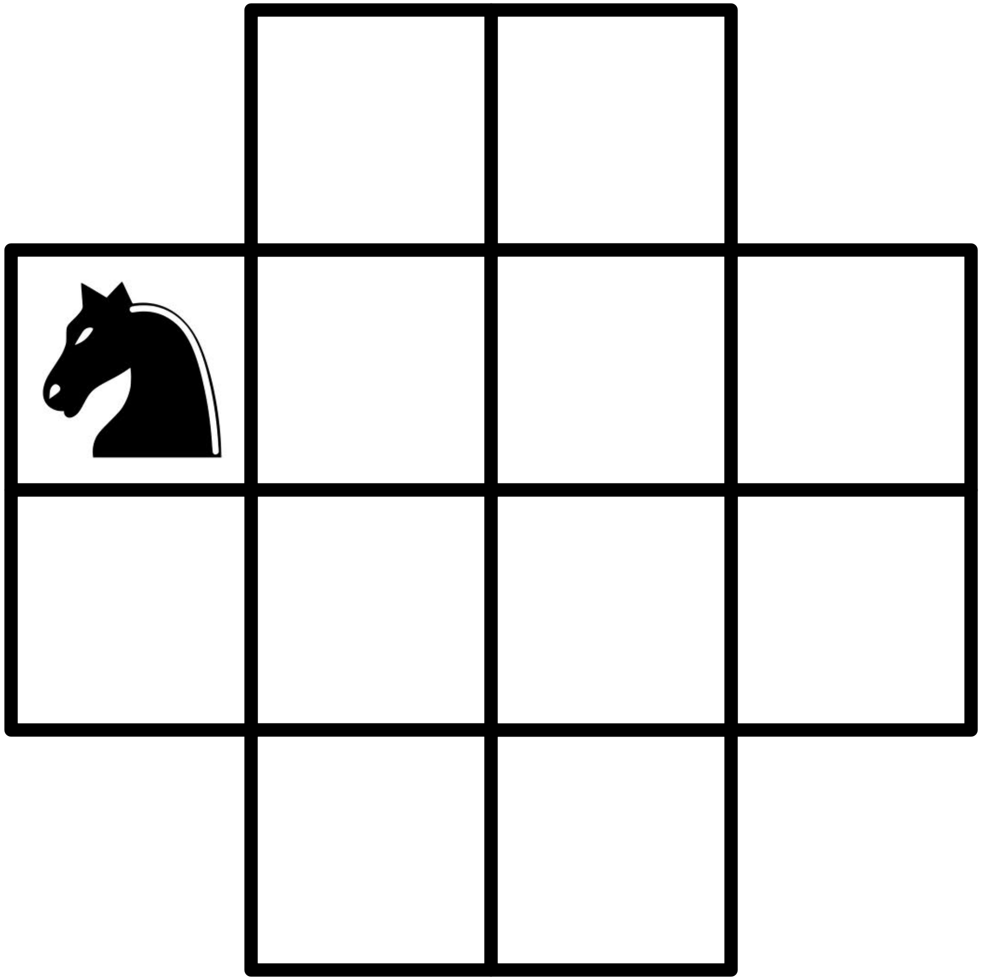


[1995 Pentium Pro, www.tayloredge.com/museum]

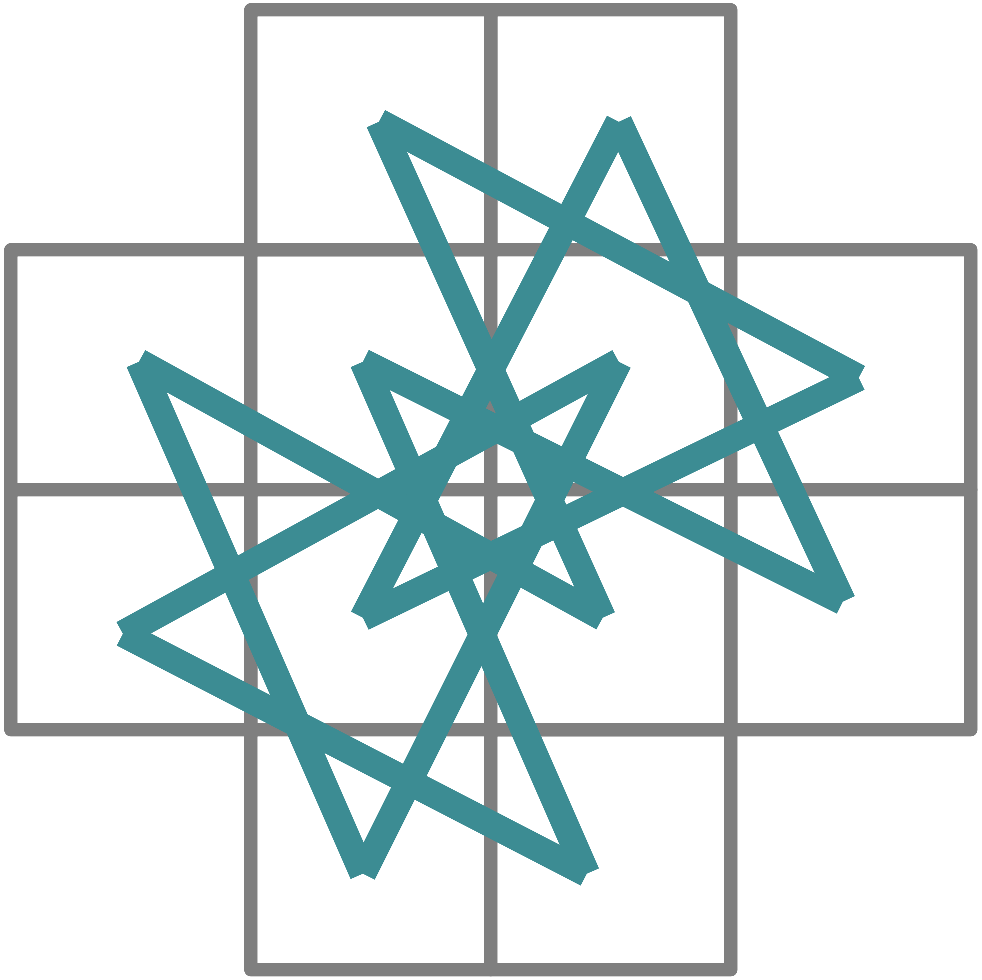


[NIST gold ion trap on aluminum-nitride backing, Y.Colombe/NIST]

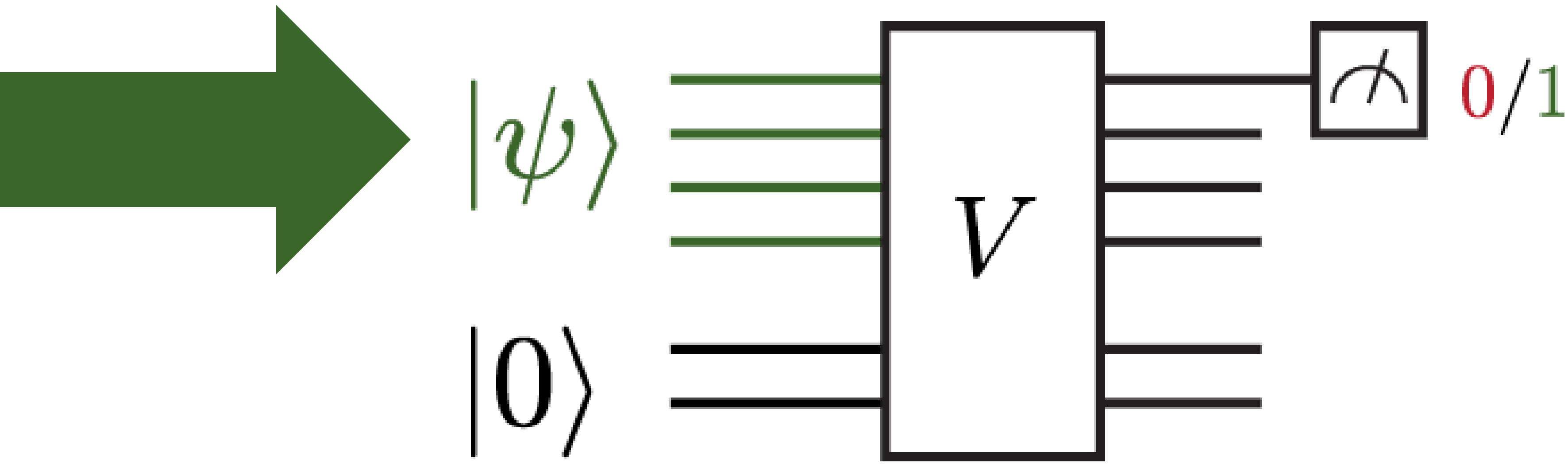
1 An NP-complete problem: Hamiltonian path



1 An NP-complete problem: Hamiltonian path

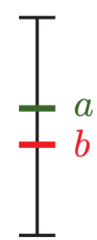


3 The QMA protocol

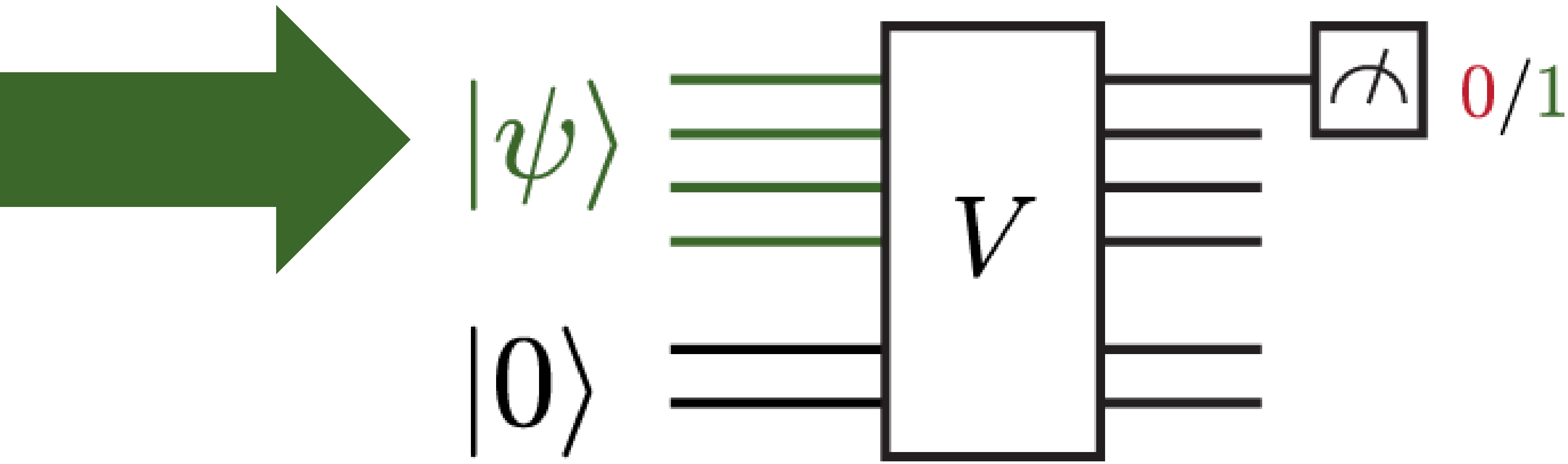


YES? Accept a good proof with $p > a$.

NO? Probability of accepting $p < b$.

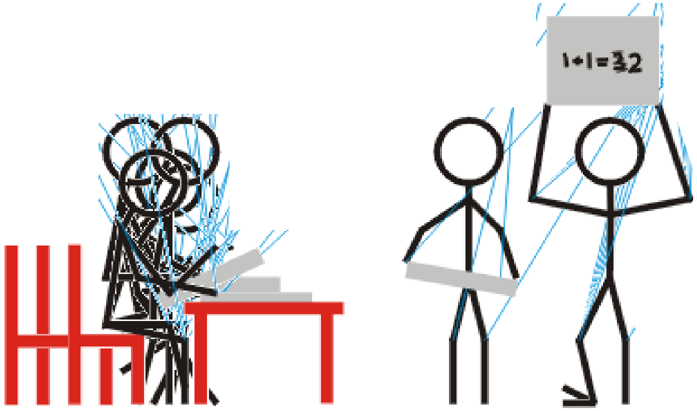


3 A QMA-hard question

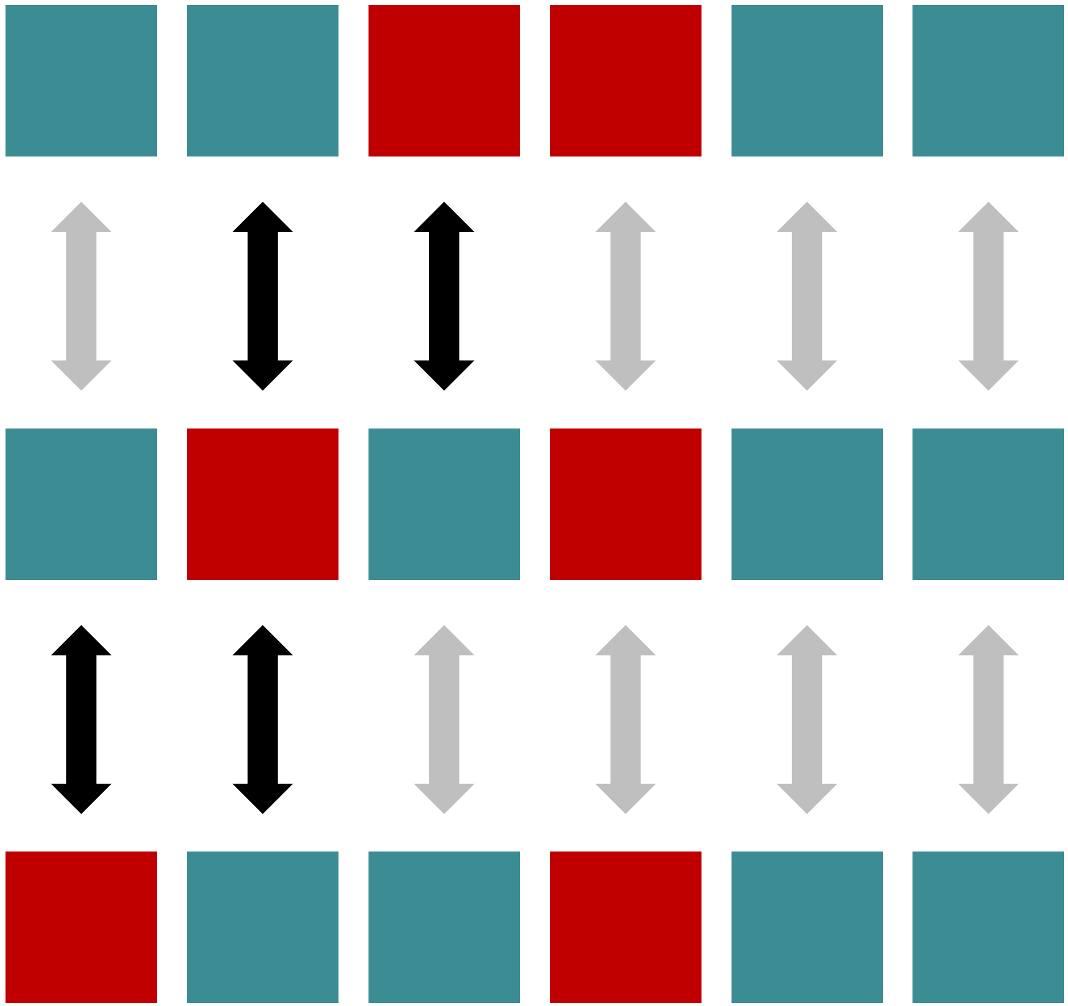


Could we feed this quantum verifier something that likely outputs 1?

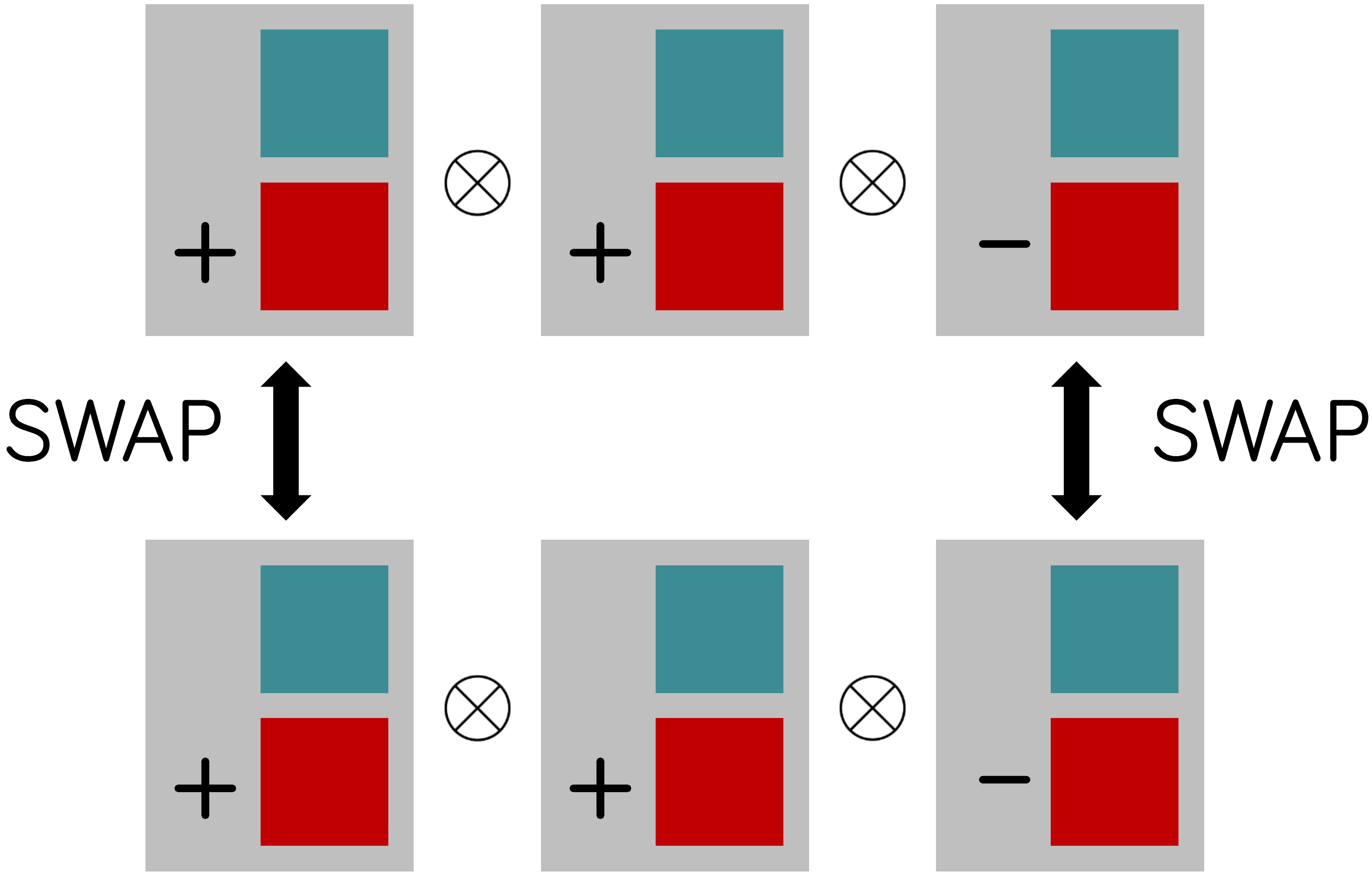
3 Snapshots of a computation



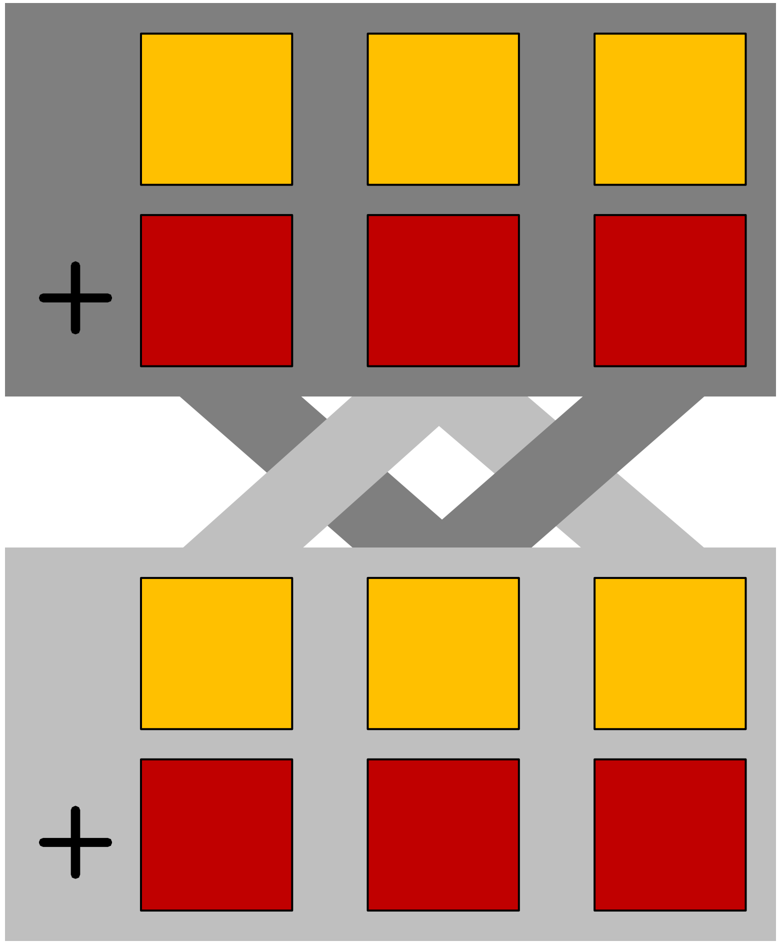
Locally comparing strings.



Locally comparing product states: SWAP.

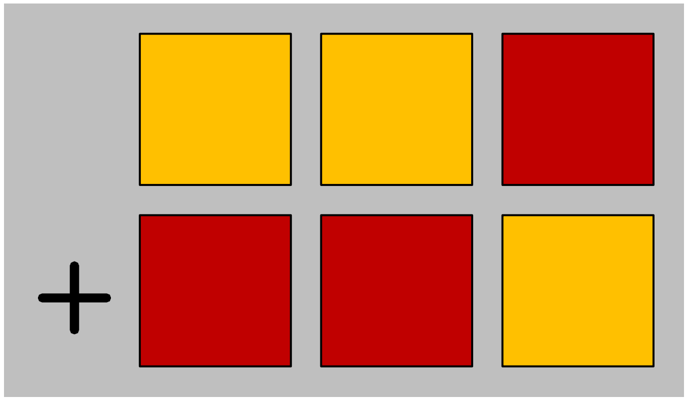


Locally comparing entangled states?

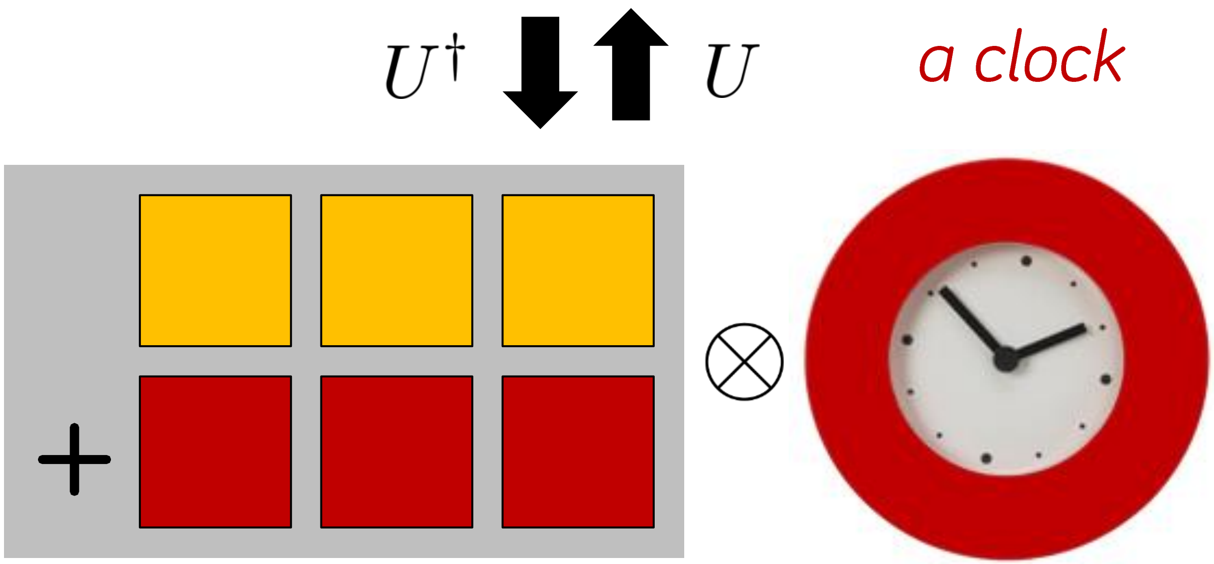


UGH!

1 The data & the clock

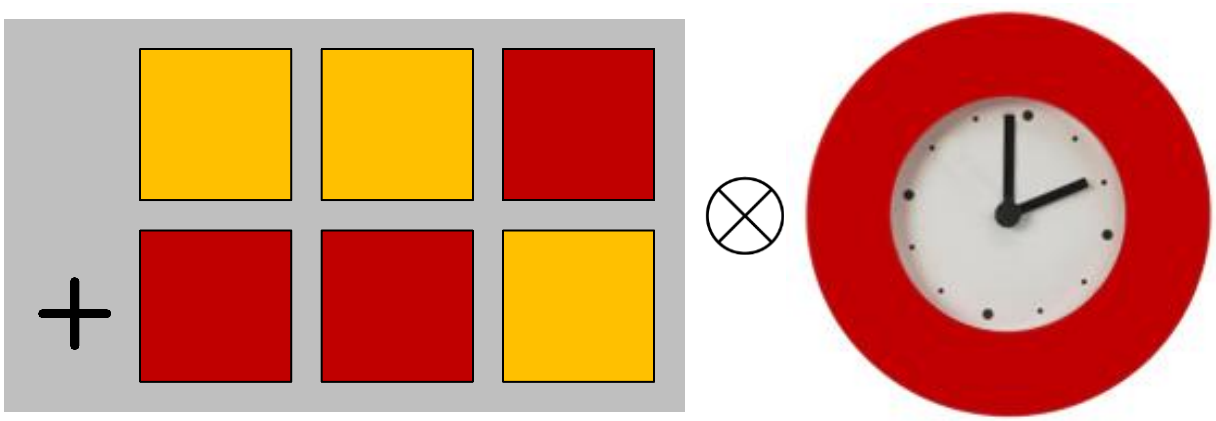


Hard to compare directly (locally).

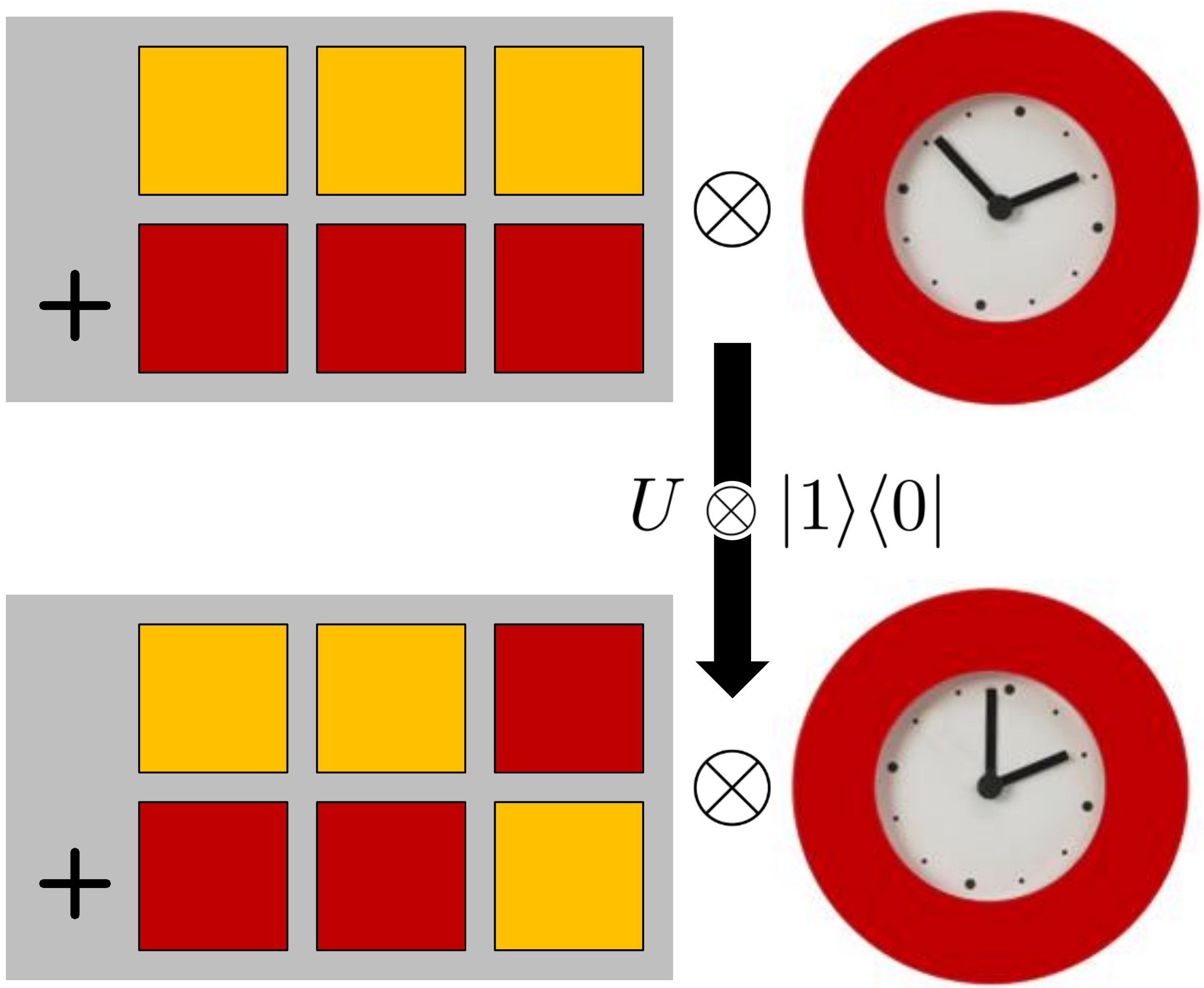


1 The data & the clock

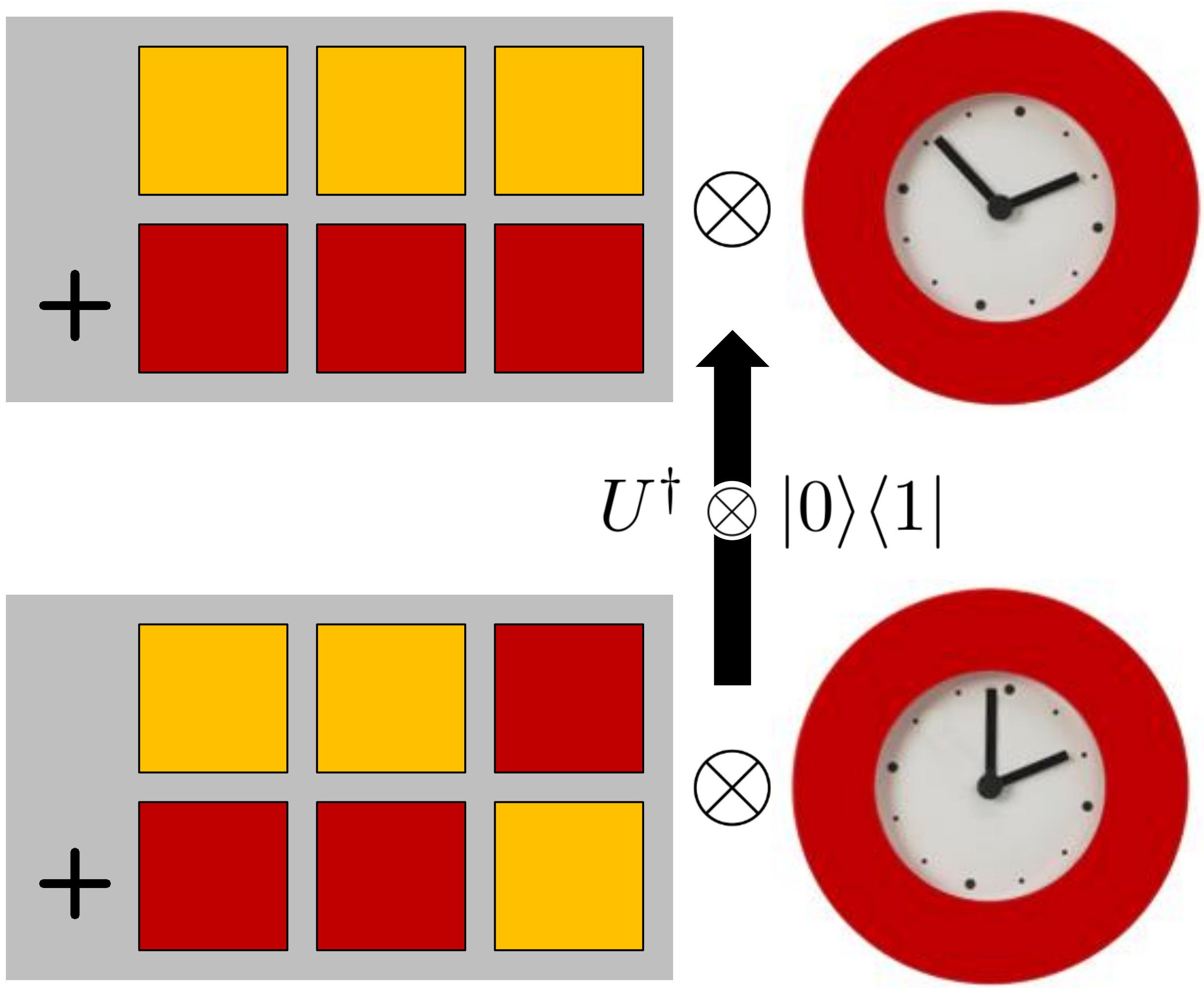
a clock



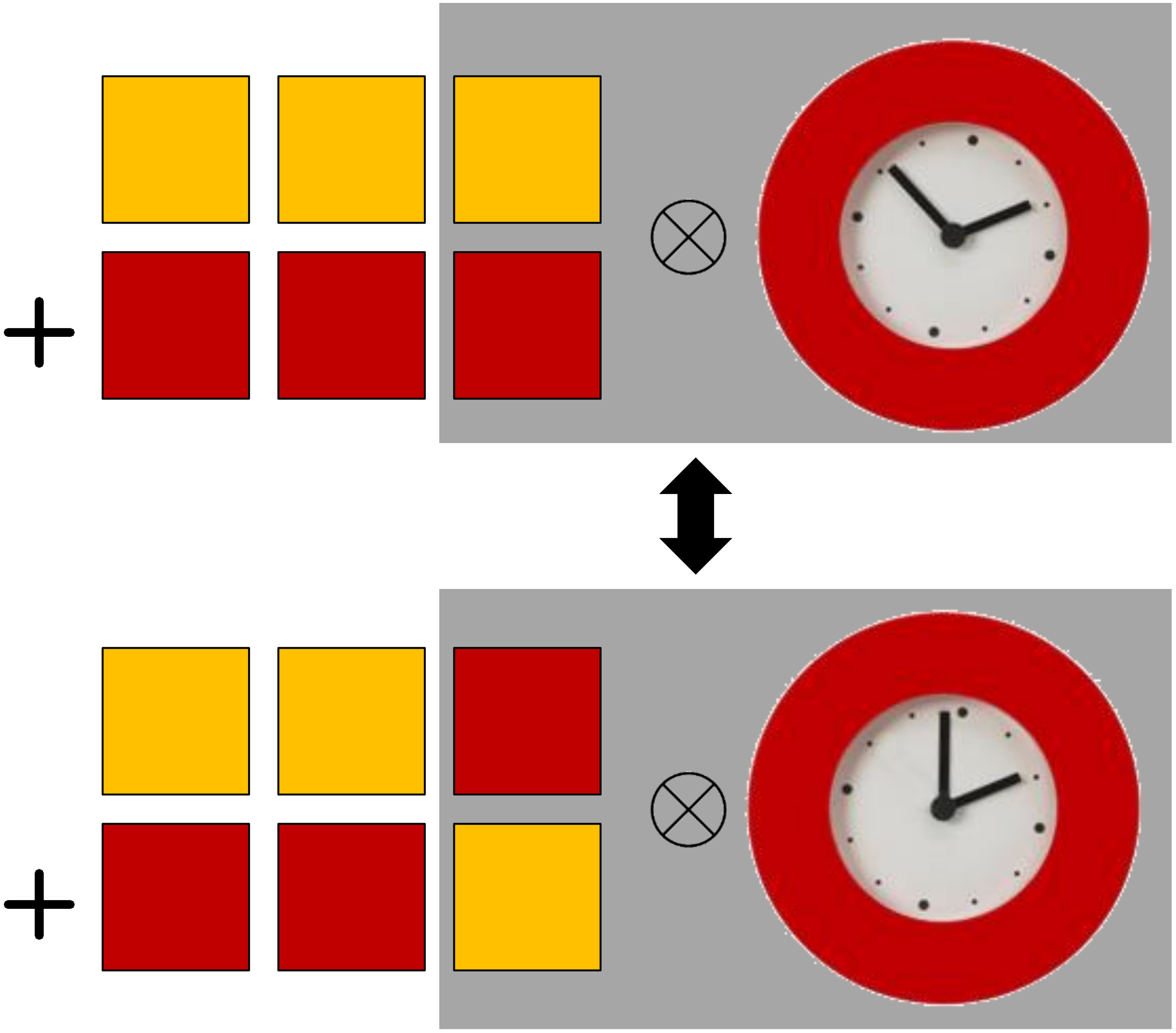
1 The data & the clock



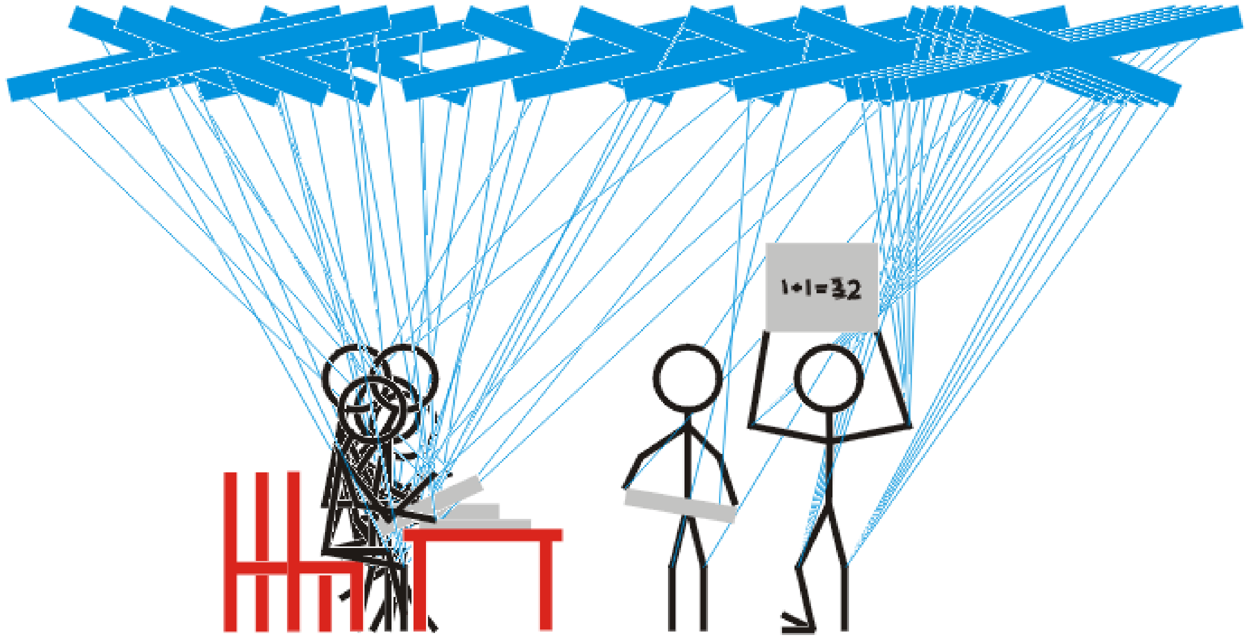
1 The data & the clock



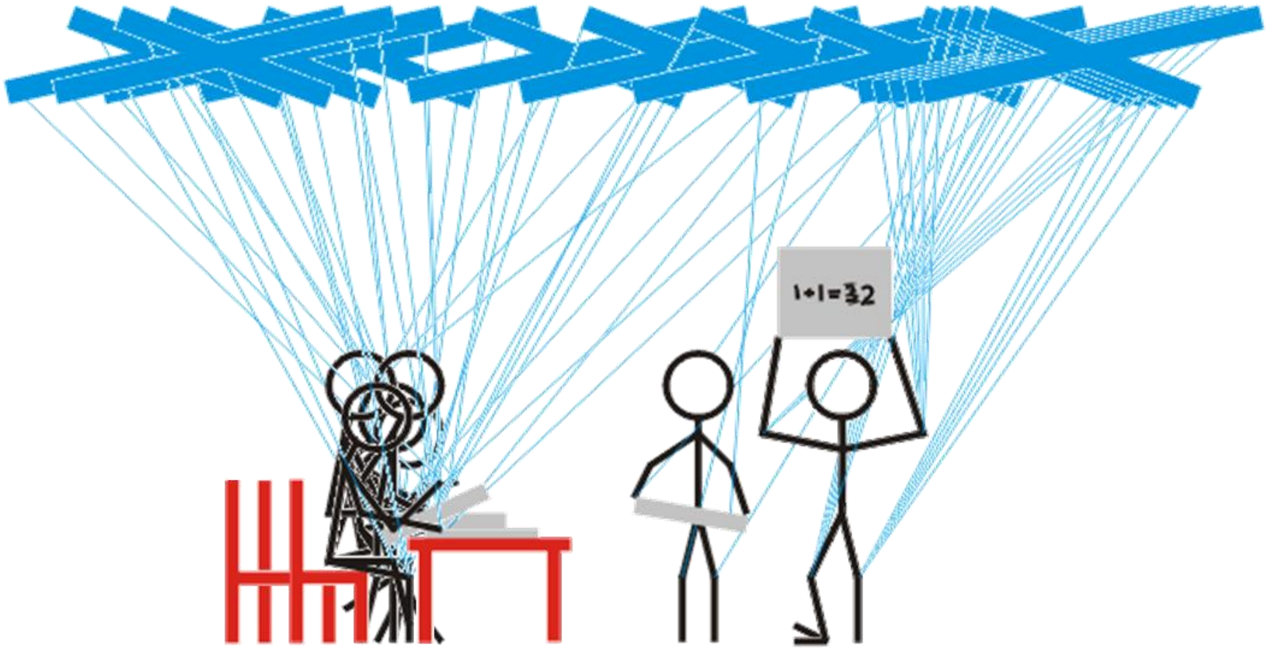
1 The data & the clock



1 Snapshots of a computation & a “clock”



1 The history state



$$|\psi_{hist}\rangle = \frac{1}{\sqrt{T+1}} \sum_{t=0}^{T} |\varphi_t\rangle \otimes |t\rangle$$

$$|\varphi_t\rangle = U_t \cdots U_1 |\varphi_0\rangle$$

1 The history state: a ground state

Π_j  $= 0$

$$|\psi_{hist}\rangle = \frac{1}{\sqrt{T+1}} \sum_{t=0}^{T} \underbrace{|\varphi_t\rangle}_{U_t \cdots U_1 |\varphi_0\rangle} \otimes |t\rangle$$

1 Do we have a history state?

k-local

c-o-n-d-i-t-i-o-n-s

clock encoding

state progression

$$|\varphi_t\rangle \otimes |t\rangle$$

$$|\varphi_{t+1}\rangle \otimes |t+1\rangle$$

$$|\psi_{hist}\rangle = \frac{1}{\sqrt{T+1}} \sum_{t=0}^{T} |\varphi_t\rangle \otimes |t\rangle$$

1 Checking if a state is an accepted history

k-local

c-o-n-d-i-t-i-o-n-s

clock encoding

state progression

initialization

$$|\cdots 0\rangle \otimes |0\rangle$$

$$|\varphi_t\rangle \otimes |t\rangle$$
$$|\varphi_{t+1}\rangle \otimes |t+1\rangle$$

output

$$|\cdots 1\rangle \otimes |T\rangle$$

$$|\psi_{hist}\rangle = \frac{1}{\sqrt{T+1}} \sum_{t=0}^{T} |\varphi_t\rangle \otimes |t\rangle$$

1 Run the clock, apply gates ... with a local clock

$$|\varphi_{t-2}\rangle \otimes |t-2\rangle$$

$$|\varphi_{t-1}\rangle \otimes |t-1\rangle$$

$$|\varphi_{t}\rangle \otimes |t\rangle$$

$$|\varphi_{t+1}\rangle \otimes |t+1\rangle$$

$$|\varphi_{t+2}\rangle \otimes |t+2\rangle$$

$$|\varphi_{t+3}\rangle \otimes |t+3\rangle$$

? ? ?

- YES

ground state

- NO

lower bound on the ground state energy

good
clock
states

not
clock
states

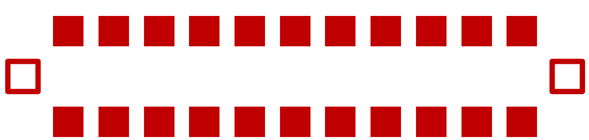
history states

non-uniform
superpositions

history states

a polynomially small gap

$\Delta = O\left(L^{-2}\right)$



history states

well	badly
initialized history states	

well

initialized histories

accepted states

well

initialized histories

accepted states

$H_A + H_B$

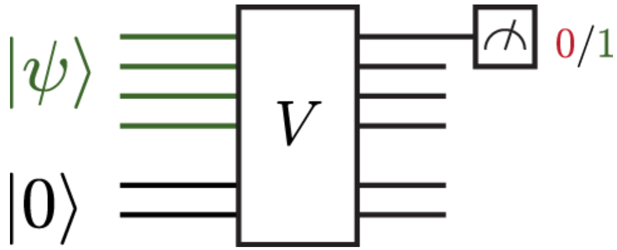
$$\lambda_0 \geq \sin^2 \frac{\vartheta}{2} \times \min(\Delta_A, \Delta_B)$$

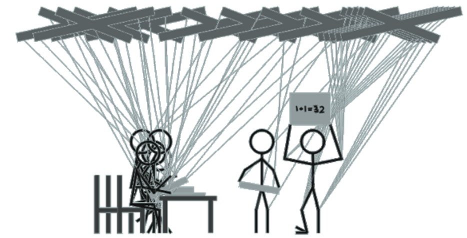
L^{-2}

L^{-1}

1 LH and QMA verification

$$H_{clock} + H_{init} + H_{prop} + H_{out}$$





NO V is unlikely to accept anything (ϵ)

any state has energy

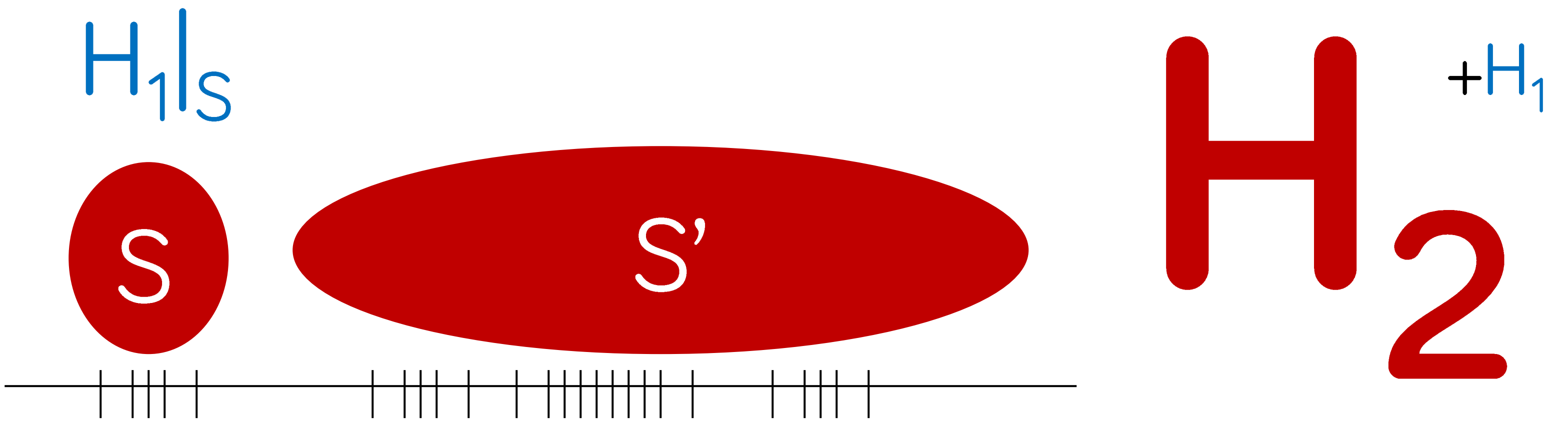
$$\langle \eta | H | \eta \rangle \geq \frac{c\left(1-\sqrt{\epsilon}\right)}{L^3}$$

YES some proof is likely (1-ϵ) accepted

the history for the proof

$$\langle \psi_{hist} | H | \psi_{hist} \rangle \leq \frac{\epsilon}{L+1}$$

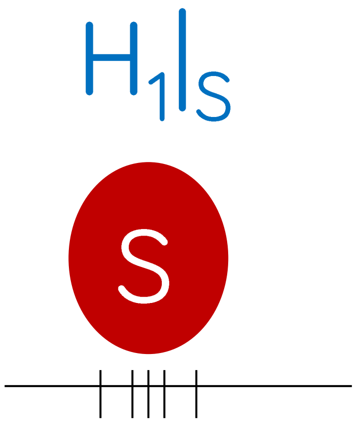
1 The projection lemma to estimate eigenvalues



Lemma 1 *Let $H = H_1 + H_2$ be the sum of two Hamiltonians operating on some Hilbert space $\mathcal{H} = \mathcal{S} + \mathcal{S}^{\perp}$. The Hamiltonian H_2 is such that $\mathcal{S}$ is a zero eigenspace and the eigenvectors in $\mathcal{S}^{\perp}$ have eigenvalue at least $J > 2\|H_1\|$. Then,*

$$\lambda(H_1|_{\mathcal{S}}) - \frac{\|H_1\|^2}{J - 2\|H_1\|} \leq \lambda(H) \leq \lambda(H_1|_{\mathcal{S}}).$$

1 The projection lemma to estimate eigenvalues

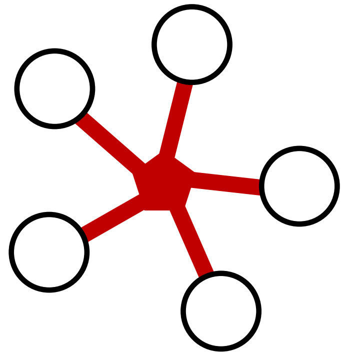


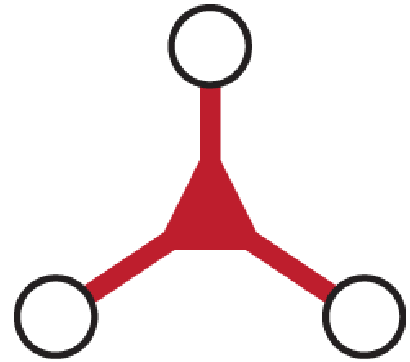
$$|1\rangle\langle 0| + |0\rangle\langle 1|$$

$$|1110000\rangle$$
$$|1111000\rangle$$
$$|1111100\rangle$$

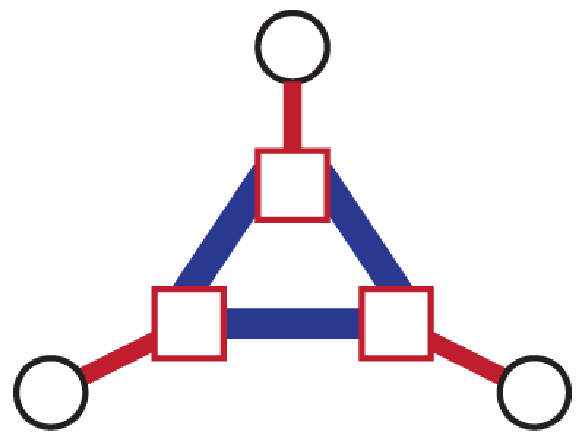
1 Projection lemma, perturbation gadgets

- 3-local H. that works just as the 5-local one in the good subspace



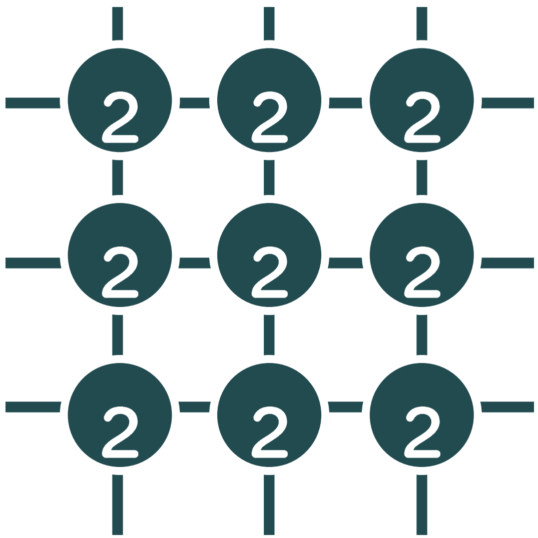


- 2-local … from effective interactions



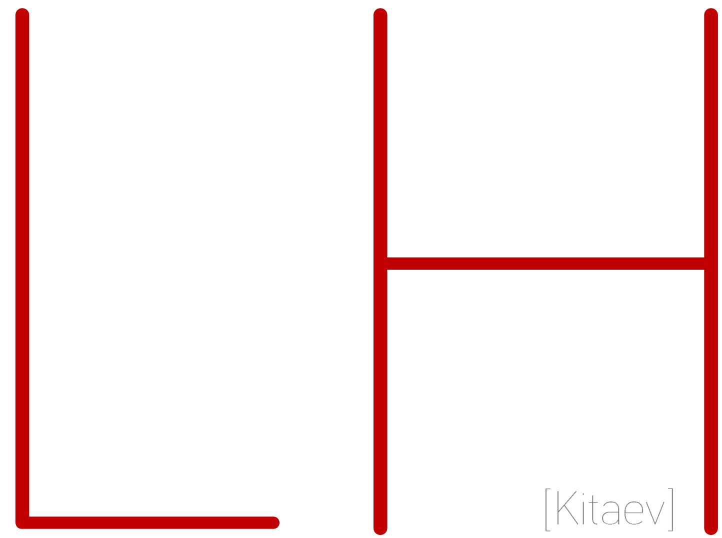
[Kempe, Kitaev, Regev '03]

1 2-local Hamiltonian is QMA-complete

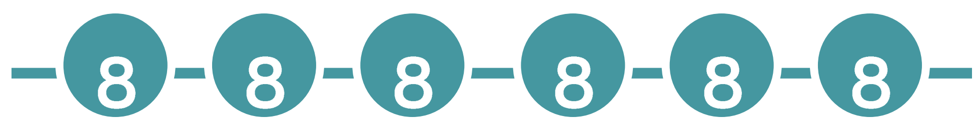


[Oliveira, Terhal '04]

a global minimum

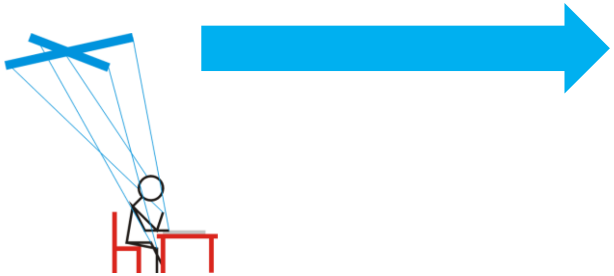


$$\sum H_{jk}$$



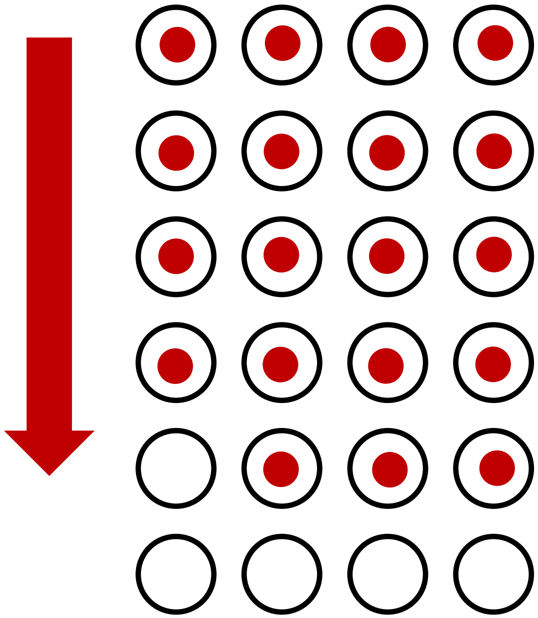
[Hallgren, N, Narayanaswami '13]

clock/work registers



[Kempe, Kitaev, Regev]

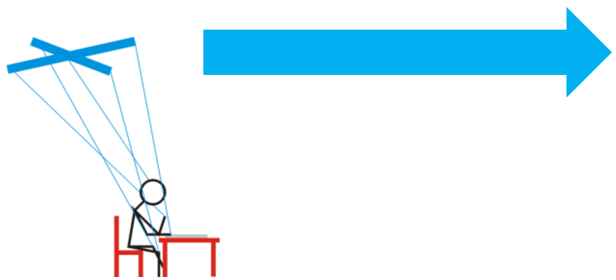
a geometric clock



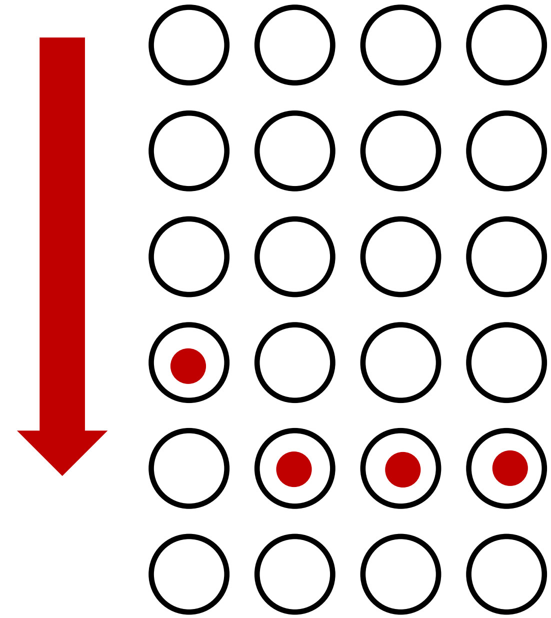
[Mizel] [Aharonov+]

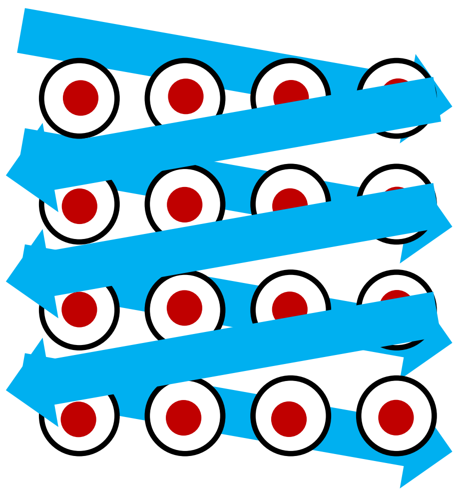
[Childs Gosset Webb]

clock/work registers

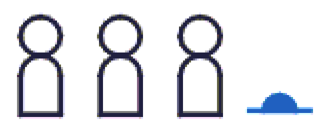


a geometric clock



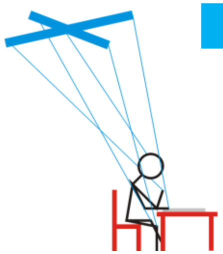


geometric locality



moving data on a line

clock/work registers



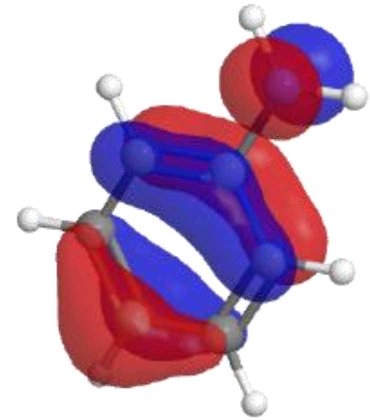
A different construction?

A stronger promise?

Nontrivial
intermediate
problems?

More interesting
hard problems?

1 Complex quantum chemistry calculations



- electronic structure
  many **e**'s, lots of possible orbitals

- DFT is QMA-c [Whitfield Schuch Verstraete 13]

$$t\sum_{ij}\sum_{\sigma\in\{\downarrow,\uparrow\}} a^\dagger_{i\sigma}a_{j\sigma} + U\sum_i a^\dagger_{i\uparrow}a_{i\uparrow}a^\dagger_{i\downarrow}a_{i\downarrow} + \sum_i \mathbf{b}_i\cdot\mathbf{S}_i \quad \text{Hubbard}$$

$$J\sum_{ij} X_iX_j + Y_iY_j + Z_iZ_j + \sum_i \mathbf{b}_i\cdot\mathbf{S}_i \quad \text{Heisenberg}$$

- approximations
  Hartree-Fock is NP-c [Schuch Verstraete 07]

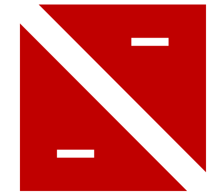
- reduced density matrices
  N-representability is QMA-c [Liu, Christandl, Verstraete 07]

1 The variants of LH

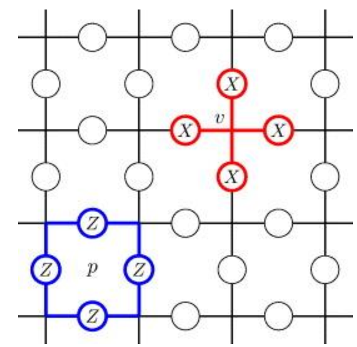
- stoquastic [Bravyi+ 06, Jordan+ 10]
  not universal for q.comp., used in AQO

$Z,\ ZZ,\ X$

~~XZ~~



- commuting
  2-local in NP [Bravyi Vyalyi 05]
  2D plaquettes in NP [Schuch 11]
  3-local (d=2, 3*) in NP [Aharonov Eldar 13]
  constructive LLL [Schwarz+ 13, Arad Sattath 13]



[Brell+'11]

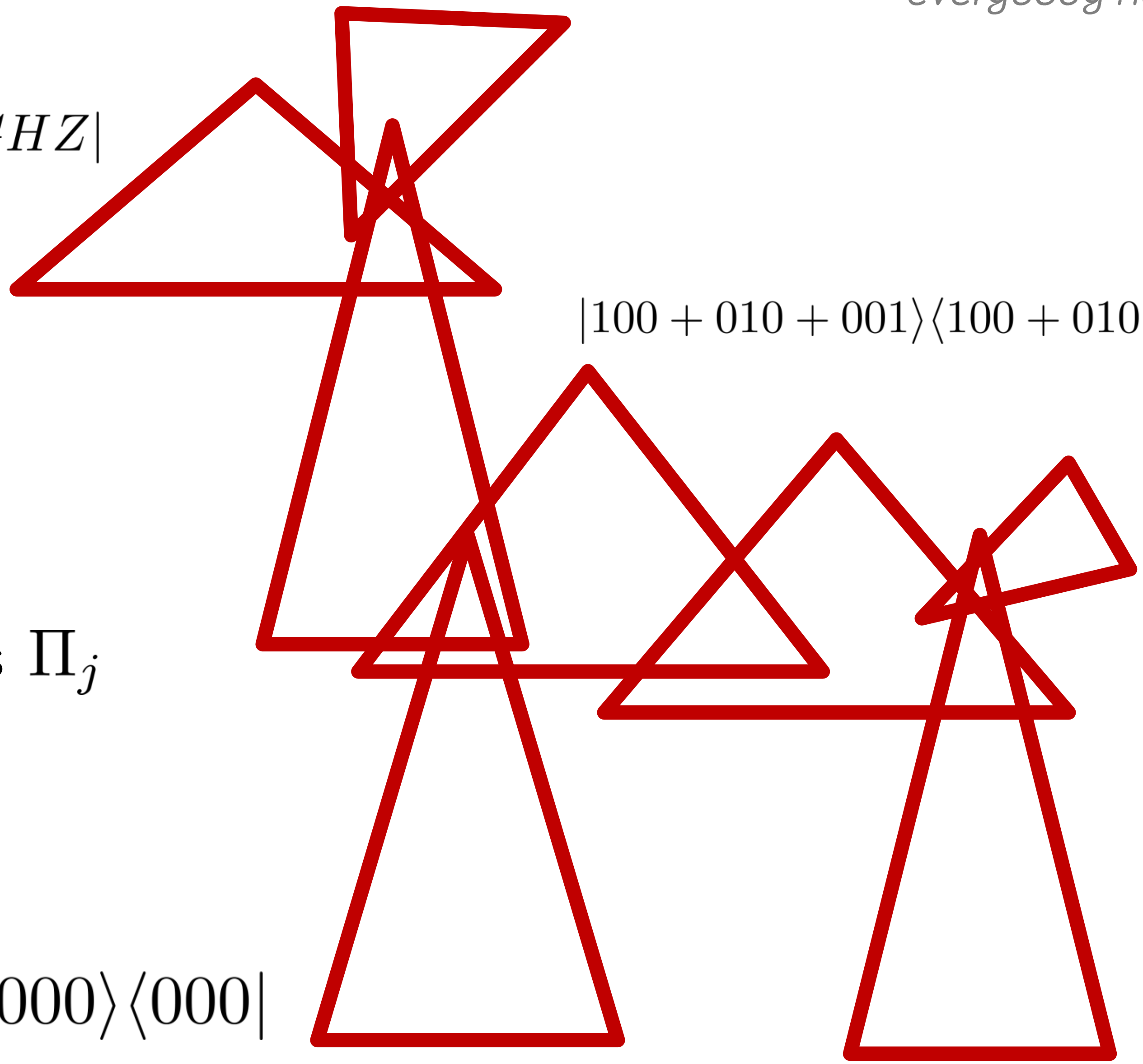
- restricted terms [Biamonte Love 07]
  dichotomy [Cubitt Montanaro 13]

- fixed interaction, general graph [Childs Gossett Webb 13]

Quantum *k*-SAT

Can we make everybody happy?

$|GHZ\rangle\langle GHZ|$



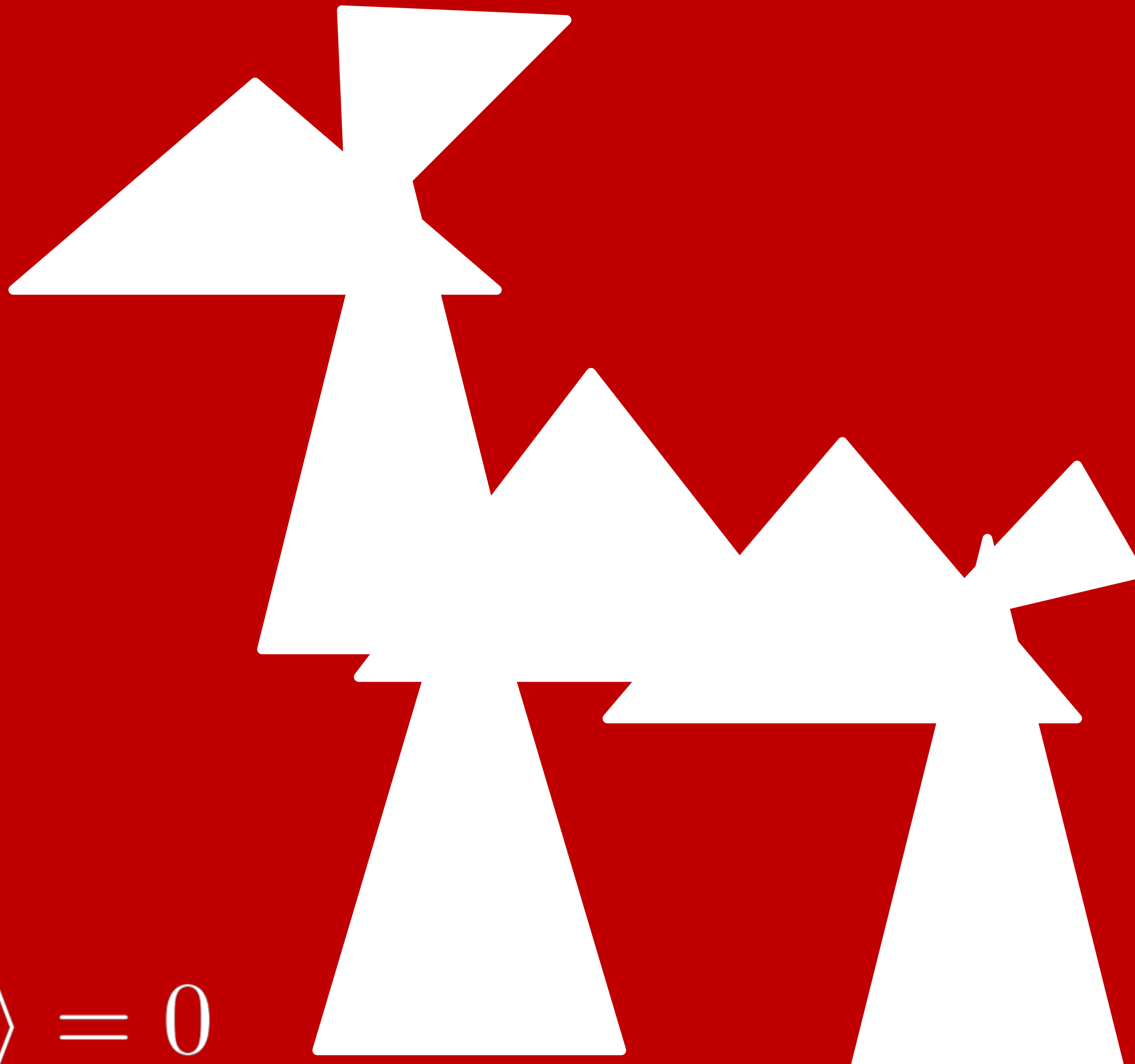
$|100+010+001\rangle\langle 100+010+001|$

- k-local projectors Π_j

$|000\rangle\langle 000|$

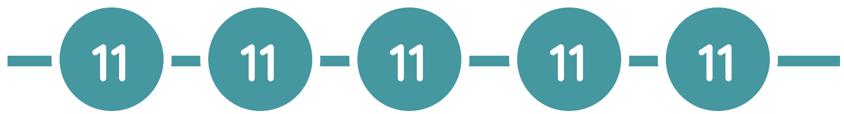
[Bravyi]

Quantum k-SAT



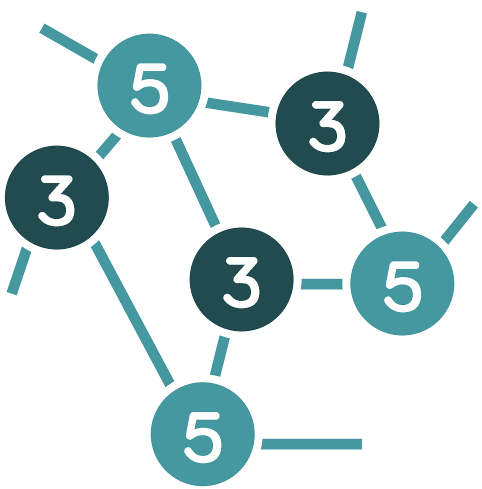
$$\Pi^j |\psi\rangle = 0$$

1 QMA$_1$-complete problems



[N. '08]

$$\Pi^j$$



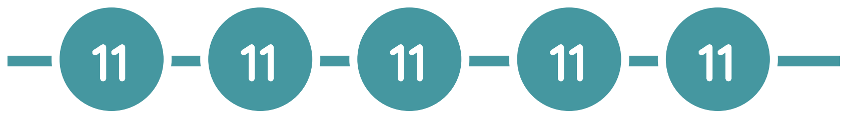
[Eldar, Regev '08]

unfrustrated

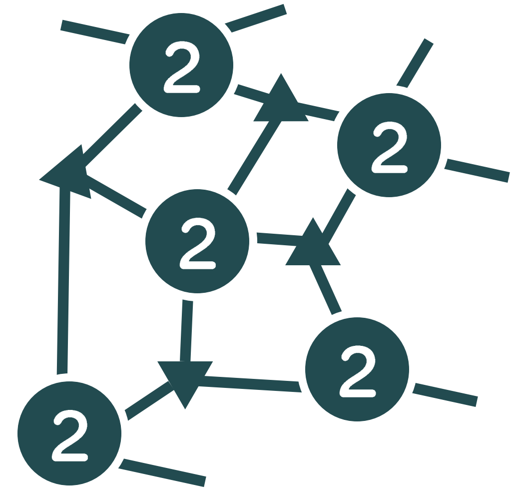
qSAT

[Bravyi]

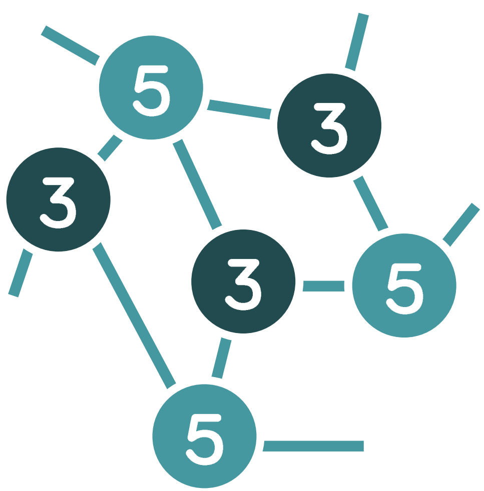
1 QMA$_1$-complete problems



[N. '08]



[Gosset, N. '13]



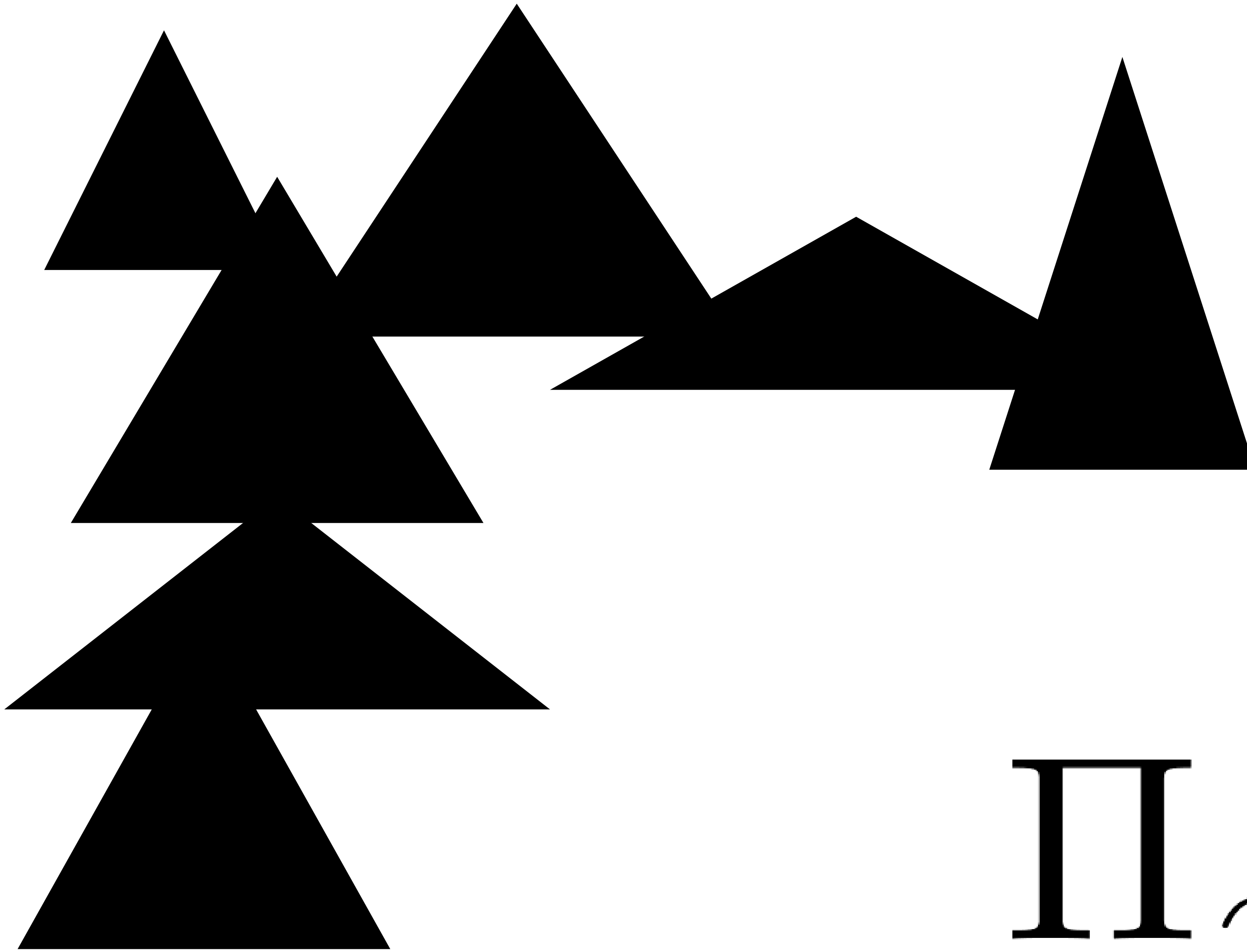
[Eldar, Regev '08]

unfrustrated

qSAT

[Bravyi]

1 Random QSAT



Π_j

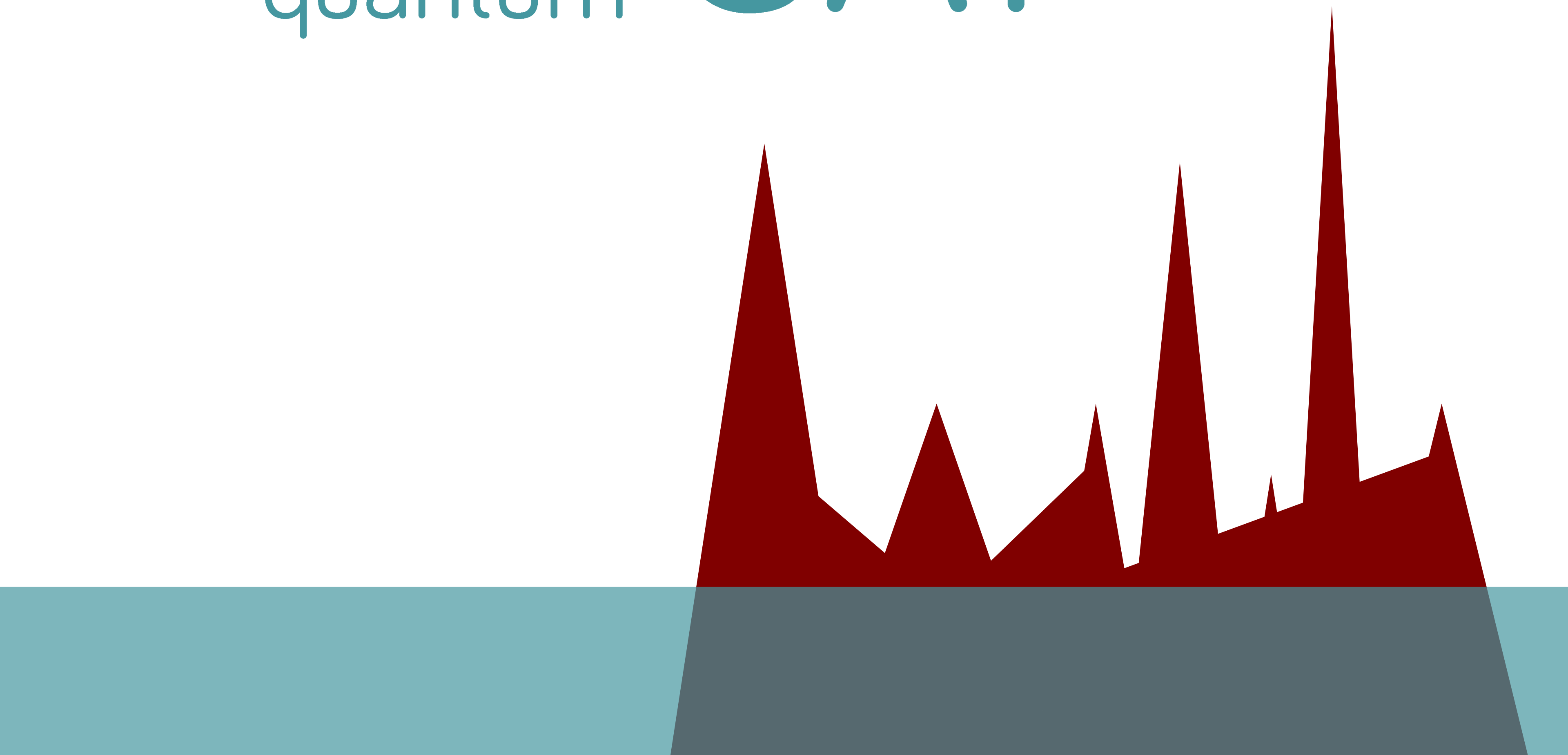
SAT

SAT

UNSAT

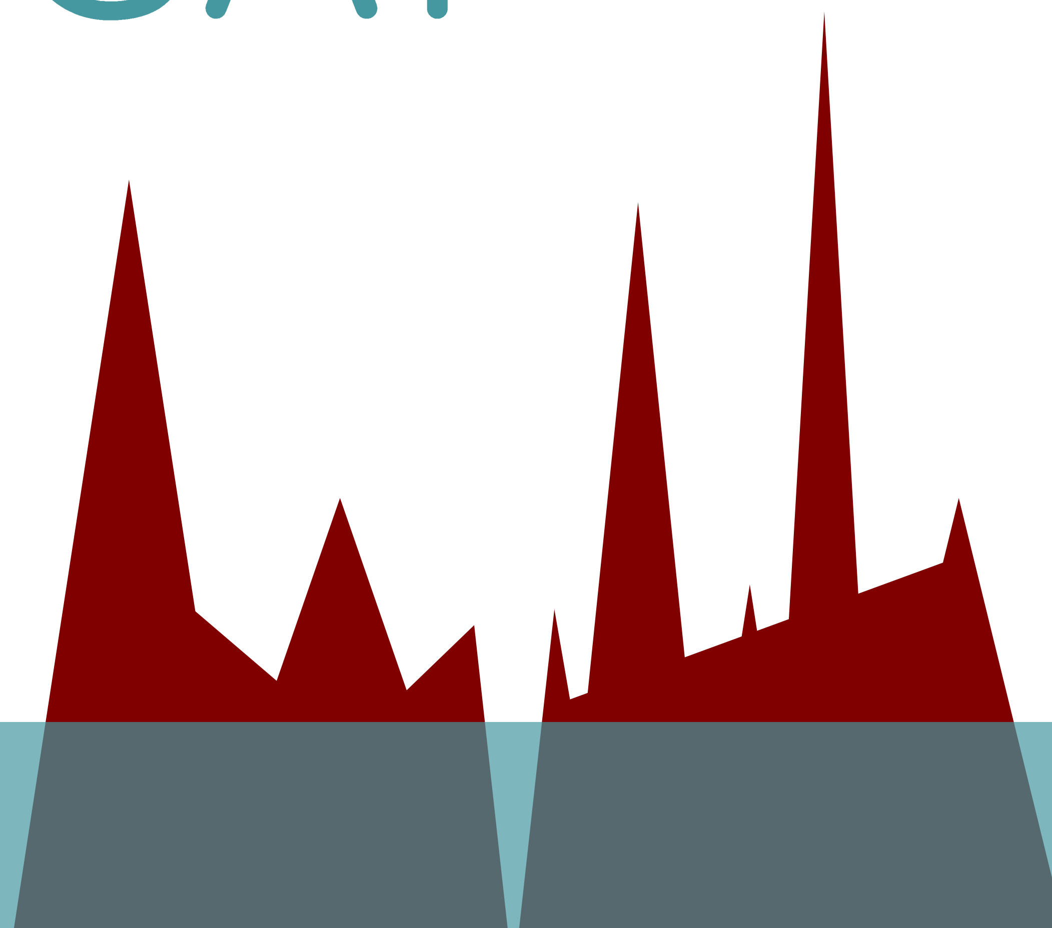
a fixed hypergraph of clauses

classical
quantum
SAT



a fixed hypergraph, worst clauses

adversary quantum SAT

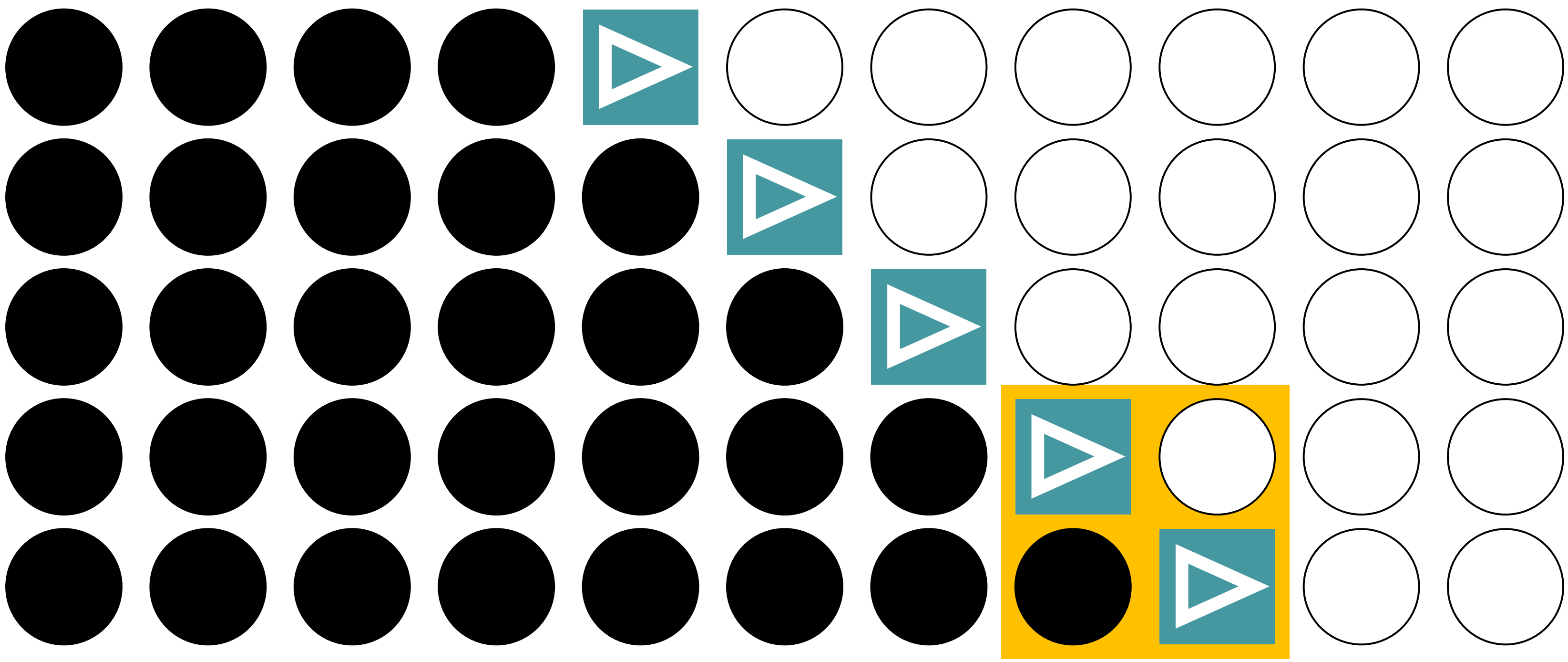


[Bardoscia Scardicchio N 13]

-l-H-a-m-i-l-t-o-n-i-a-n-s-i-n-1-D-L-o-c-a-l-H-a-m-i-l-t-o-n-i-a-n-s-i-n-1-D-L-o-c-a-l-H-a-m

-o-c-a-l-H-a-m-i-l-t-o-n-i-a-n-s-i-n-1-D-L-o-c-a-l-H-a-m-i-l-t-o-n-i-a-n-s-i-n-1-D-L-o-c-a-l-

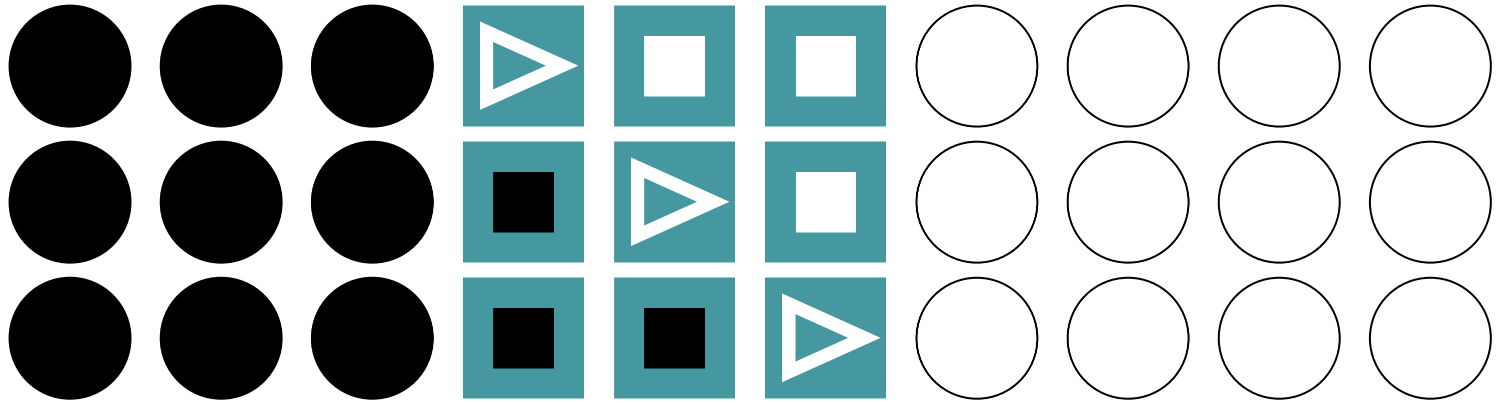
-m-i-l-t-o-n-i-a-n-s-i-n-1-D-L-o-c-a-l-H-a-m-i-l-t-o-n-i-a-n-s-i-n-1-D-L-o-c-a-l-H-a-m-i-l-t-



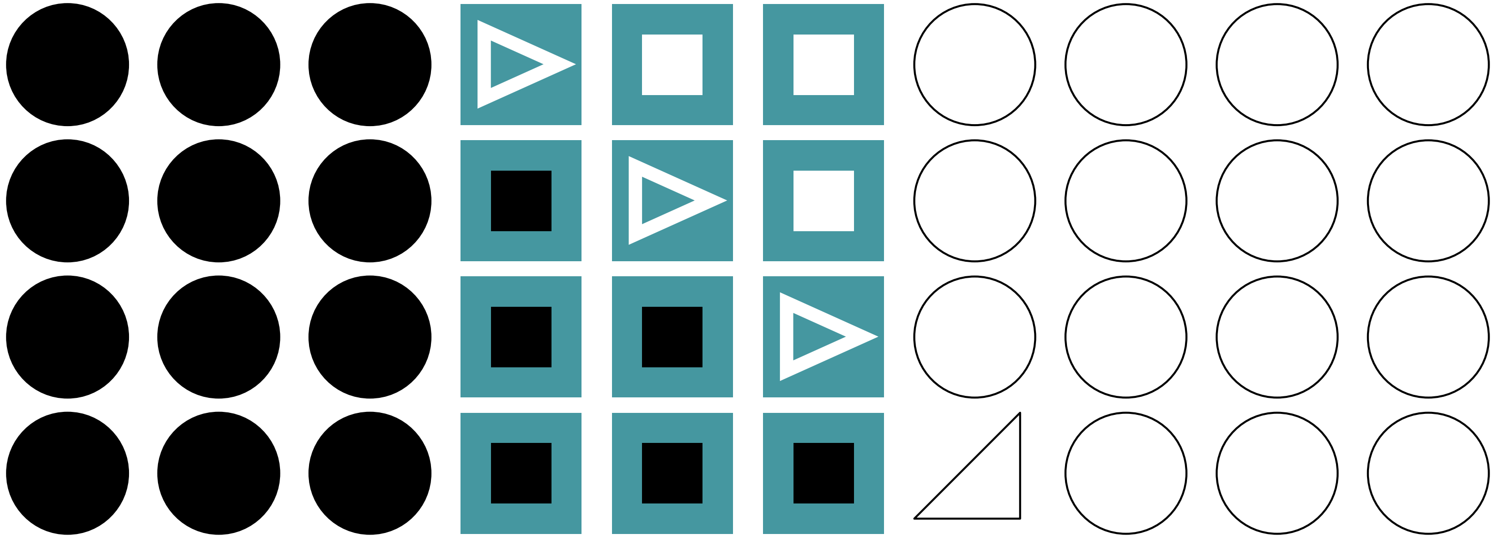
a surfer on a domain wall

the **power** of quantum systems on a line

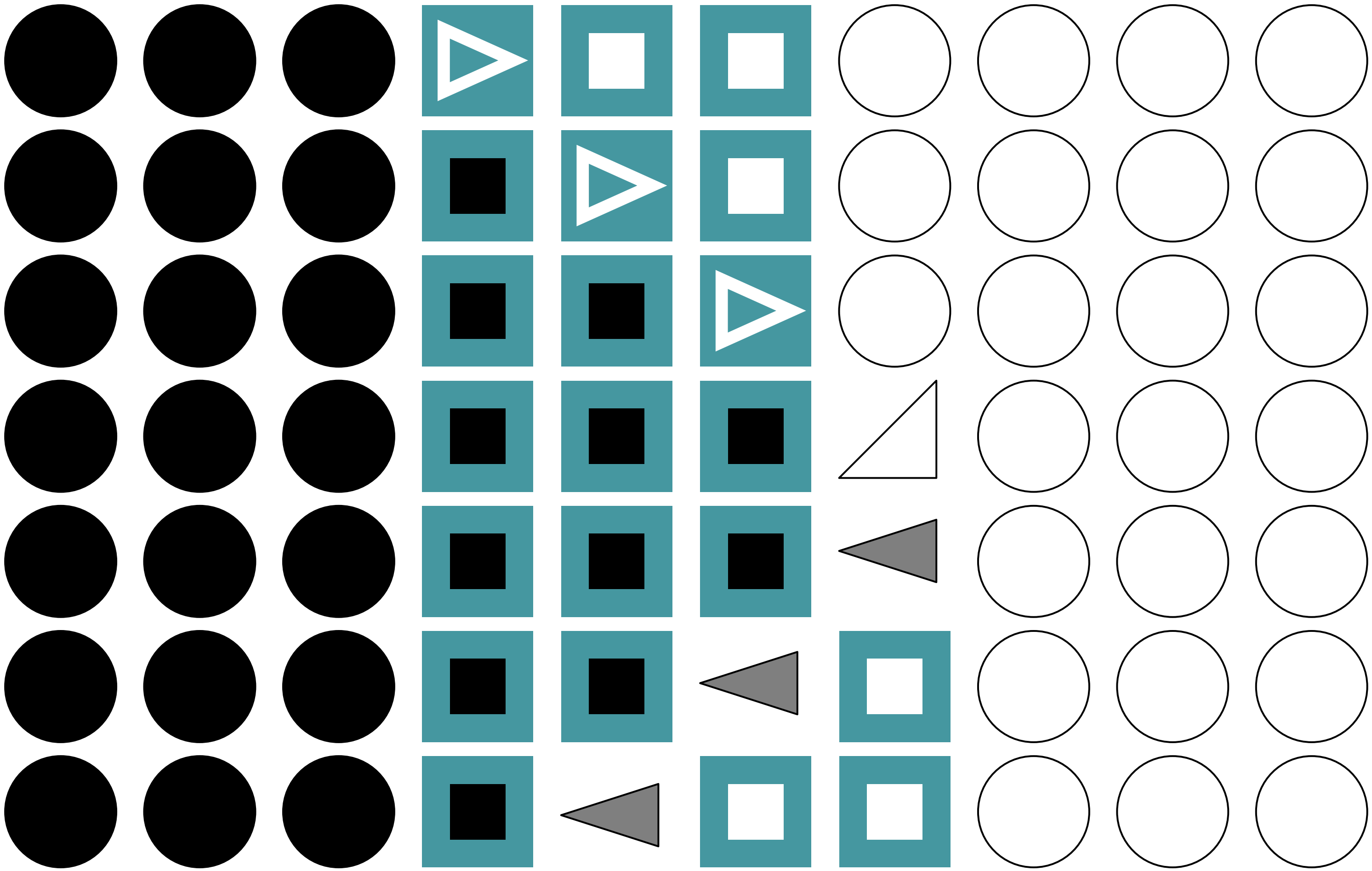
[Aharonov, Gottesman, Irani, Kempe]



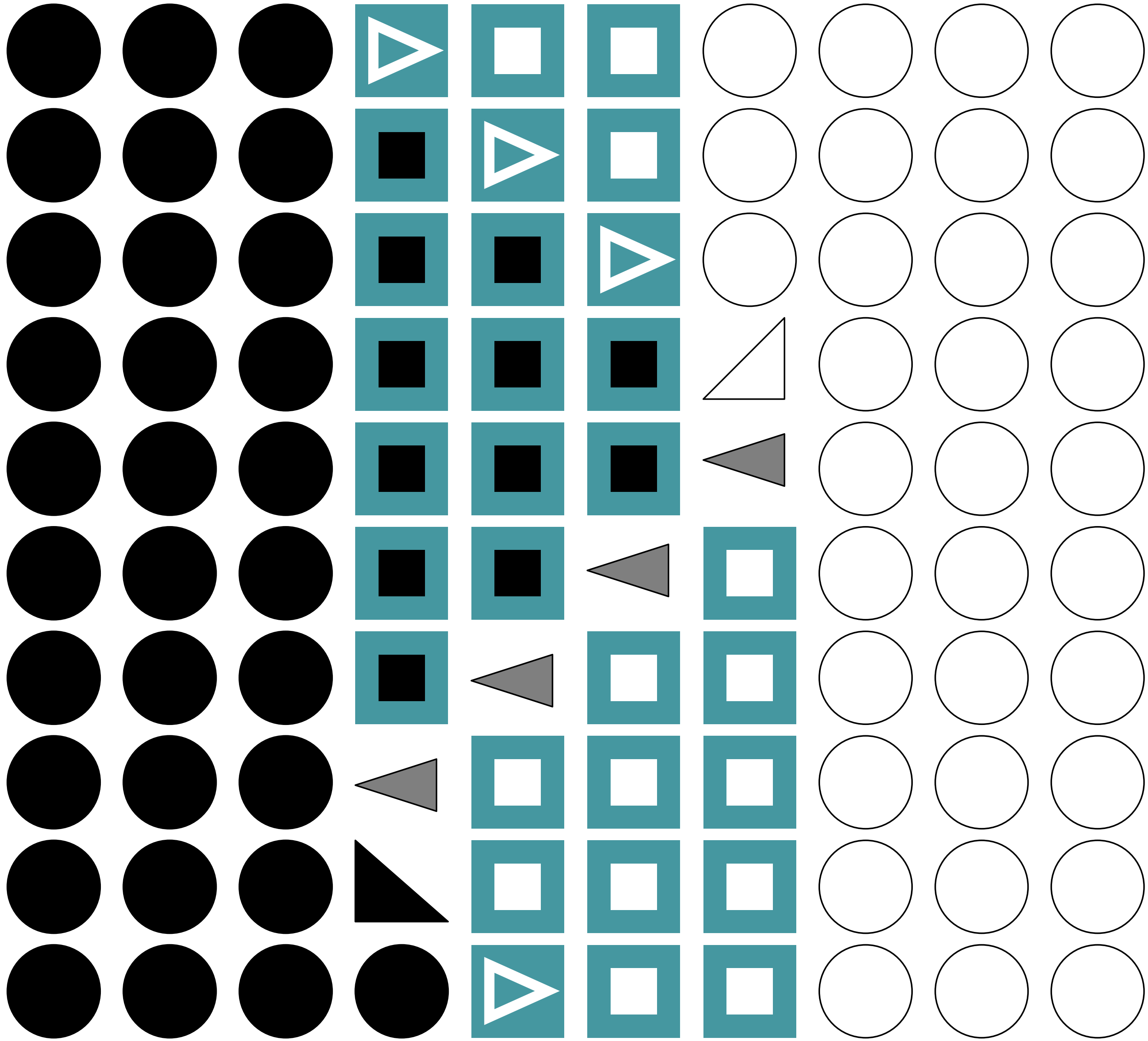
the **power** of quantum systems on a line

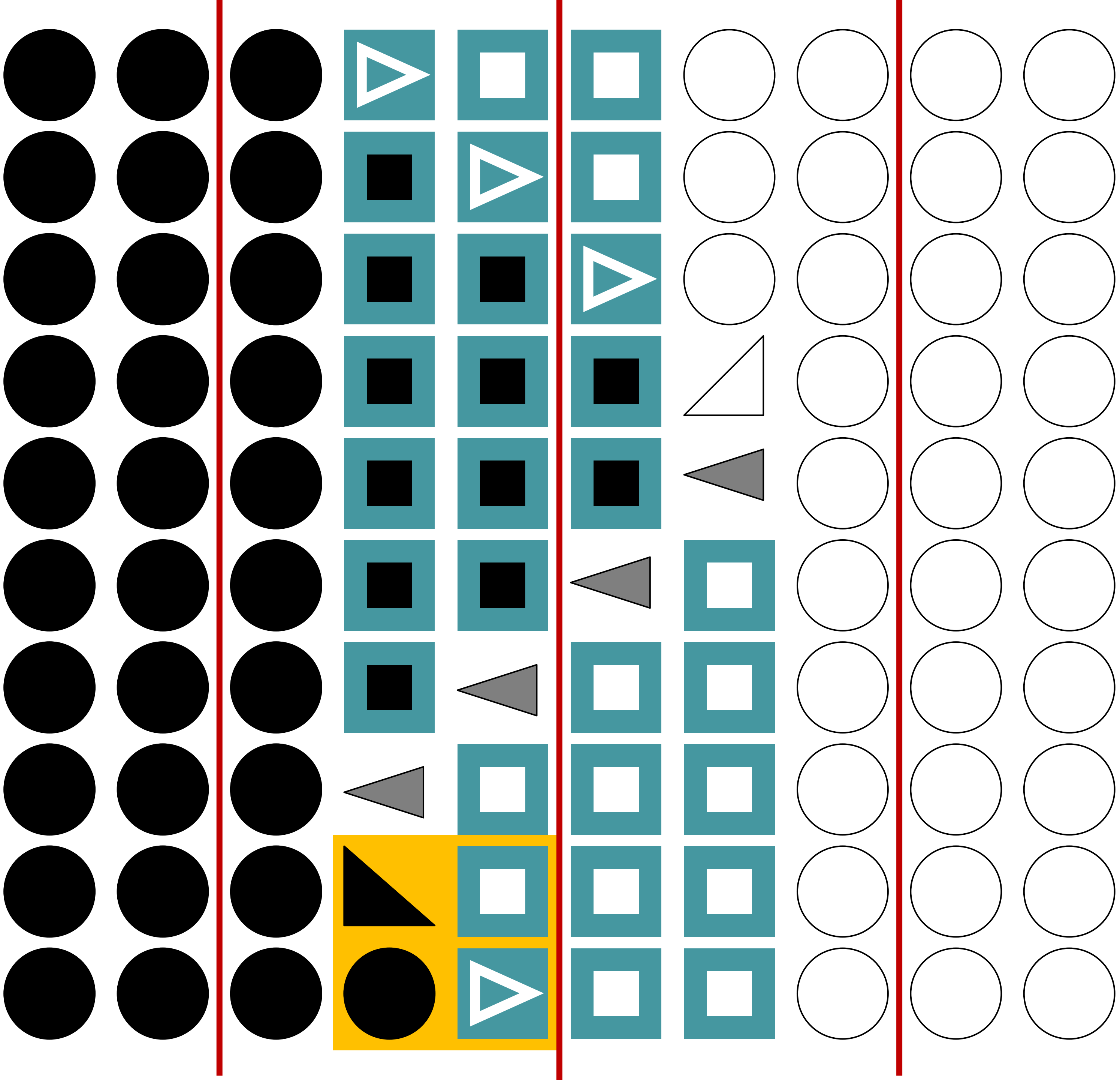


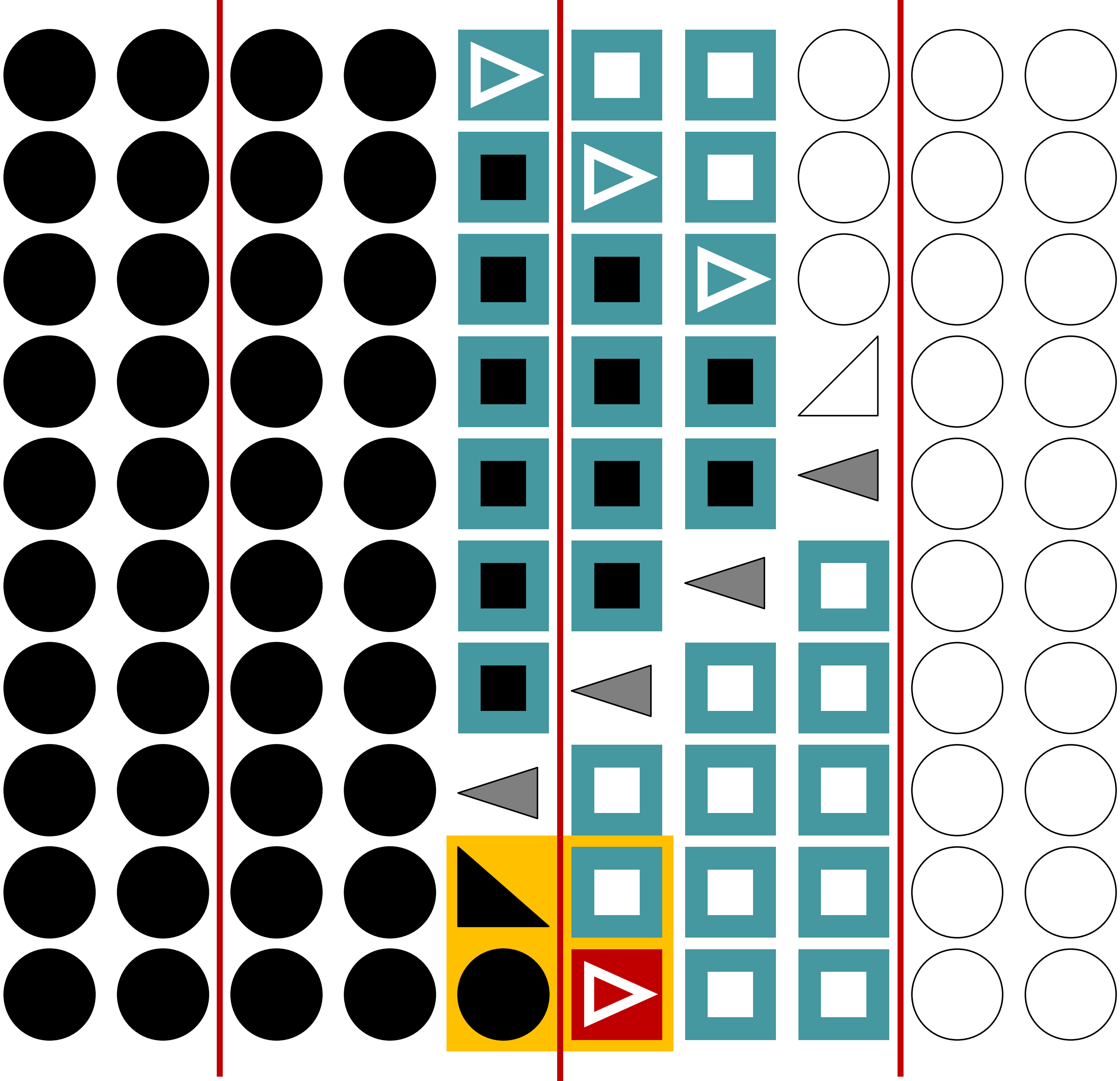
moving the data



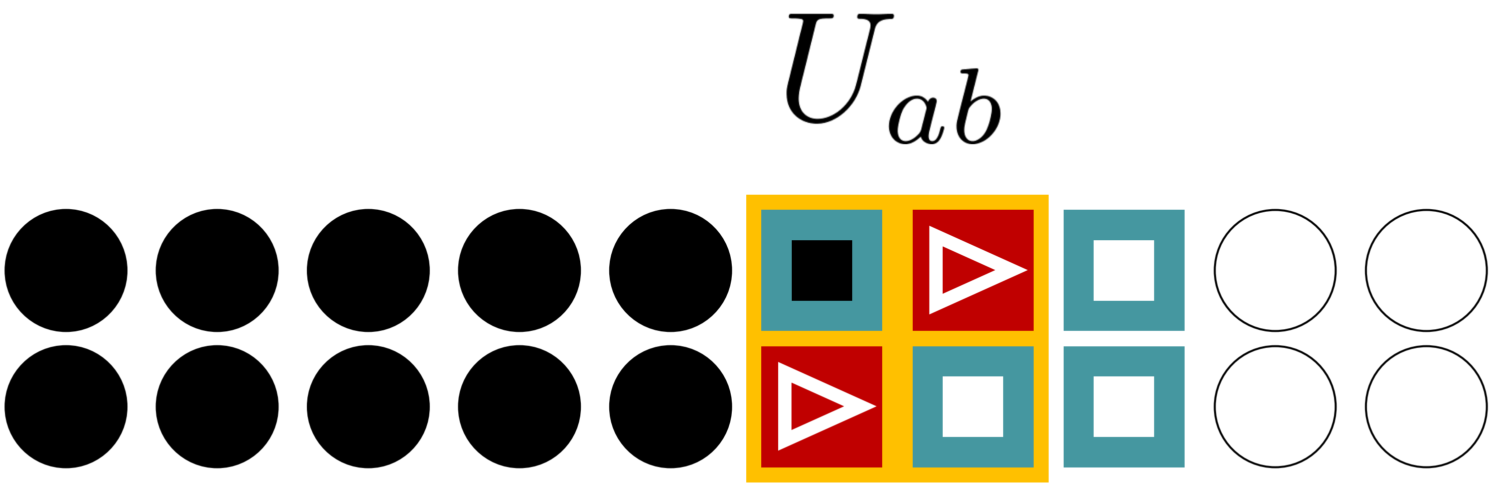
moving the data

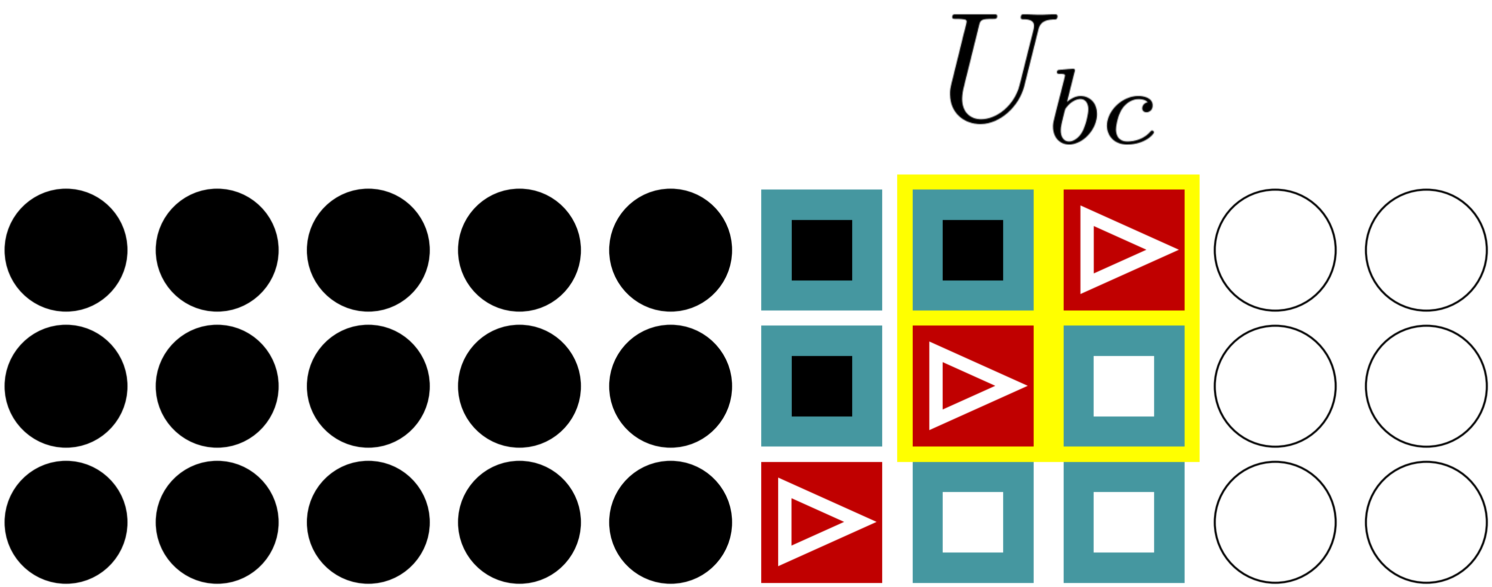




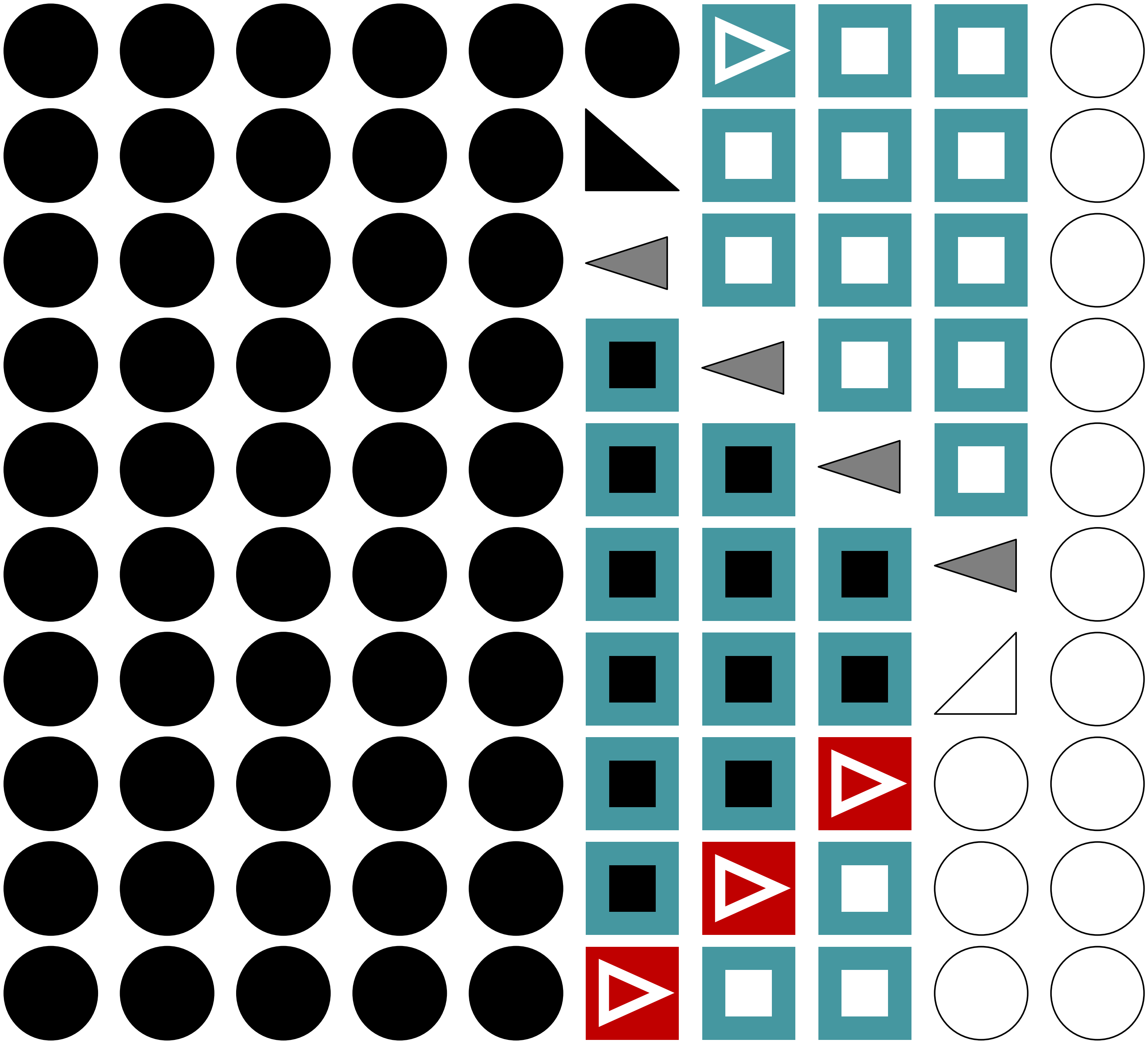


applying gates





U_{bc}



1 LH in 1D with qudits

- a unique state progression

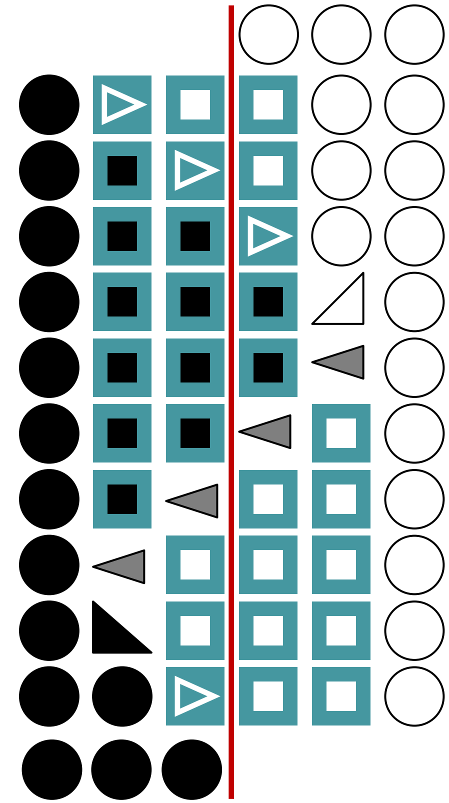
  every legal state goes
  to exactly 2 states

- an entangled ground state

  run a NP verification:
  poly(n) MPS [Schuch]

- clairvoyance

  allowed but illegal states
  evolve to forbidden ones



QMA-complete

d=13

[AGIK '06]

1 LH in 1D with qudits

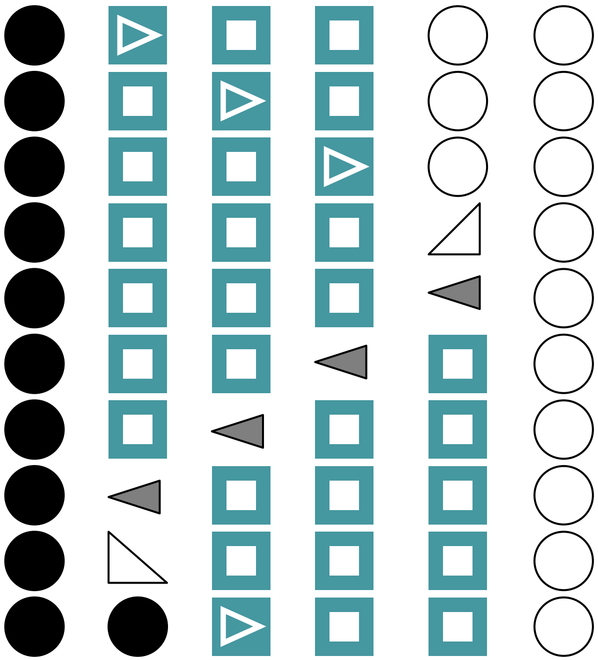
- a unique state progression

  every legal state goes
  to exactly 2 states

- an entangled ground state

  run a NP verification:
  poly(n) MPS [Schuch]

- trade space/parity
  for local dimension



QMA-complete

d=11

[N. 08] [AGIK '06]

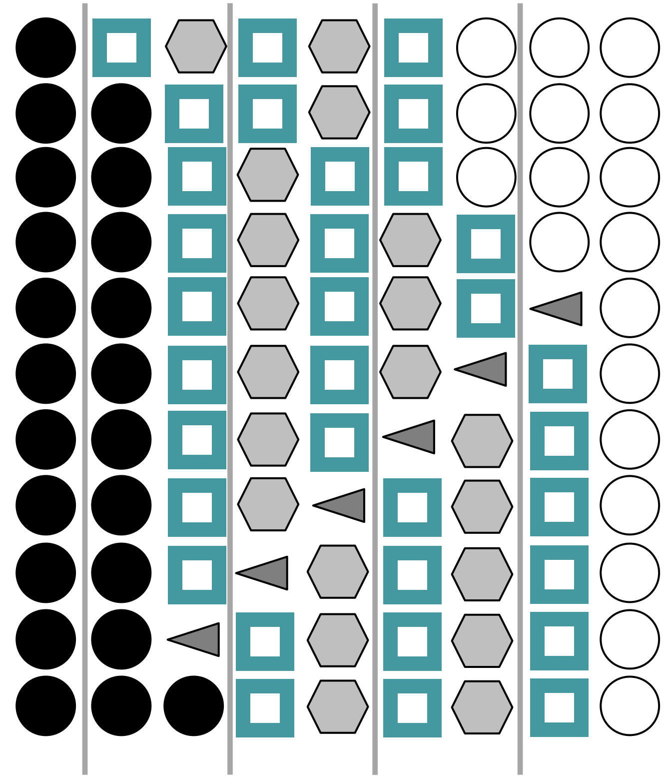
1 LH in 1D with qu$_d$its

- non-unique transitions

  bad ones caught immediately

  $$\langle\psi_{hist}|H^{(8)}_{prop}|\psi_{hist}\rangle = 0$$

- trade space/parity for local dimension

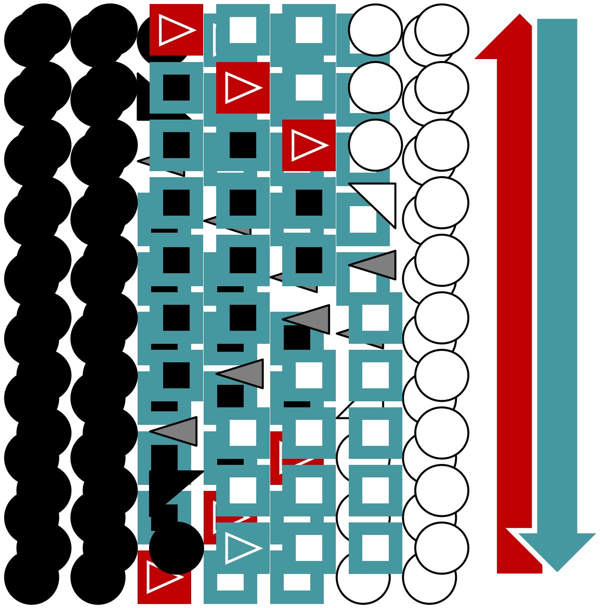


QMA-complete

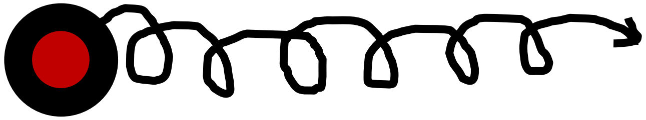
d=8

[Hallgren, N. Narayanaswami '13]

1 Translationally invariant 2-local Hamiltonian (grid)

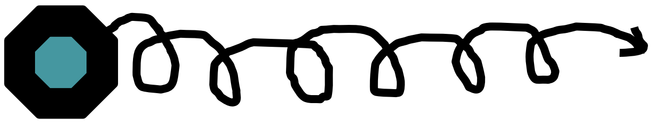


layer 1



runs a counting machine that counts and writes down N, using $\log(N)$ bits

layer 2



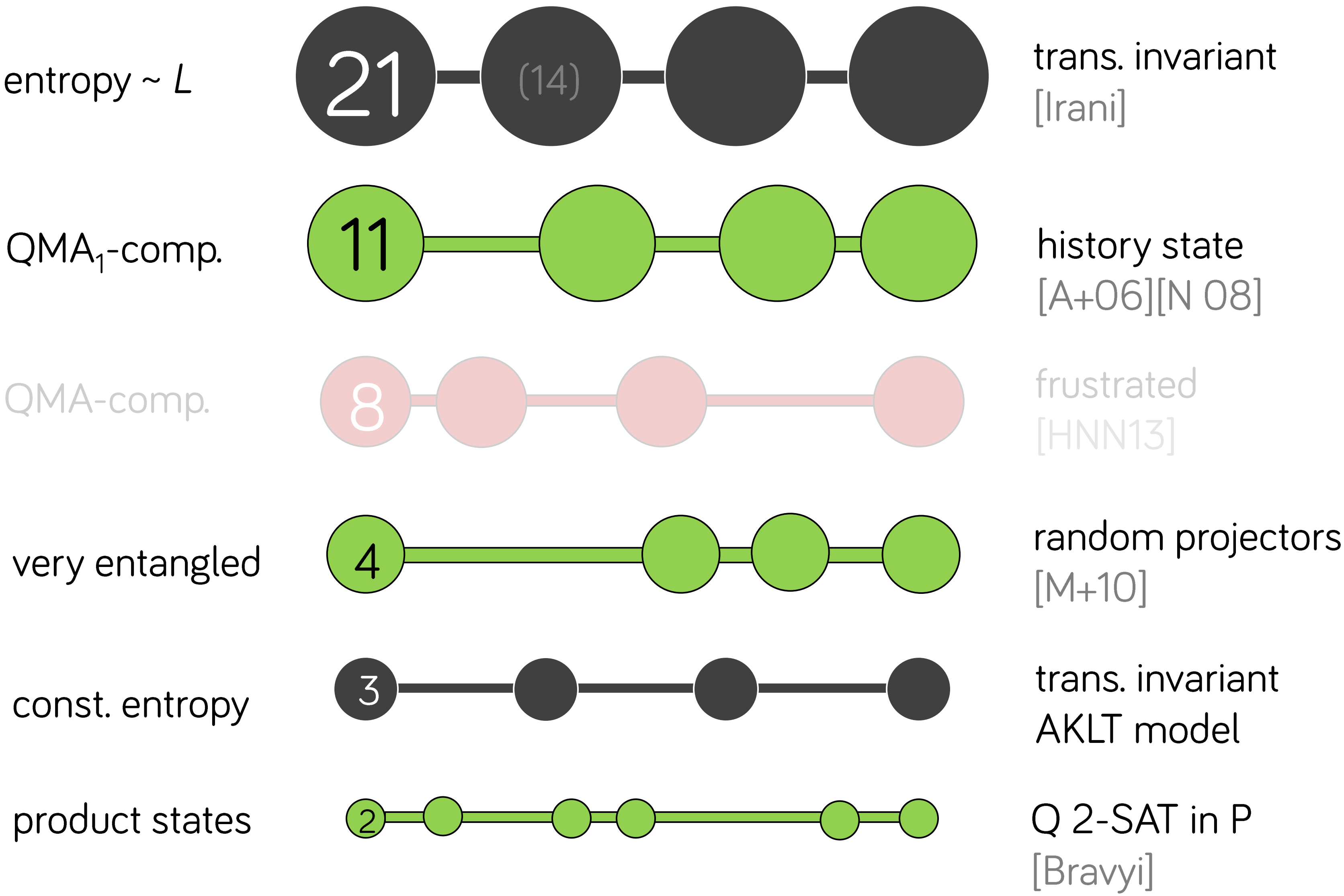
runs a universal TM on input N

- **HUGE** qudits (many kinds of tiles)
- $N \times N$ grid ... $\log(N)$ size QMA verifier circuit

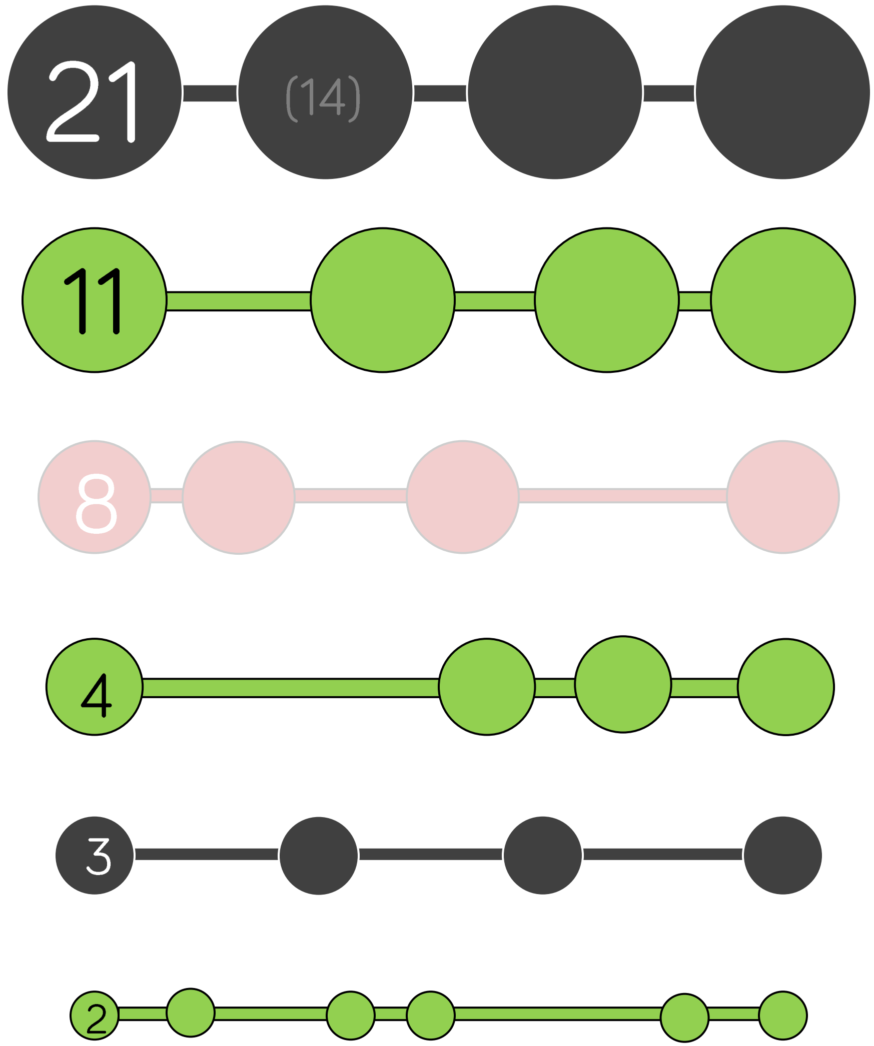
QMA$_{EXP}$-complete

[Gottesman, Irani '09]

1 Unfrustrated ground states in 1D



1 Unfrustrated ground states in 1D



entropy ~ L — trans. invariant [Irani]

QMA_1-comp. — history state [A+06][N 08]

QMA-comp. — frustrated [HNN13]

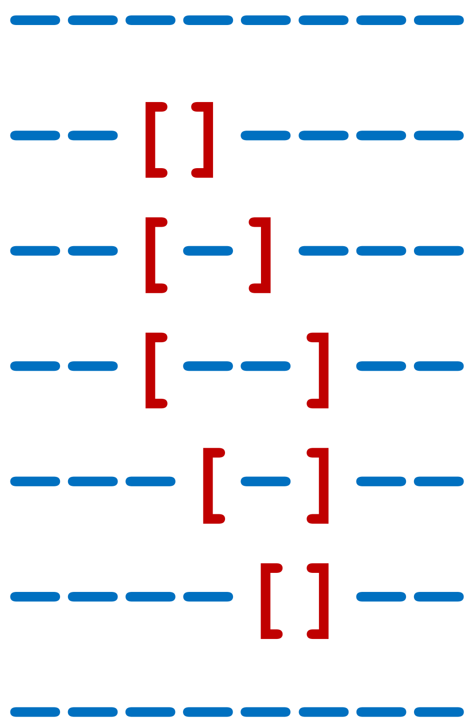
very entangled — random projectors [M+10]

■ entropy ~ log L — trans. invariant [B+'12]

product states — Q 2-SAT in P [Bravyi]

1 A qutrit chain with brackets

- 2-local transition terms



- an unfrustrated ground state, unique, entangled, 1/poly-gap

well-bracketed words

[Bravyi Caha Movassagh N Shor 12]

DMRG

[White 92]

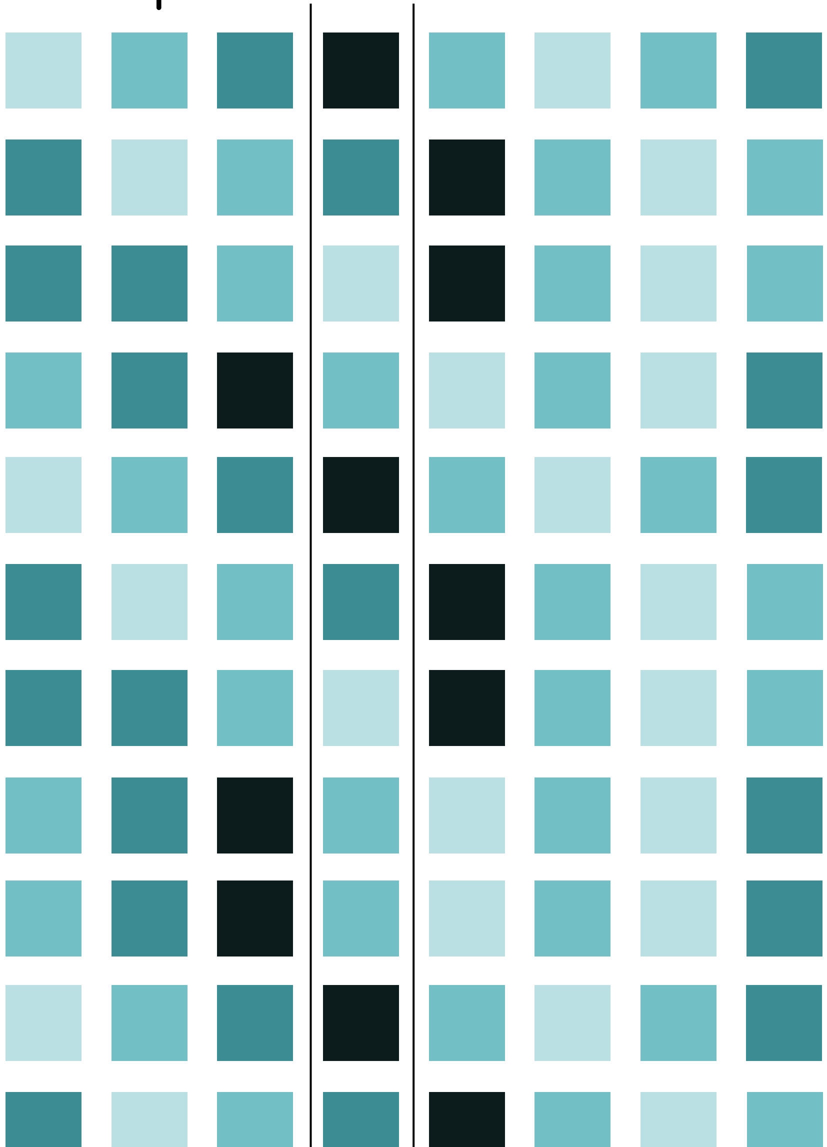
the algorithms we have

DMRG, tDMRG, TEBD, MPS, cMPS, TDVP, MERA, iPEPS, …

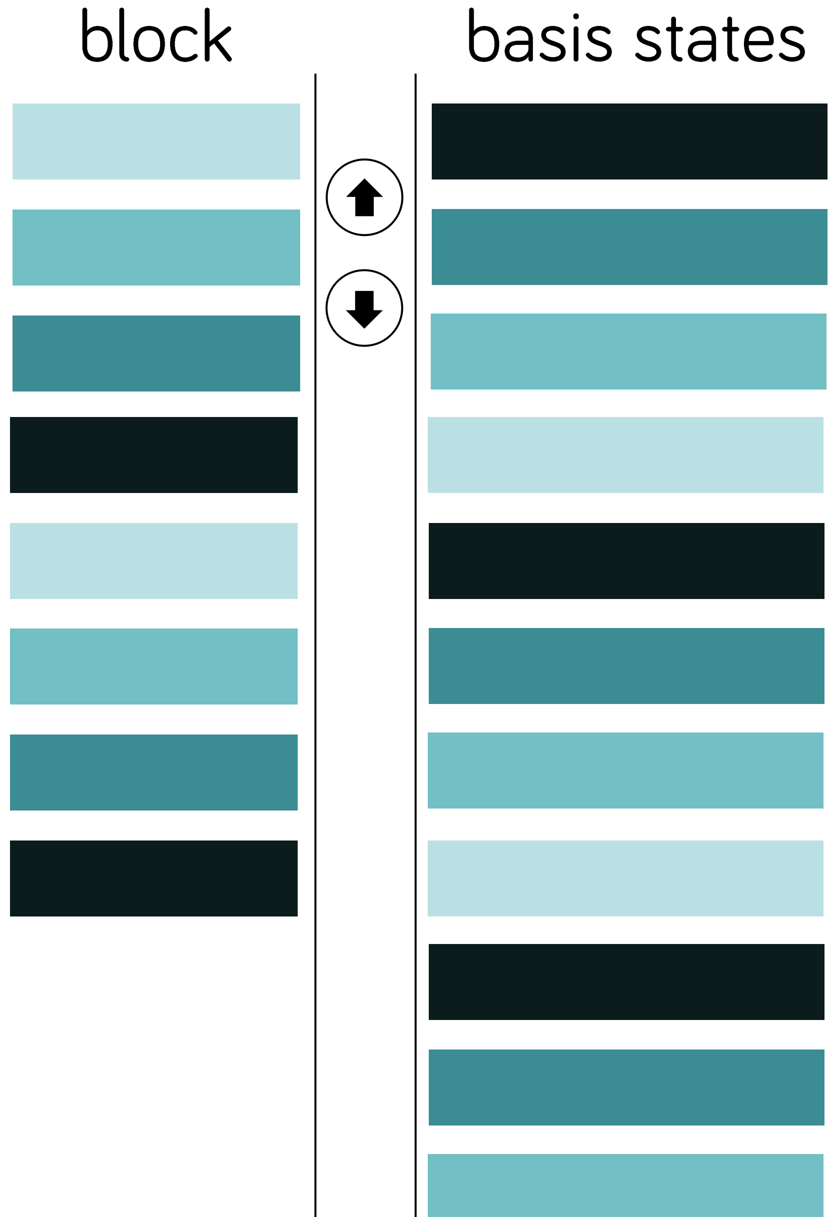
1D gapped, 2-qSAT, almost independent commuting

2 DMRG (simplified)

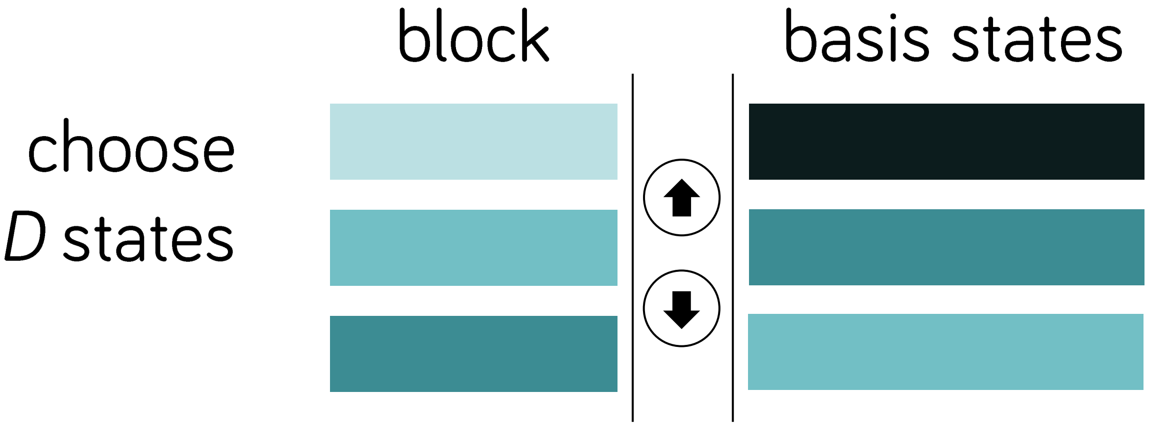
computational basis states



2 DMRG (simplified)

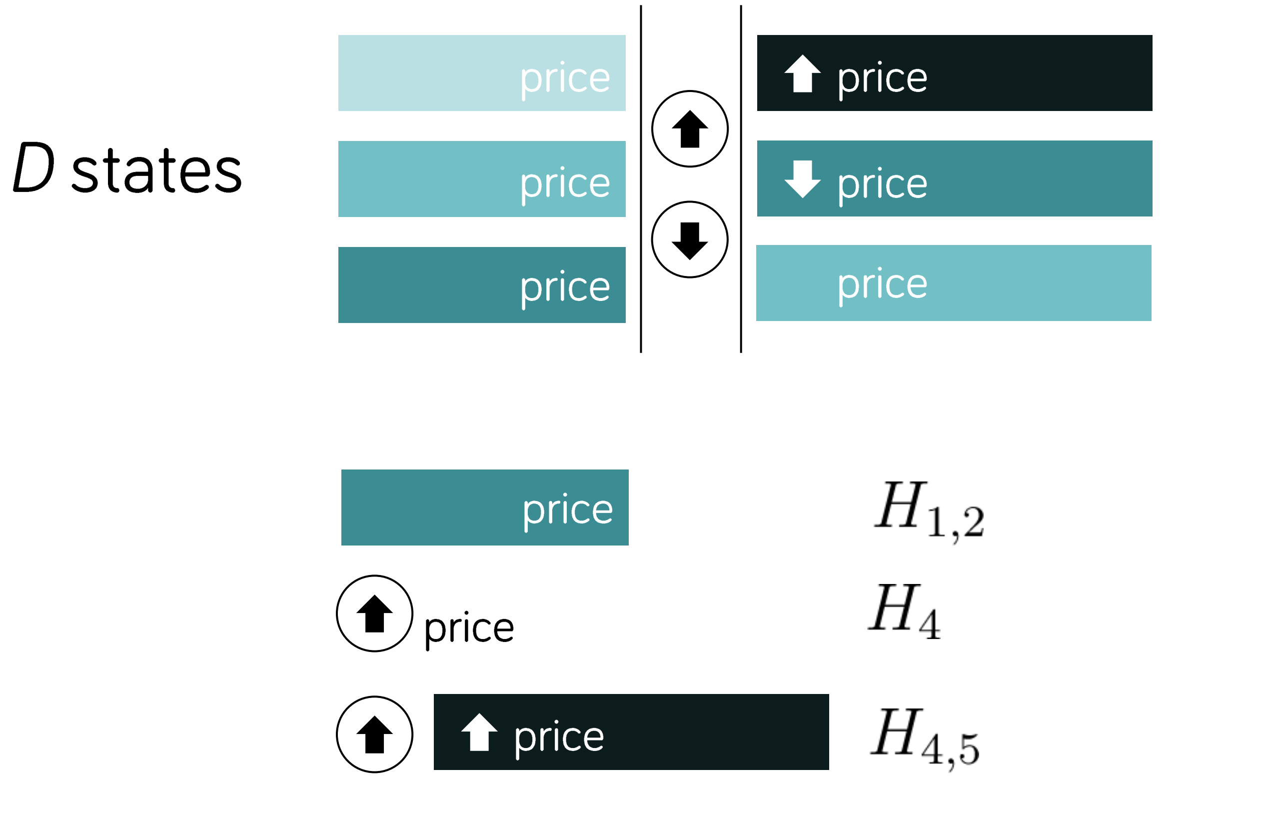


2 DMRG (simplified)



➡ doing our best within some basis ...

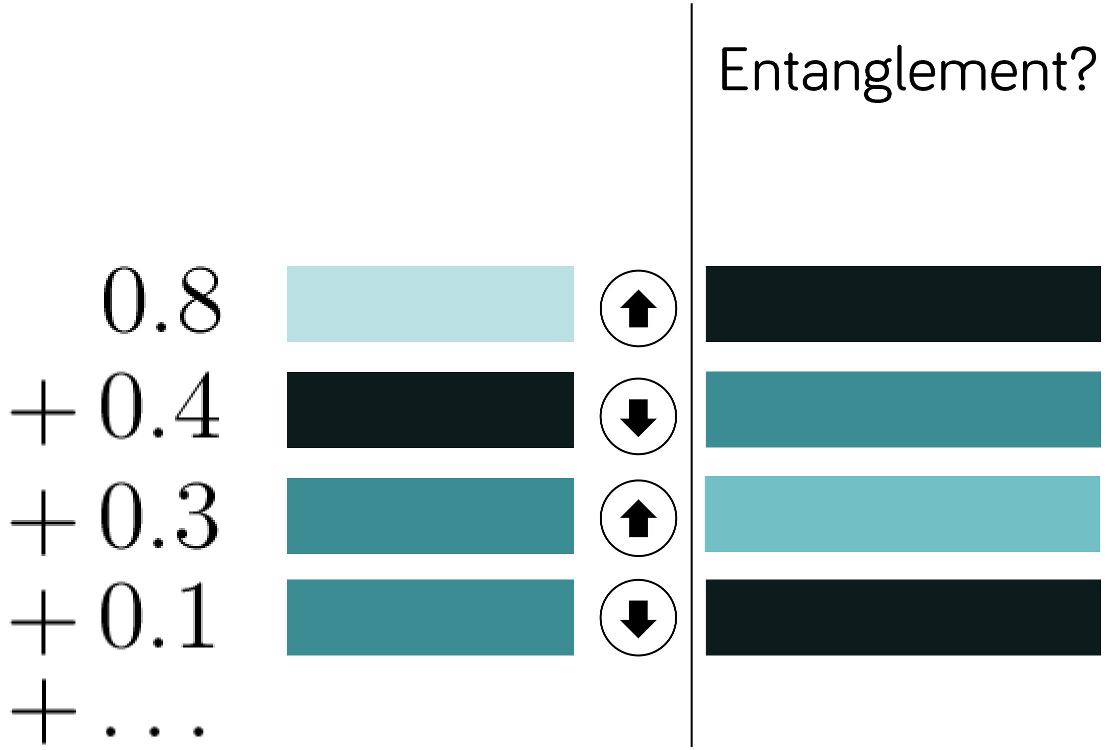
2 DMRG (simplified)



an effective Hamiltonian (dD^2)

find the best state (*Lanczos*)

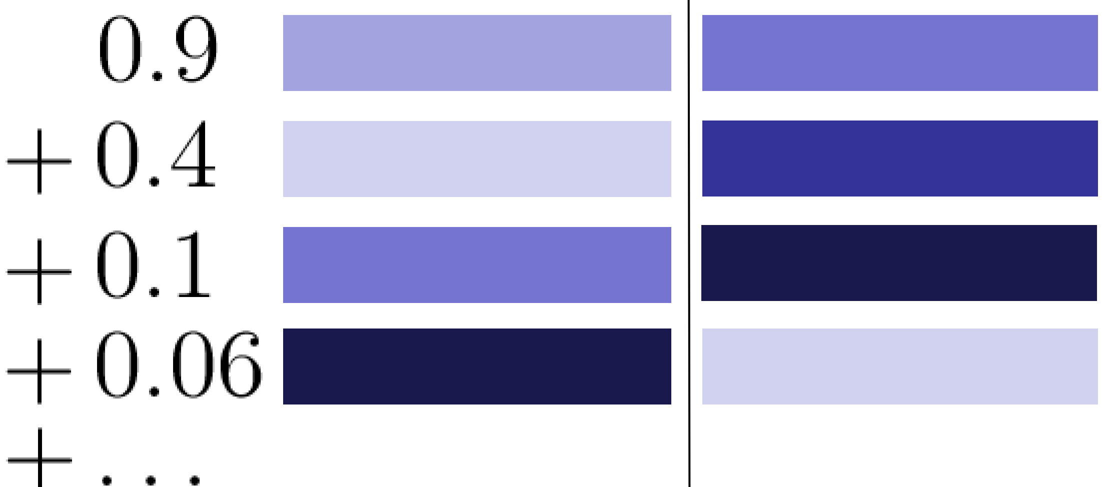
2 DMRG (simplified)



→ find the best state (*Lanczos*)

2 DMRG (simplified)

Schmidt decomposition

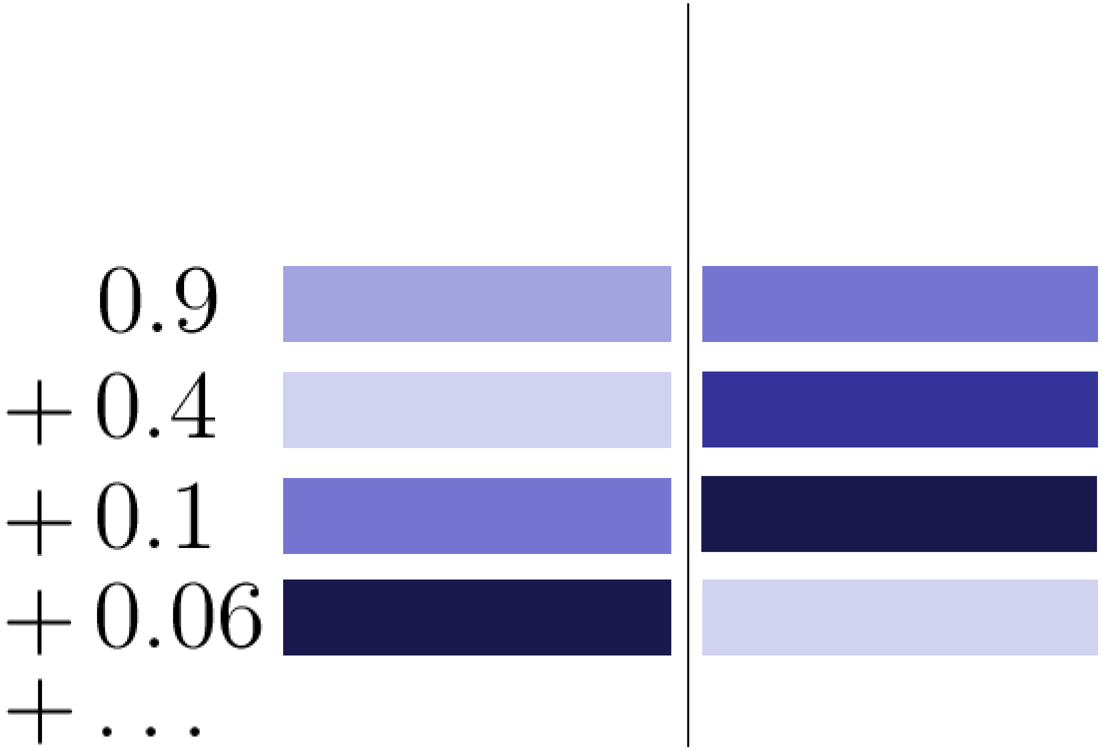


the best state

reduced density matrix

diagonalize it (or just QR)

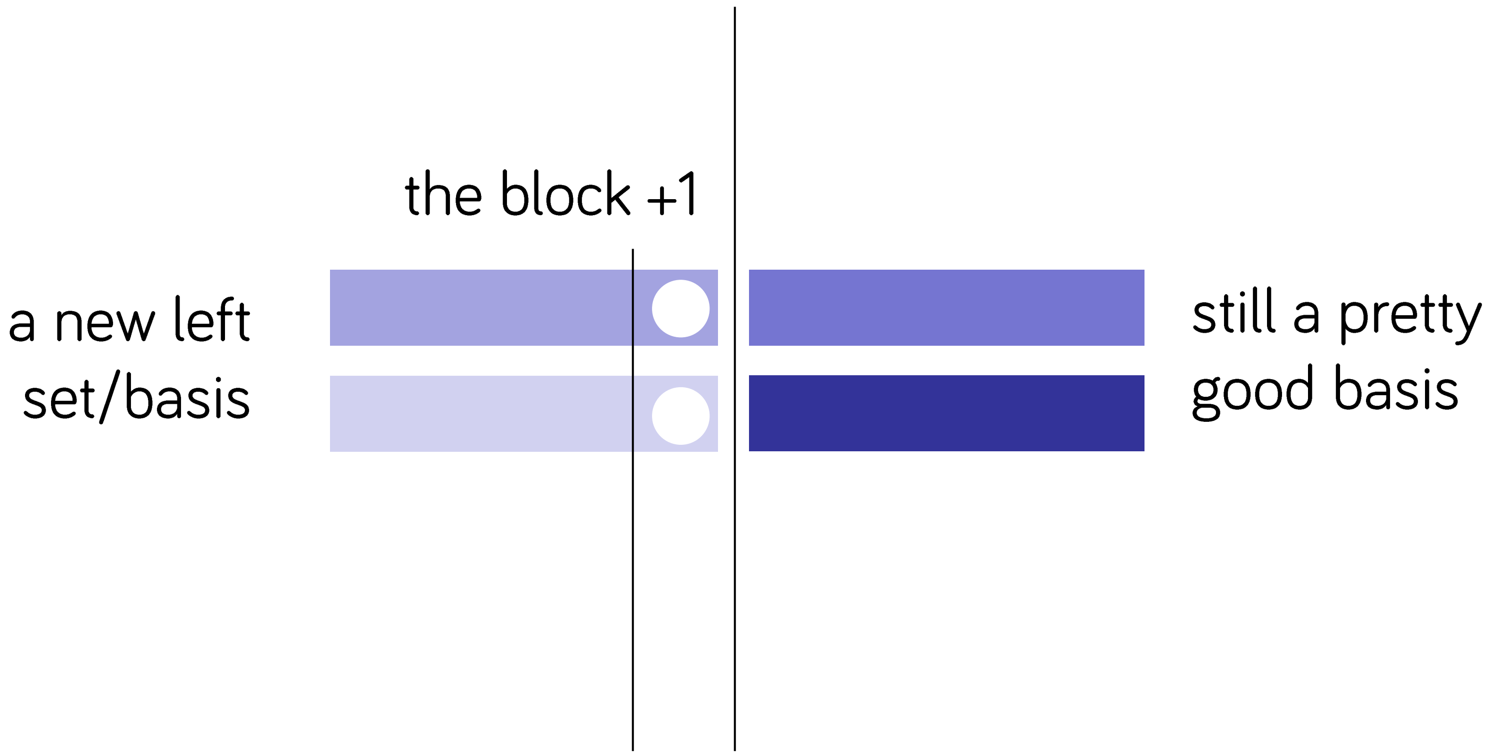
2 DMRG (simplified)



still a pretty good state

→ truncate the state

2 DMRG (simplified)



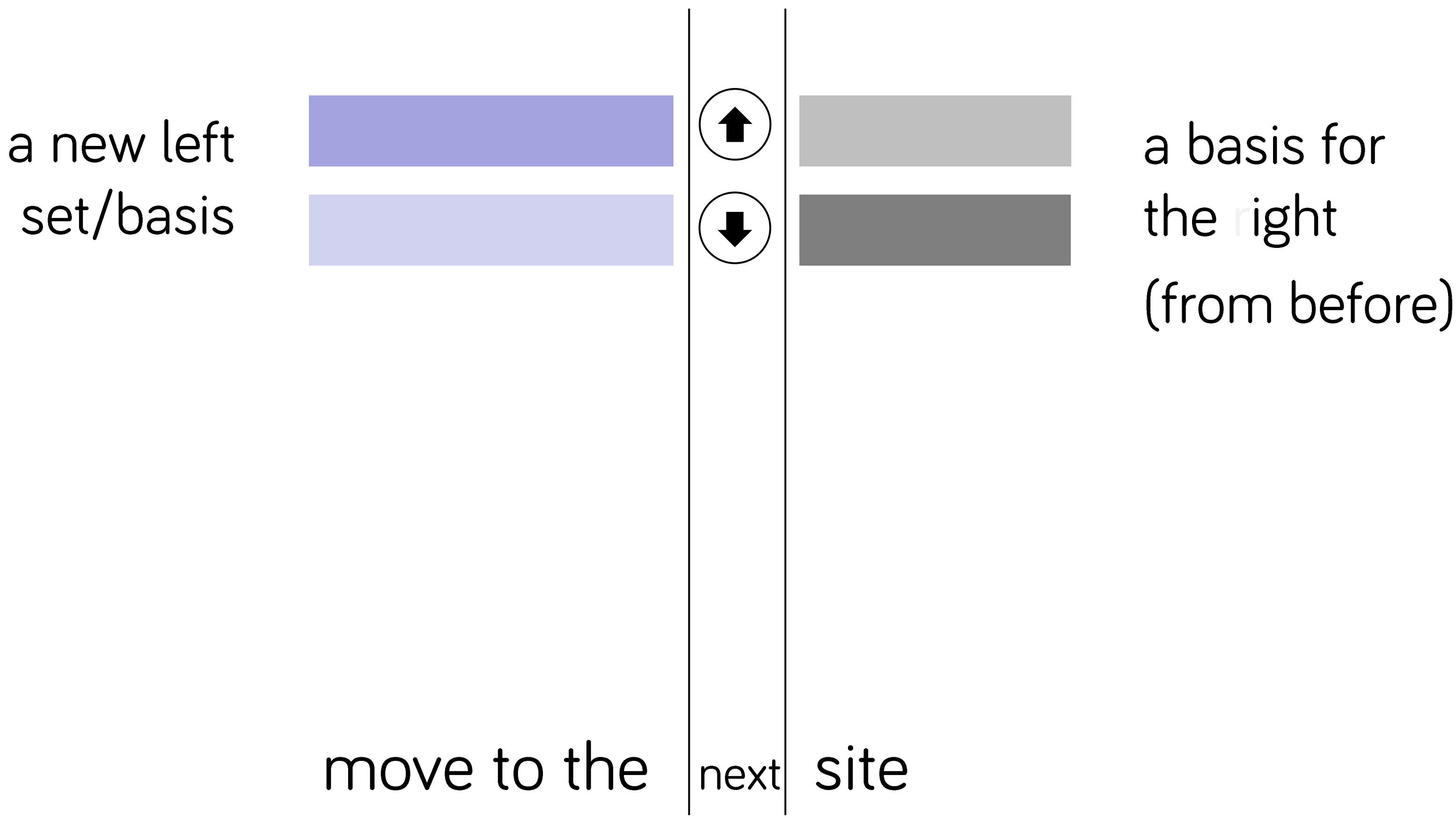
truncate the basis

2 DMRG (simplified)

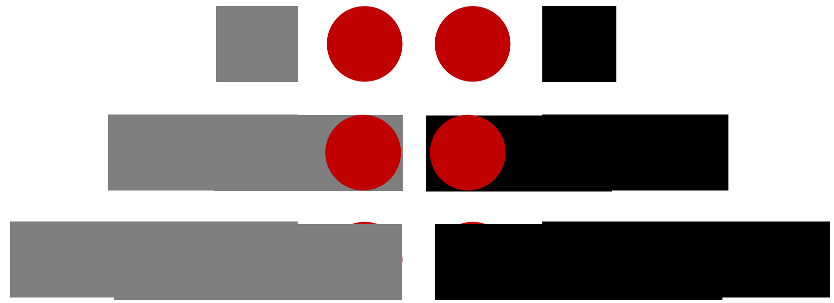
a new left set/basis

➡ form a new set for block +1
recalculate the costs

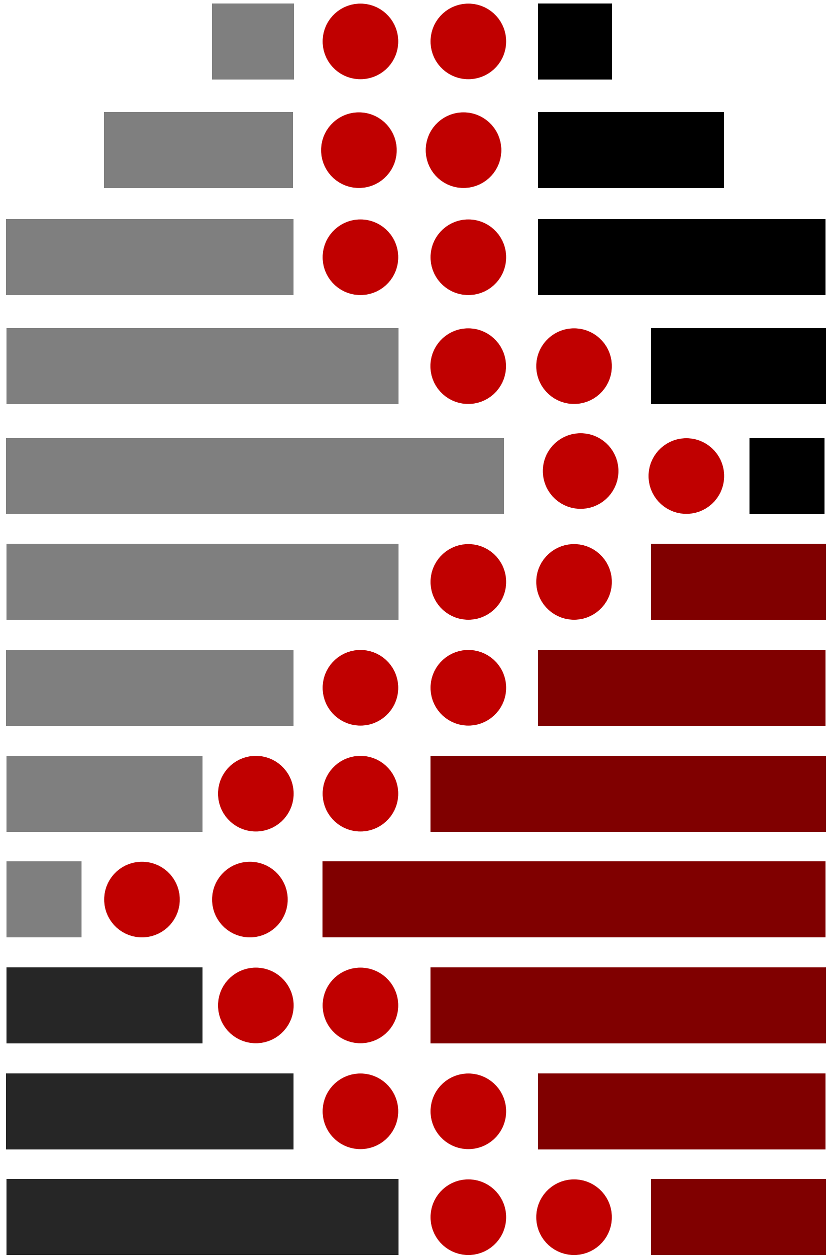
2 DMRG (simplified)



2 Build & sweep



2 Build & sweep

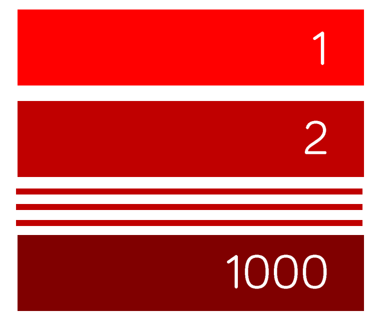


2 DMRG works fantastically in 1D

- a critical benchmark
  (AF Heisenberg chain)

100 *spins*
300 *states*
1 *sweep*
3 *minutes*
$\mathbf{10^{-13}}$ *relative error*

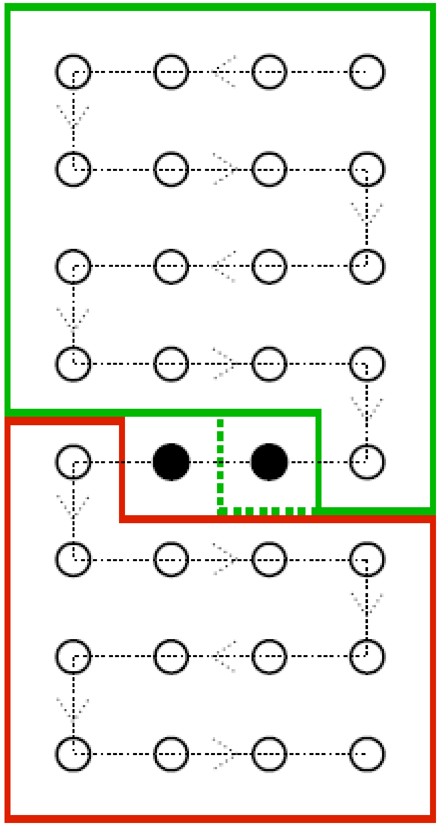
[A. Gendiar]

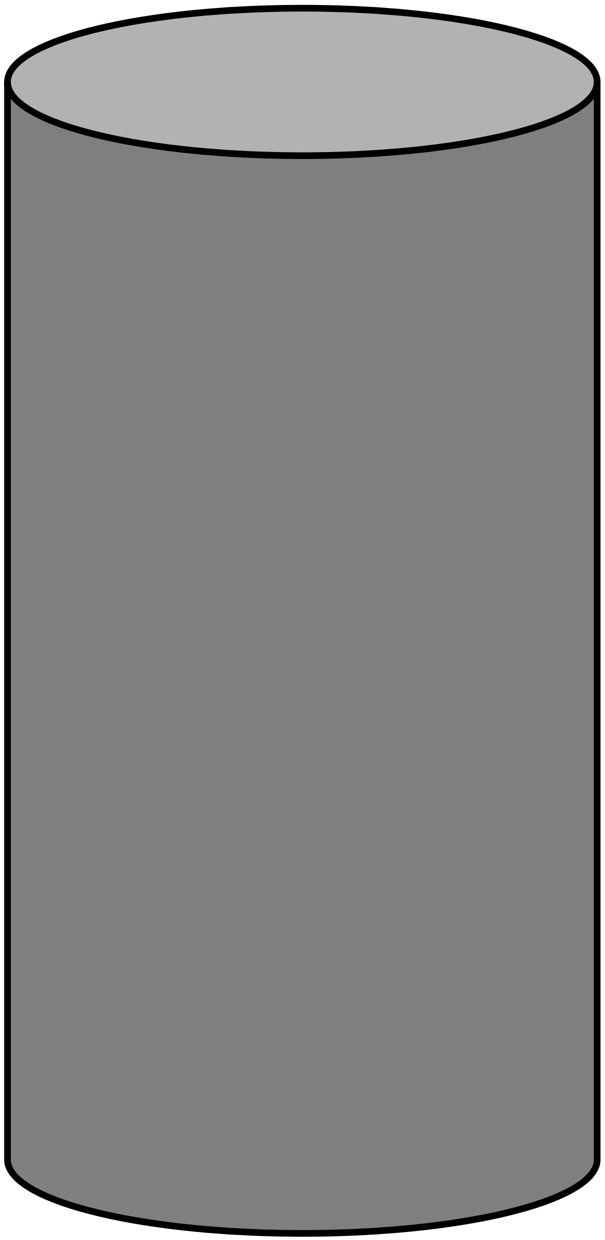


- get the excitations too

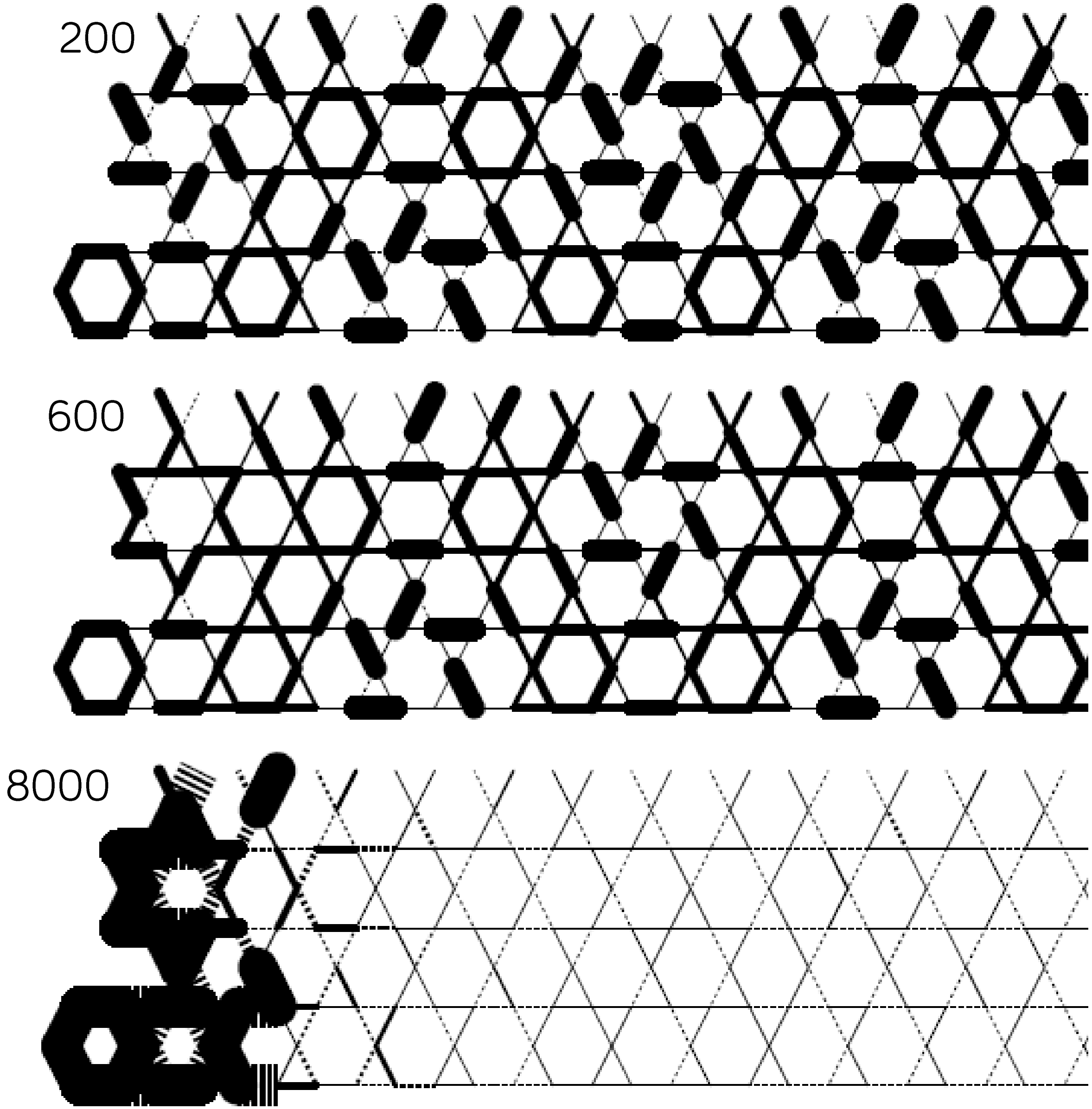
- slowdown?
  big spins (Hubbard: interacting fermions + spin)
  non-tree geometry
  open boundary conditions

[Schollwoeck 11: *DMRG in the age of MPS*]





[N. Mori]

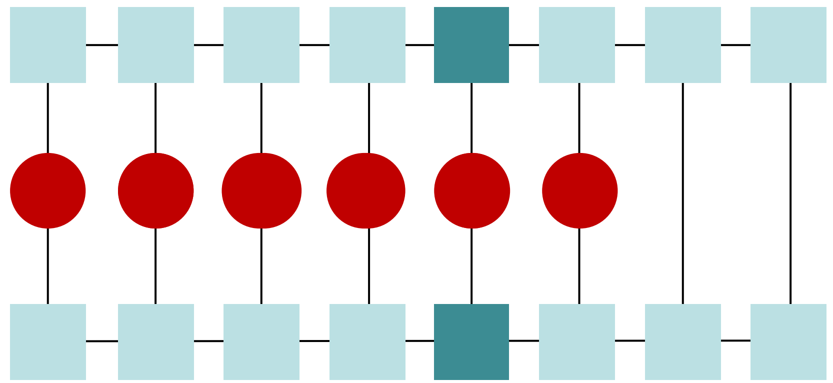


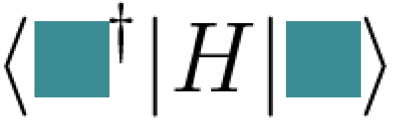
Kagome lattice, Heisenberg AF spin-½

spin liquid instead of HVBC

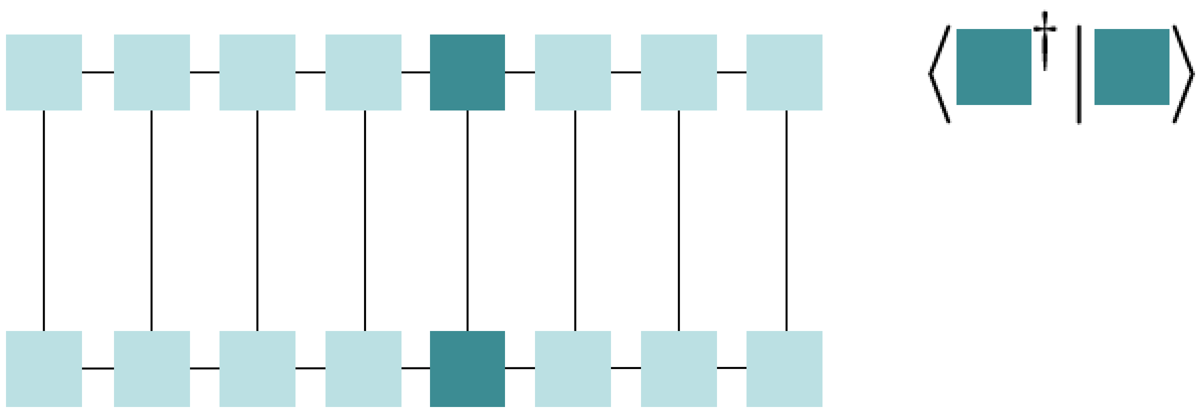
[Yan, Huse, White 11]

2 Variational MPS





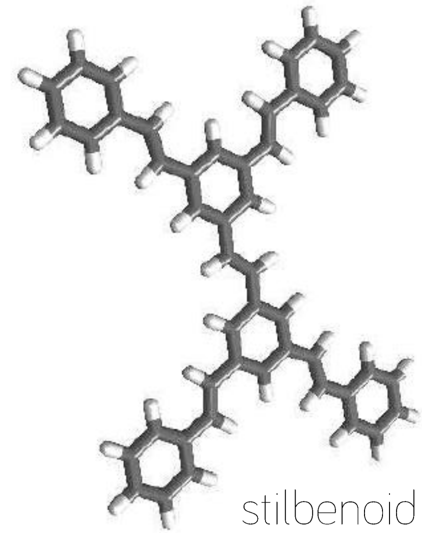
2 Variational MPS



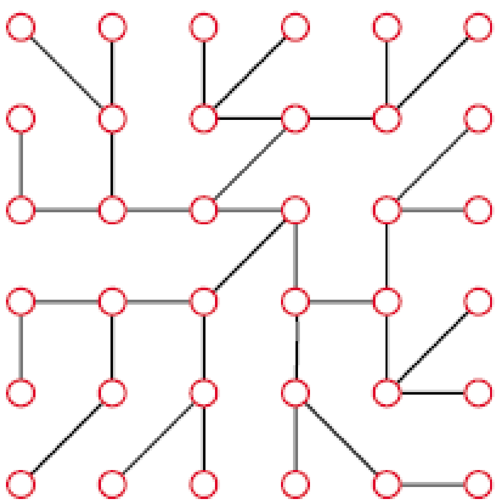
2 Tree Tensor Networks

- electronic structure calculations
  orbitals, 4-local interactions

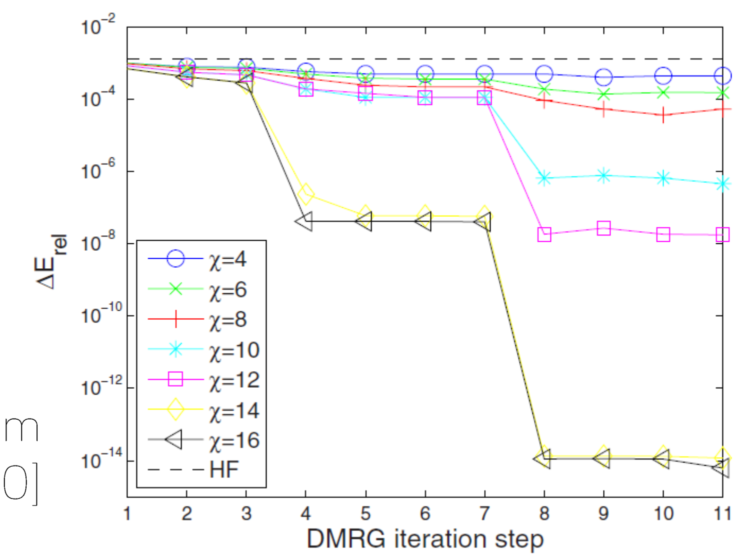
- shorter distances (log *N*)
  assign the tree wisely
  more indices ...



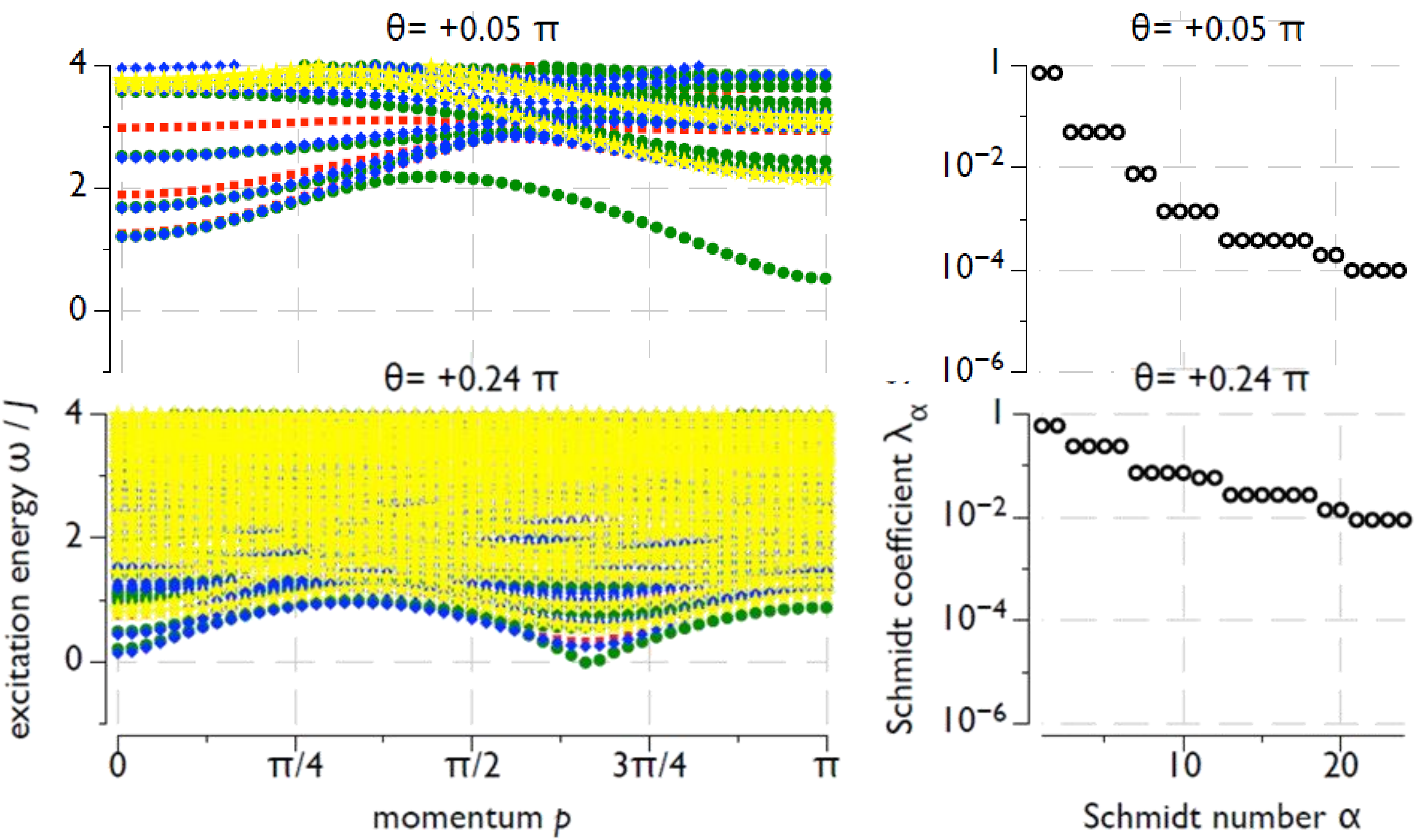
stilbenoid
dendrimers
[Nakatani Chan 13]



berylium
[Murg+ 10]



2 Post-MPS: to tangent space & beyond (TDVP)

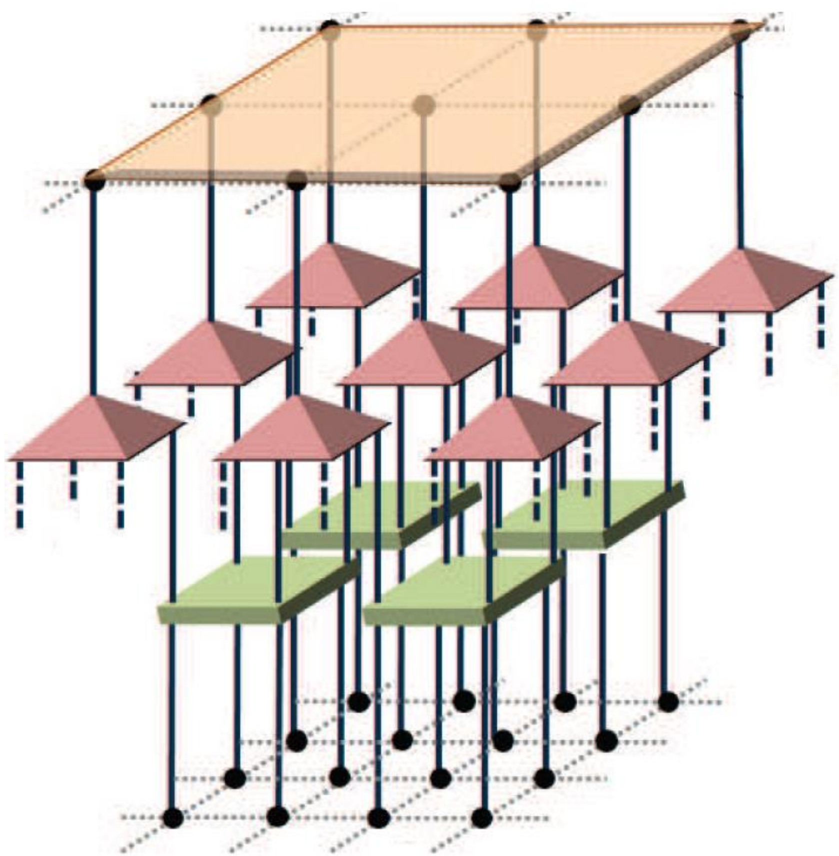


$$\hat{H}_{\mathrm{BB}} = J \sum_{n \in \mathbb{Z}} \cos\theta \left(\hat{S}_n \cdot \hat{S}_{n+1}\right) + \sin\theta \left(\hat{S}_n \cdot \hat{S}_{n+1}\right)^2$$

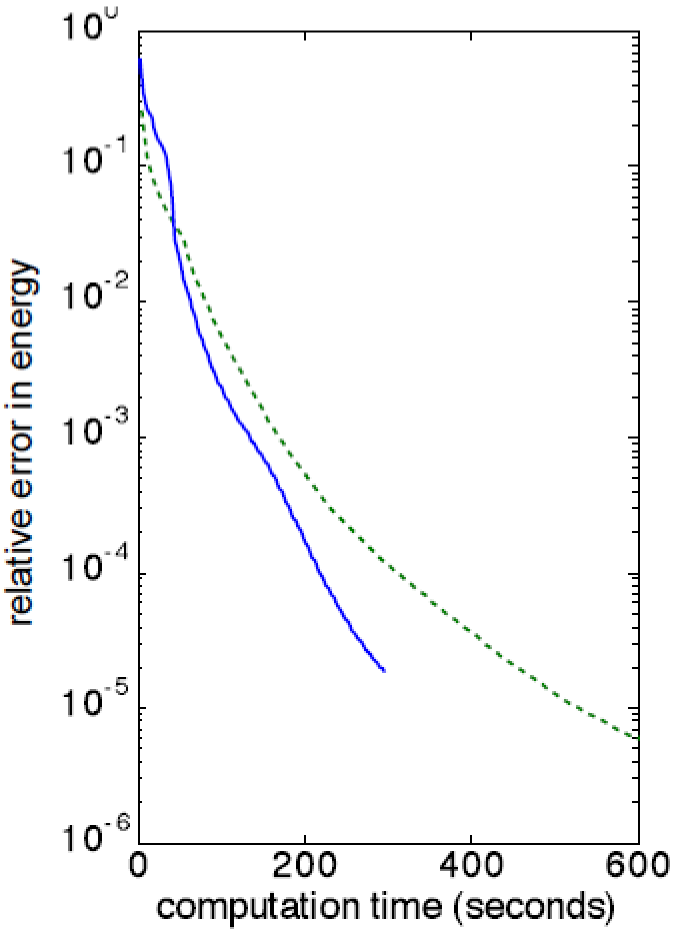
bilinear-biquadratic, s=1 Heisenberg

[Haegeman Osborne Verstraete 13]

2 MERA: renormalization + disentangling

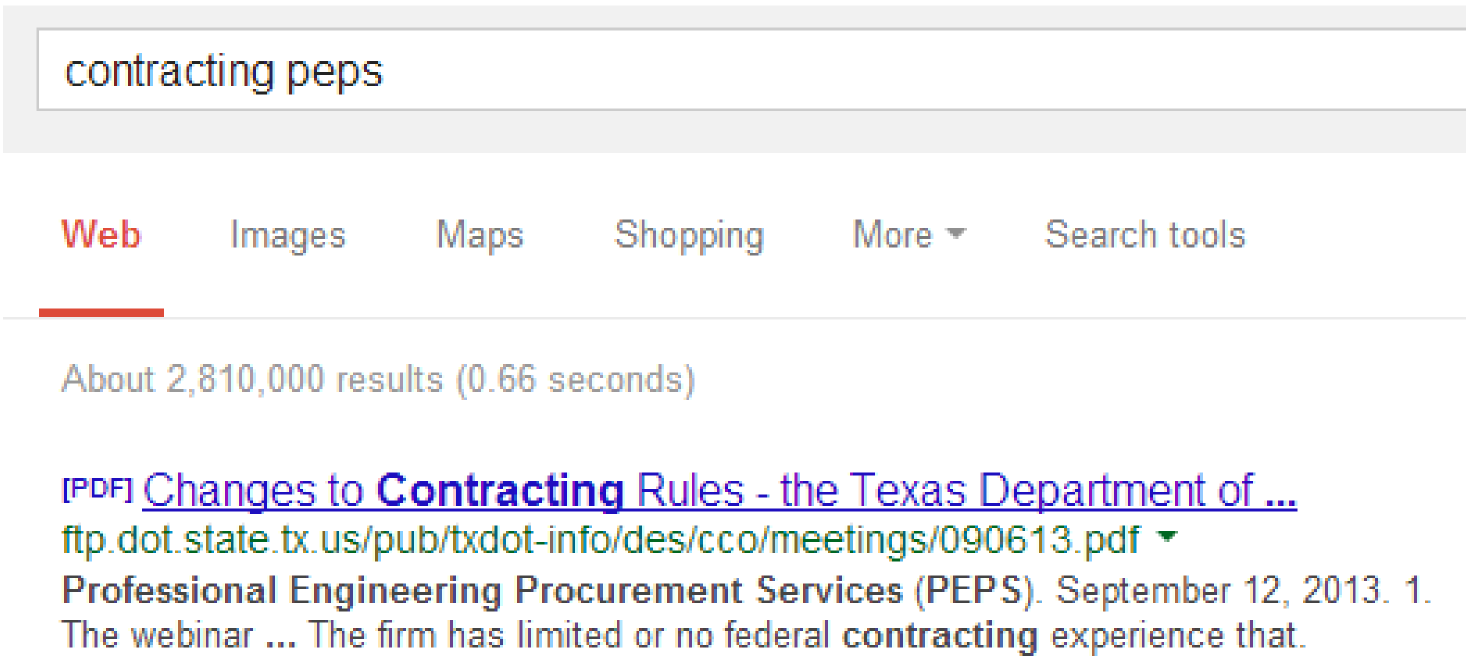


[Evenbly Vidal 13]



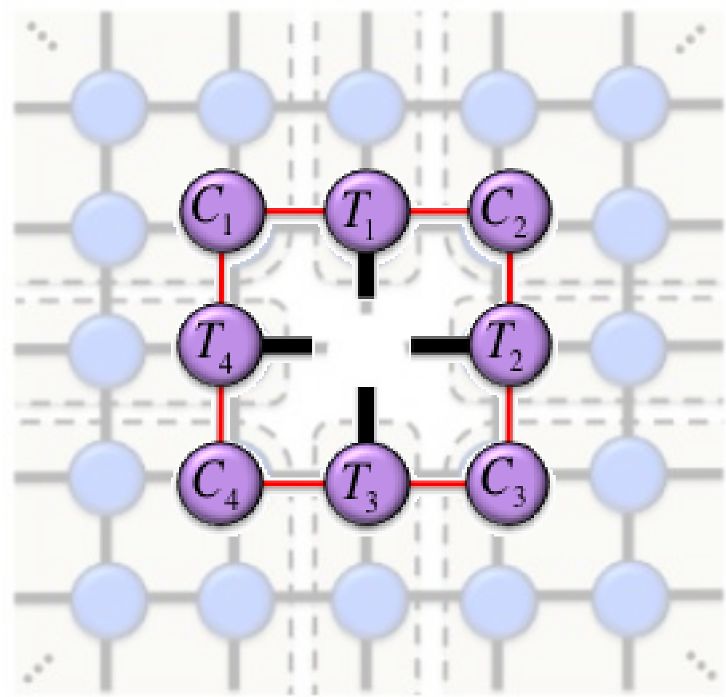
[Evenbly Pfeifer 13]
critical Ising, N=72

2 Contracting PEPS: not a disease

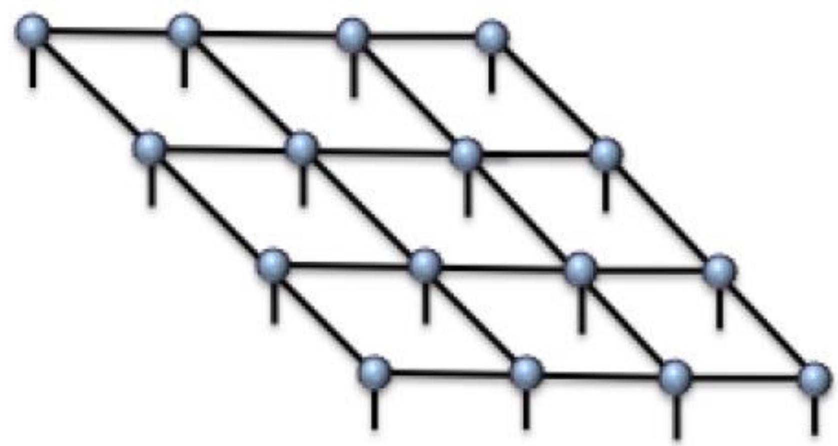


2 Contracting iPEPS approximately

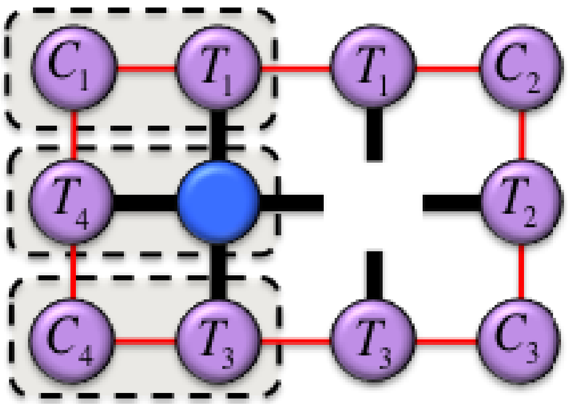
- [Lubasch Cirac Bañuls 13] simple, edge, cluster, …
- CTMRG like (infinite lattice)



[R. Orús]

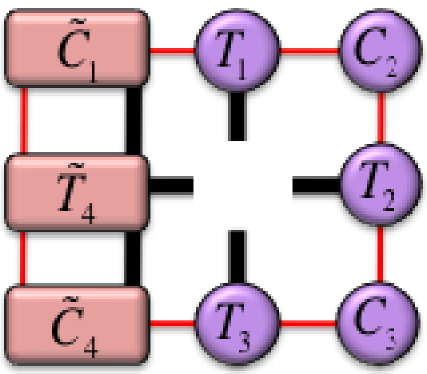


2 Contracting iPEPS approximately



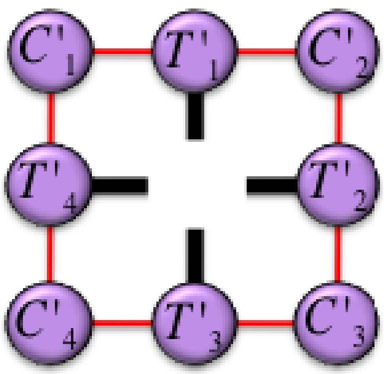
[R. Orús]

2 Contracting iPEPS approximately



[R. Orús]

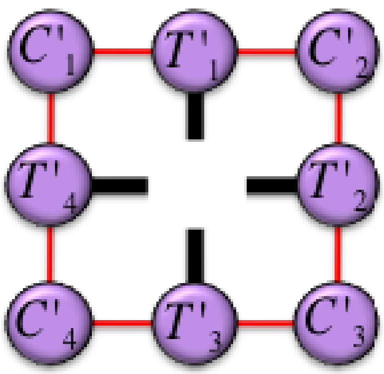
2 Contracting iPEPS approximately



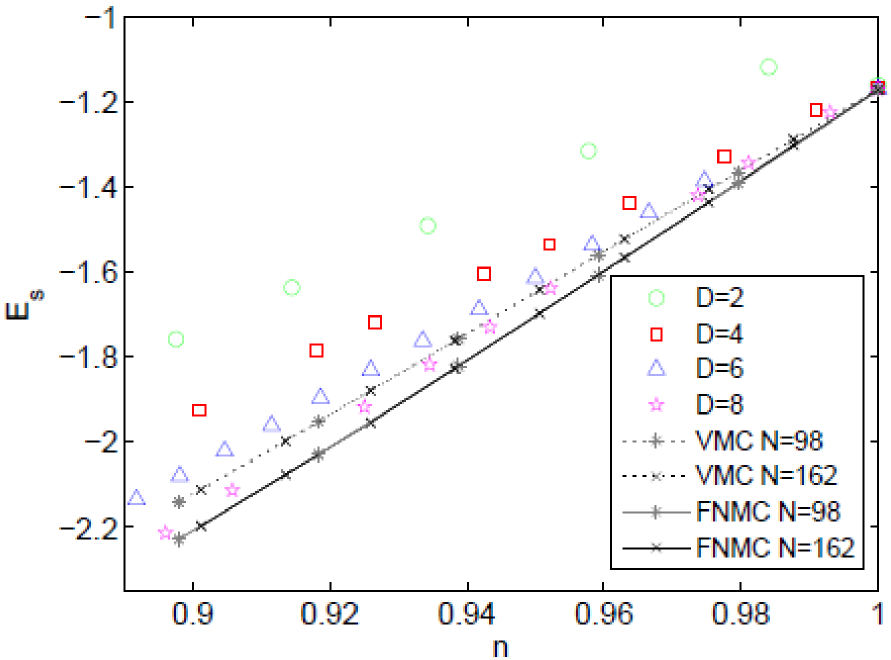
[R. Orús]

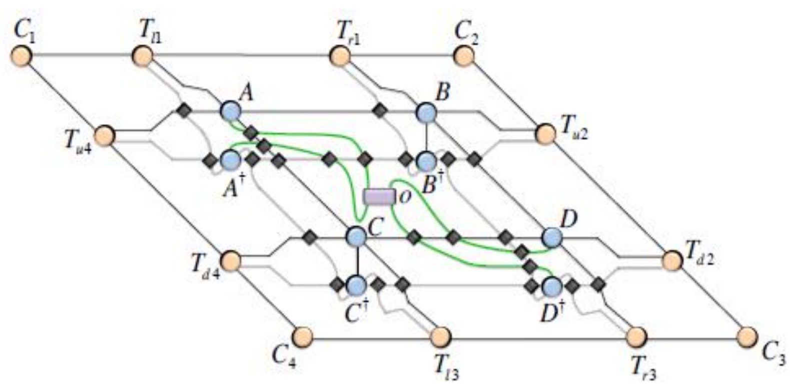
2 Contracting iPEPS

fermionic, t-t'-J model: next nearest neighbor [Corboz Jordan Vidal 10]

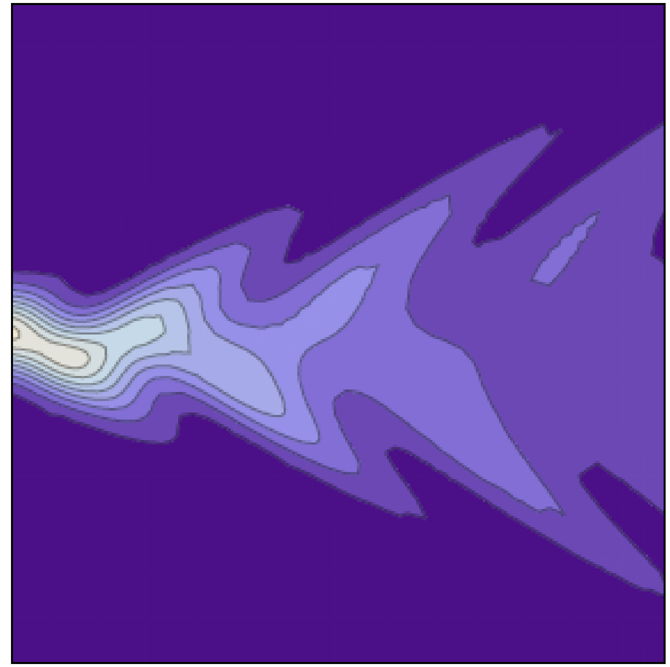


[R. Orús]





[Angelakis+ 14]



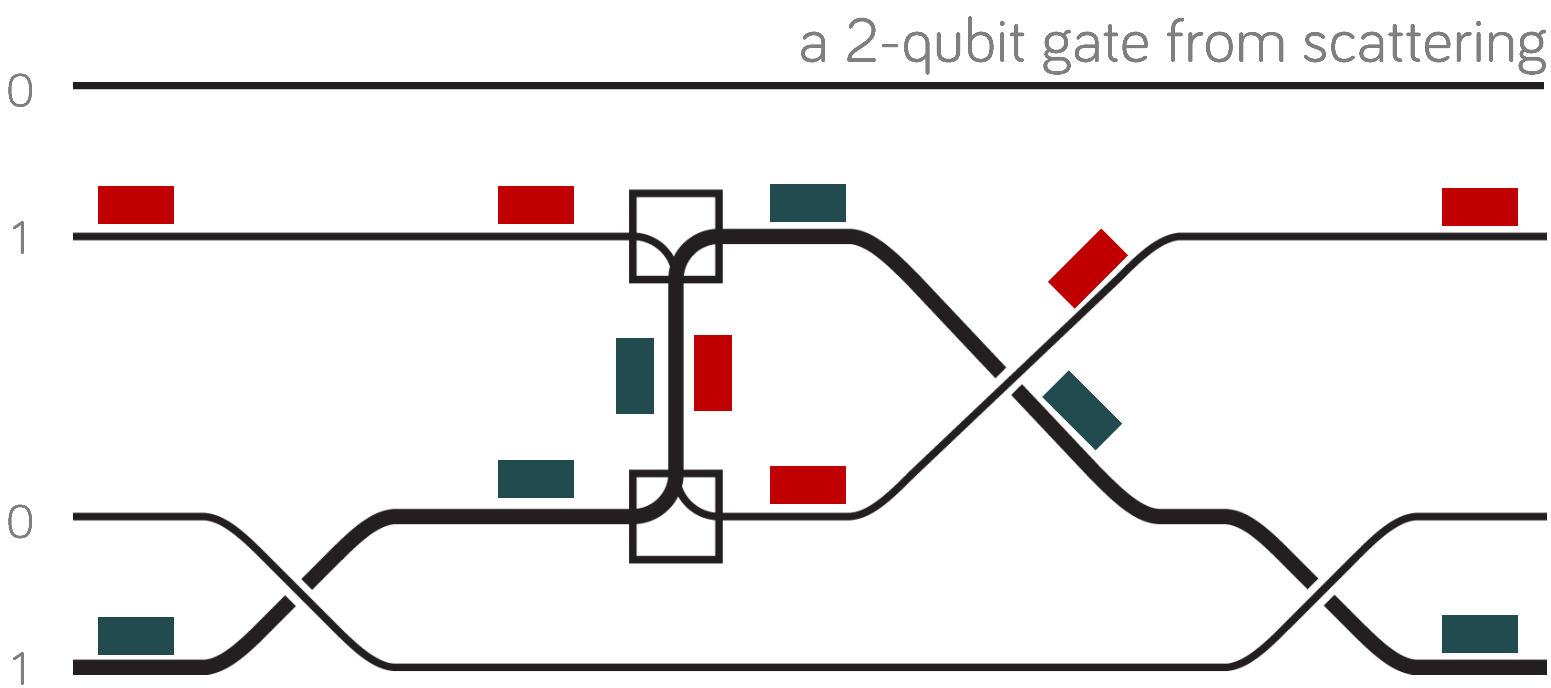
making a **computer**
or a **simulator**

3 Computing by scattering

- multiparticle walk
  Bose-Hubbard
  scattering on a graph
  [Childs Gosset Webb 12]

$$H = t \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1)$$

hopping — repulsion



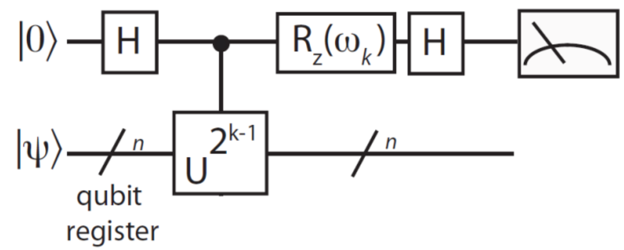
3 (Towards) quantum chemistry on a quantum computer

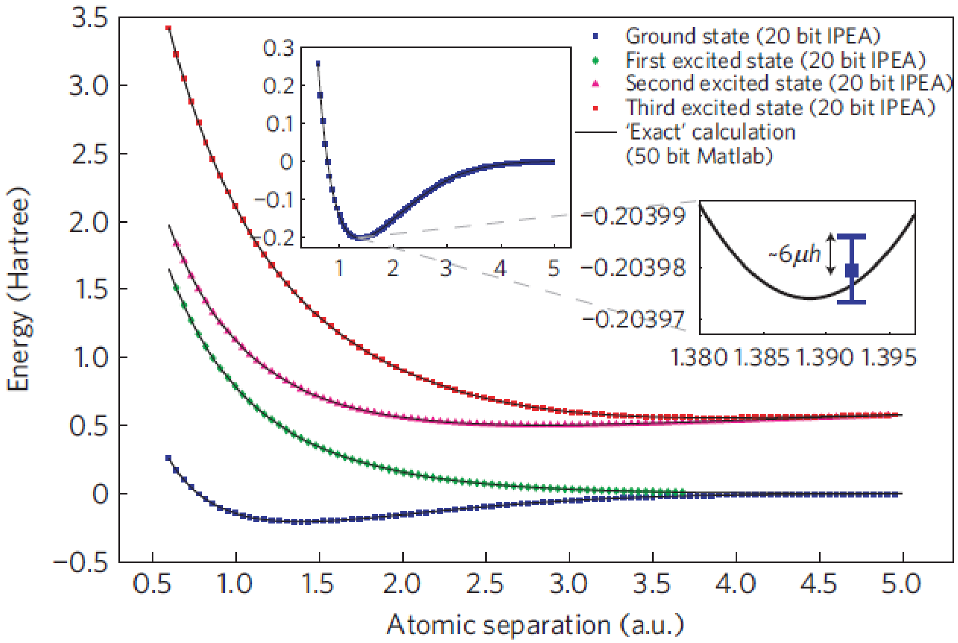
- **H_2 energies** [Lanyon+ 10]

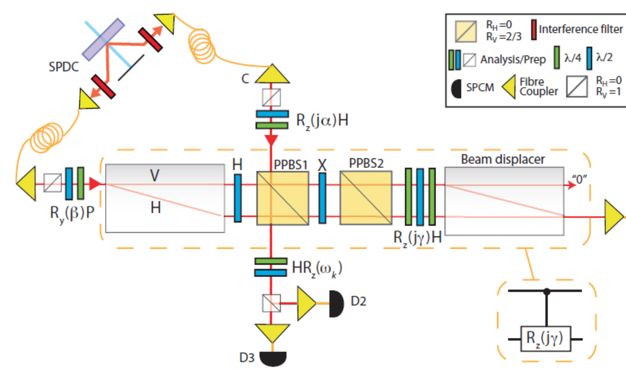
  a small basis of orbitals

  2 photons

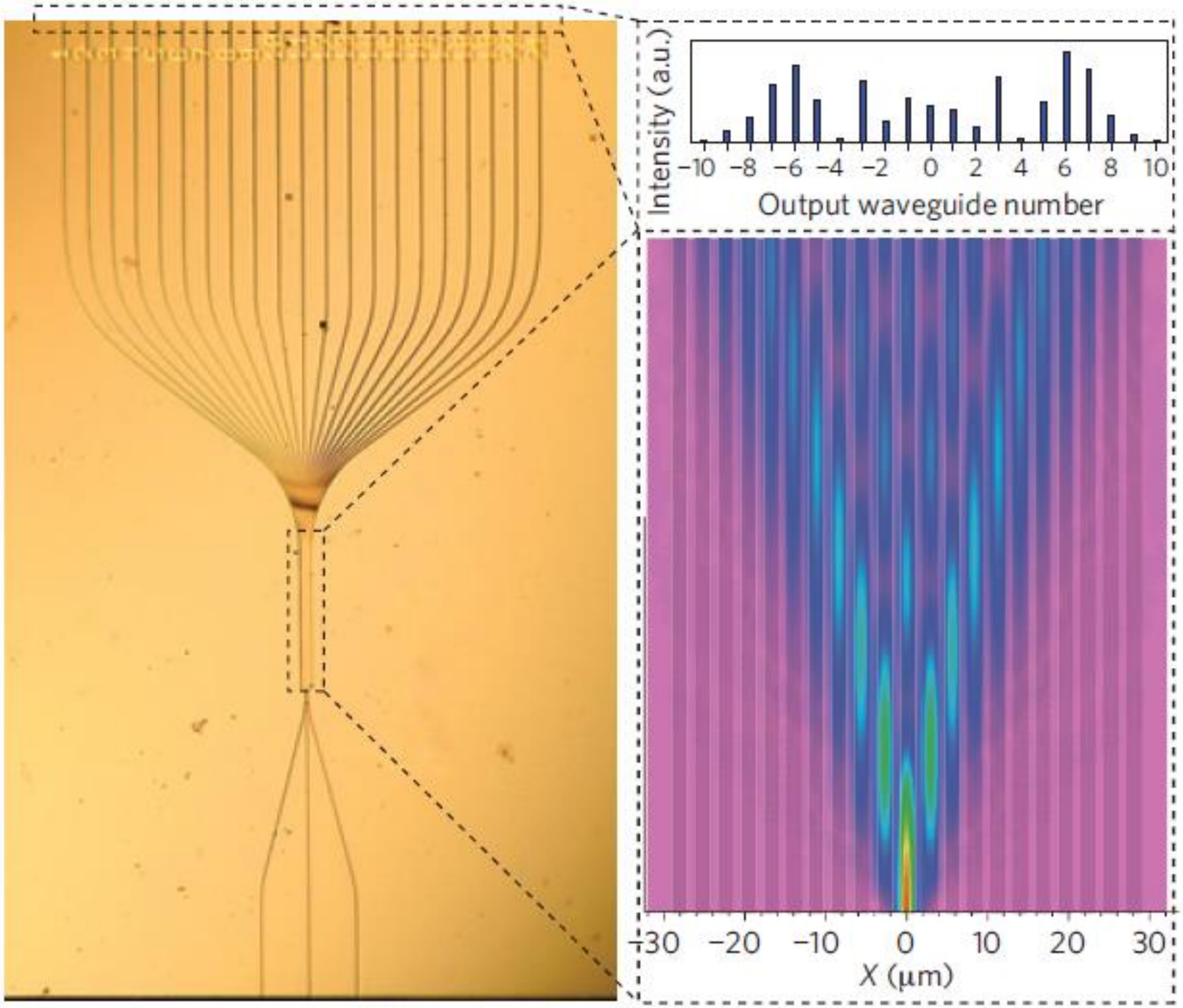
  iterative phase estimation







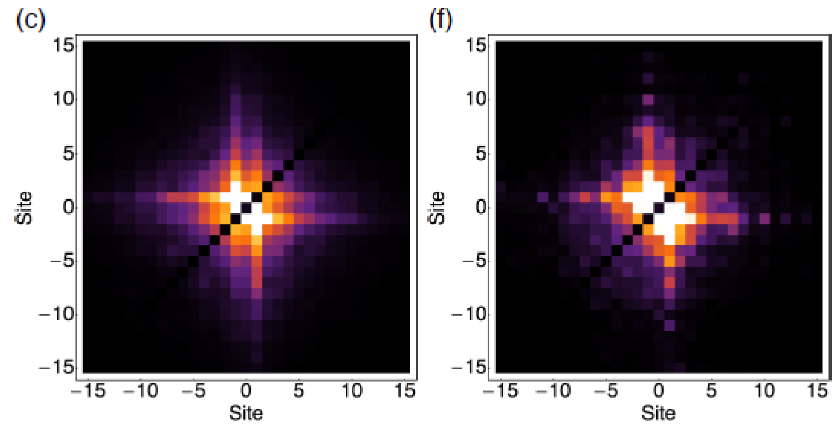
3 Photonic simulators: quantum walks



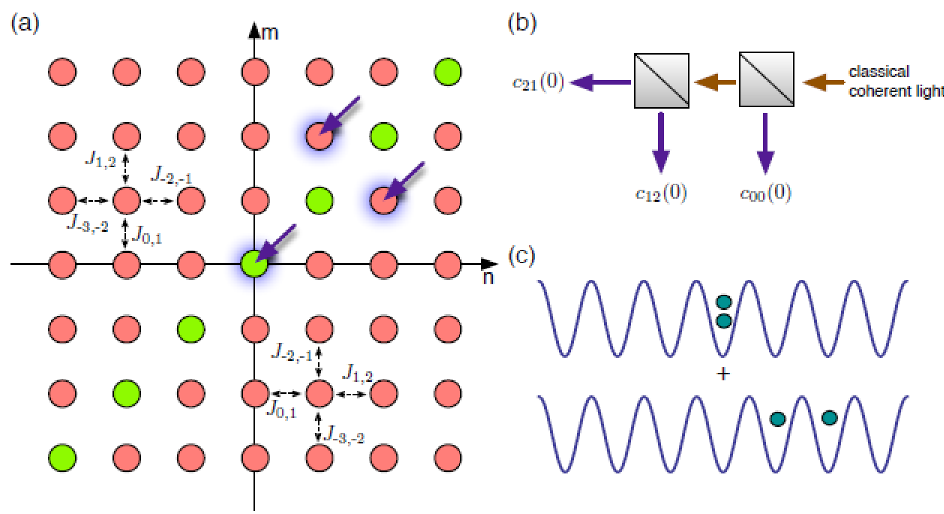
[Peruzzo + 10]

3 Linear photonic lattices

- 2 interacting particles in 1D simulated by light in a 2D waveguide array

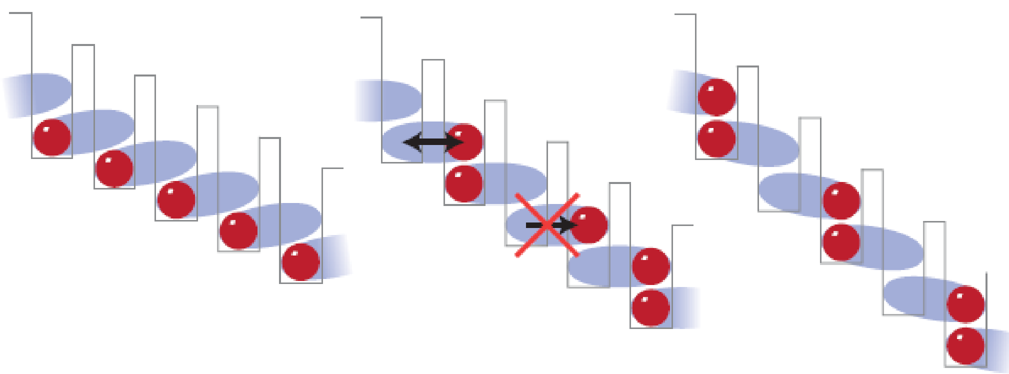


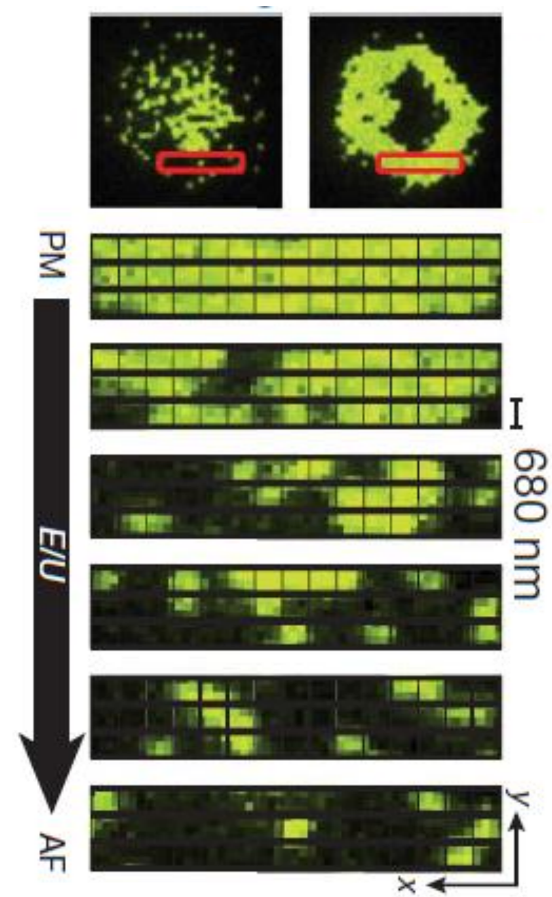
correlations, disorder, 1D
[Lee Rai Noh Angelakis 13]



3 Quantum simulators

- an antiferromagnetic spin chain
  [Simon Bakr Ma Tai Preiss Greiner 11]
  atoms in a 2D optical lattice
  tilting ... tuning the interaction

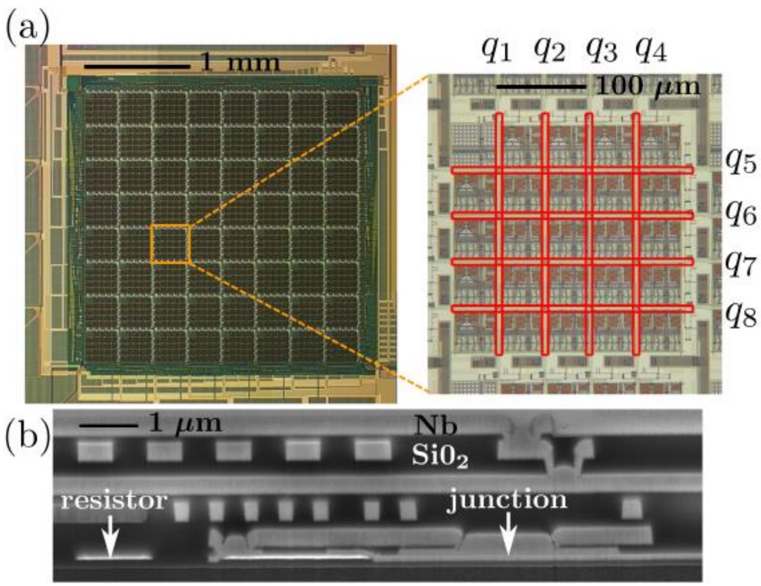


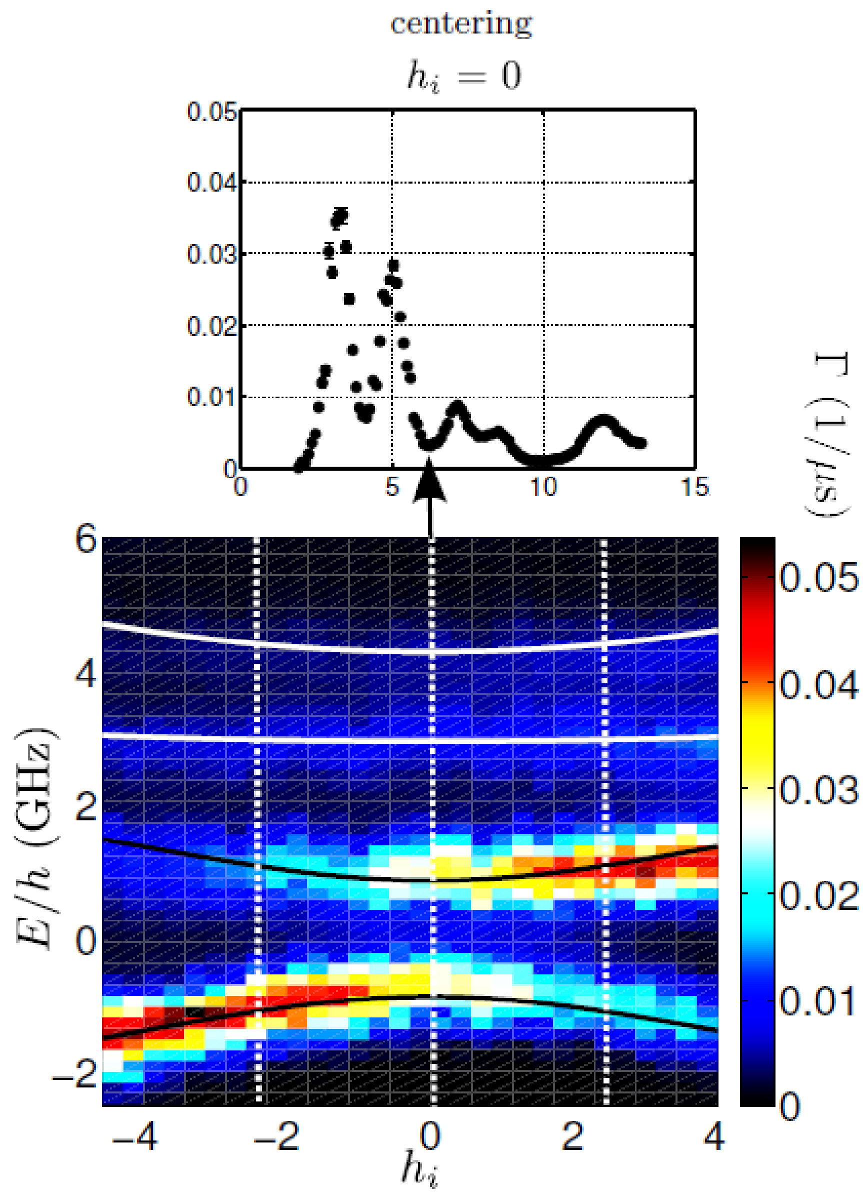


[wire

3 Superconducting programmable simulators (D-WAVE)

- quantum annealing
  [Lanting+ 14]
  showing coherence
  in 2, 8 qubits





Quantum Physics

Defining and detecting quantum speedup

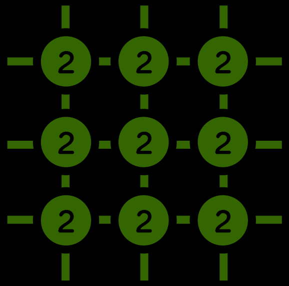
Troels F. Rønnow, Zhihui Wang, Joshua Job, Sergio Boixo, Sergei V. Isakov, David Wecker, John M. Martinis, Daniel A. Lidar, Matthias Troyer

(Submitted on 13 Jan 2014)

The development of small-scale digital and analog quantum devices raises the question of how to fairly assess and compare the computational power of classical and quantum devices, and of how to detect quantum speedup. Here we show how to define and measure quantum speedup in various scenarios, and how to avoid pitfalls that might mask or fake quantum speedup. We illustrate our discussion with data from a randomized benchmark test on a D-Wave Two device with up to 503 qubits. Comparing the performance of the device on random spin glass instances with limited precision to simulated classical and quantum annealers, we find no evidence of quantum speedup when the entire data set is considered, and obtain inconclusive results when comparing subsets of instances on an instance-by-instance basis. Our results for one particular benchmark do not rule out the possibility of speedup for other classes of problems and illustrate that quantum speedup is elusive and can depend on the question posed.

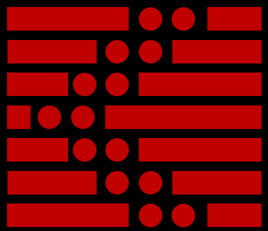
1 local hamiltonian

its simple & difficult variants



2 the algorithms

what works well & what we wish we had



3 let's make it work

computers & simulators