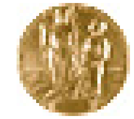
many-body physics & complexity 1

tough & interesting questions

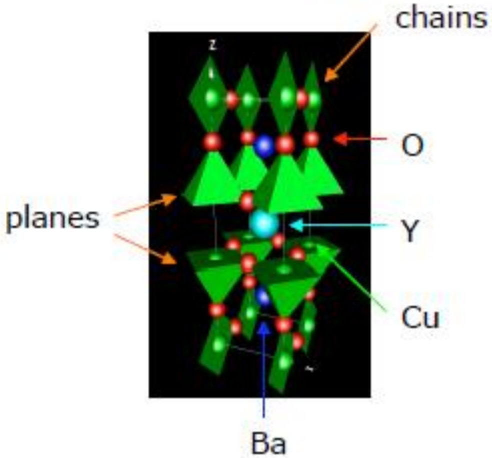
Daniel Nagaj
universität wien

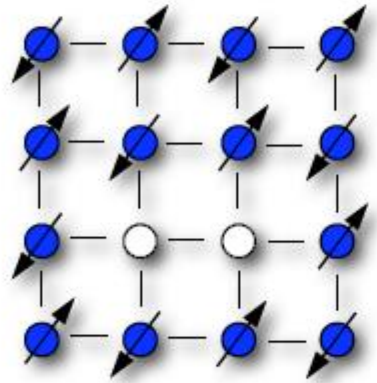


Bednorz & Müller, 1987

High Tc superconductors & Quantum Magnets

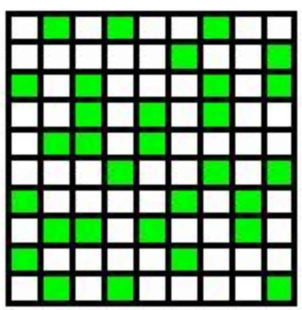
$YBa_2Cu_3O_7$

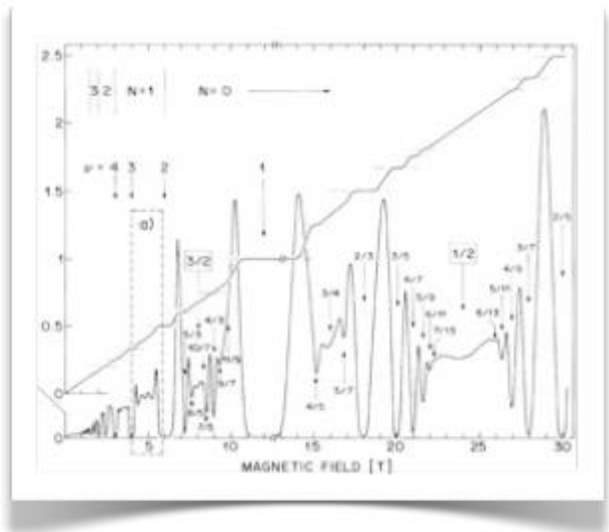




Fractional Quantum Hall Effect

$$\nu = 1/3$$





Stoermer, Tsui, Laughlin, 1998

[slide: A.Lauchli]

investigate
& explain

construct
something

Hamiltonians

1 Many-body systems & their Hamiltonians

MACROSCOPIC PROPERTIES

m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-i-c r-u-l-e-s m-i-c-r-o-s-c-o-p-

density, heat capacity, magnetization, correlations, spectrum …

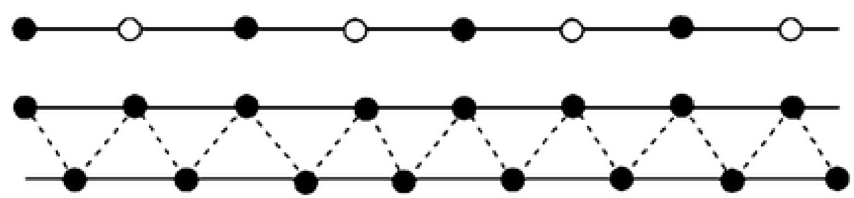
1 Many-body systems & their Hamiltonians

- a model of interactions

  non-interacting = 1-body

$E(s_1 \ldots s_n)$ strings

$\hat{H}|\psi_k\rangle = E_k|\psi_k\rangle$ spins, bosons, fermions



- a **local** Hamiltonian

$\cdots + H_{a,b,c,d} + \cdots$ few-body

$\cdots + H_{k,k+2} + \cdots$ short-range

long-range, many interactions: Aram

1 Geometry matters

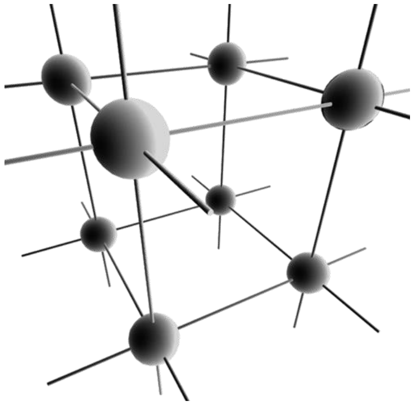
- some lattice

  1D Ising, antiferromagnetic

0/1 strings

$$E(s) = \sum_j s_j s_{j+1} - h \sum_j s_j$$

1 Geometry matters



[Melcom, de.wikipedia]

- some lattice

  3D Ising

$$E(s) = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_j s_j$$

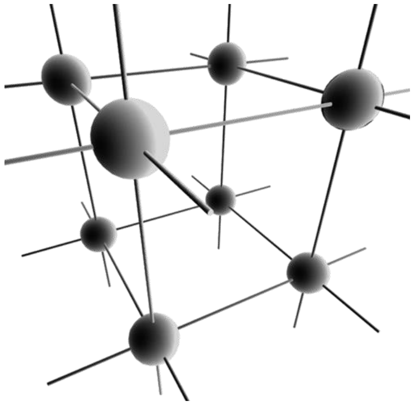
- lattice dimensionality:
  visit n^d points in n steps

1 Geometry matters

- some lattice

  3D Ising, spin glass

$$E(s) = -\sum_{\langle i,j \rangle} J_{ij}\, s_i s_j - h \sum_j s_j$$



[Melcom, de.wikipedia]

1 Geometry matters

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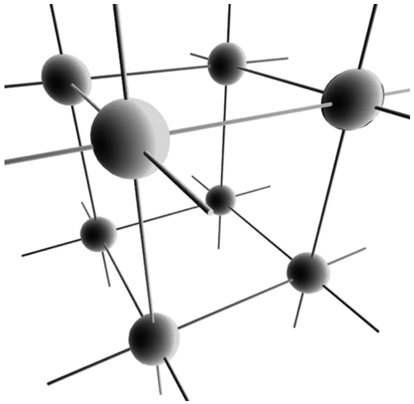


[Melcom, de.wikipedia]

1D Heisenberg (classical)

$$H = -\sum_j J_j \, \vec{s}_j \cdot \vec{s}_{j+1}$$

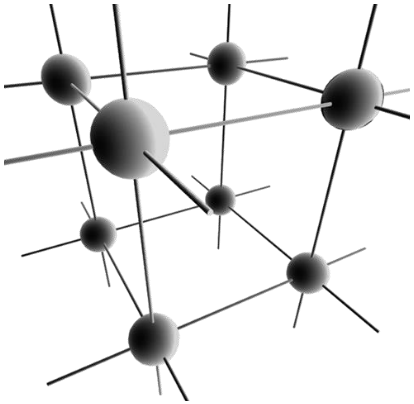
3D vectors

1 Geometry matters

- some lattice

3D Ising

$$E(s) = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_j s_j$$



[Melcom, de.wikipedia]

1D Heisenberg (quantum)

$$H = -\frac{1}{2} \sum_j \left(J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y + J_x \sigma_j^z \sigma_{j+1}^z \right) + h \sum_j \sigma_j^z$$

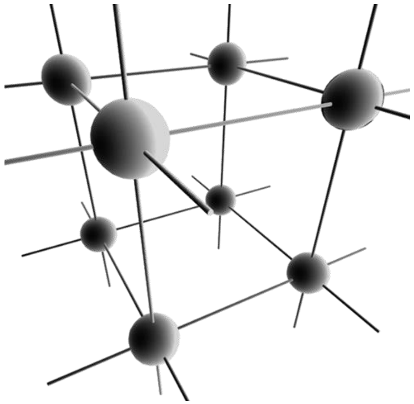
the Haldane conjecture about integer/half-integer spin

1 Geometry matters

- some lattice

3D Ising

$$E(s) = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_j s_j$$



[Melcom, de.wikipedia]

1D Heisenberg (quantum)

$$H = -\frac{1}{2} \sum_j \left(J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y + J_z \sigma_j^z \sigma_{j+1}^z \right) + h \sum_j \sigma_j^z$$

- general graphs

Bose-Hubbard

hopping　　repulsion

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

a very complex graph [Childs Gosset Webb 13]

(fixed particle number)

a lifetime with a model

Google

hubbard model

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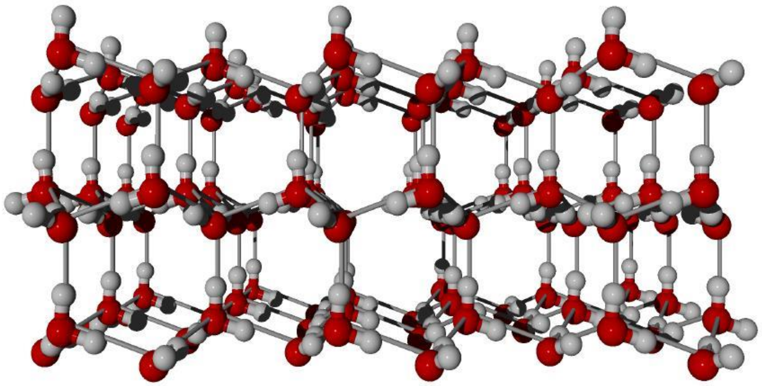
Hubbard model - Wikipedia, the free encyclopedia
en.wikipedia.org/wiki/**Hubbard_model** ▾
The **Hubbard model** is an approximate model used, especially in solid state physics, to describe the transition between conducting and insulating systems.
Theory (Narrow energy band theory) - Example: 1D chain of hydrogen ...

Bose–**Hubbard model** - Wikipedia, the free encyclopedia
en.wikipedia.org/wiki/Bose–**Hubbard_model** ▾
The Bose–**Hubbard model** gives an approximate description of the physics of interacting bosons on a lattice. It is closely related to the **Hubbard model** which **...**

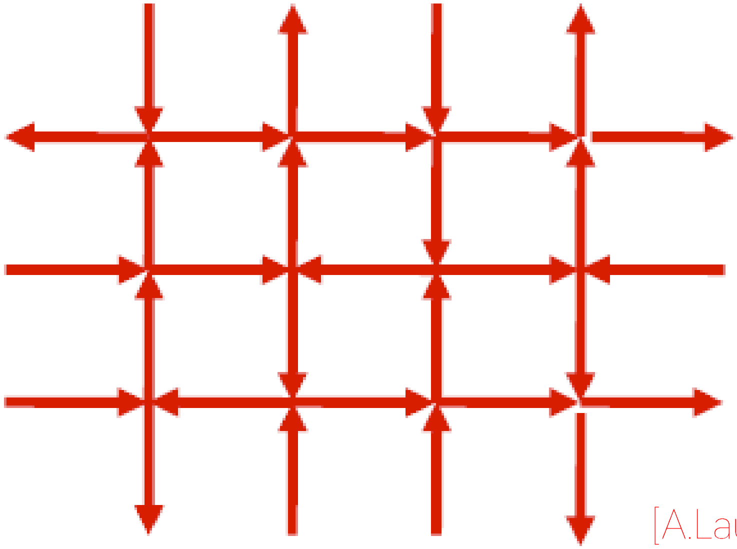
[PDF] The **Hubbard Model** for Dummies
www.physik.unizh.ch/lectures/electroncorrelations/**Hubbard**4Du.pdf ▾
Jun 13, 2007 - Electron states for the (N=8) **Hubbard model** in terms of fermionic operators: c. 1↑. †. 0 = ↑,·,·,·,·,·,·,· c. 5↓. †. 0 = ·,·,·,·,↓,·,·,·.

ice-type

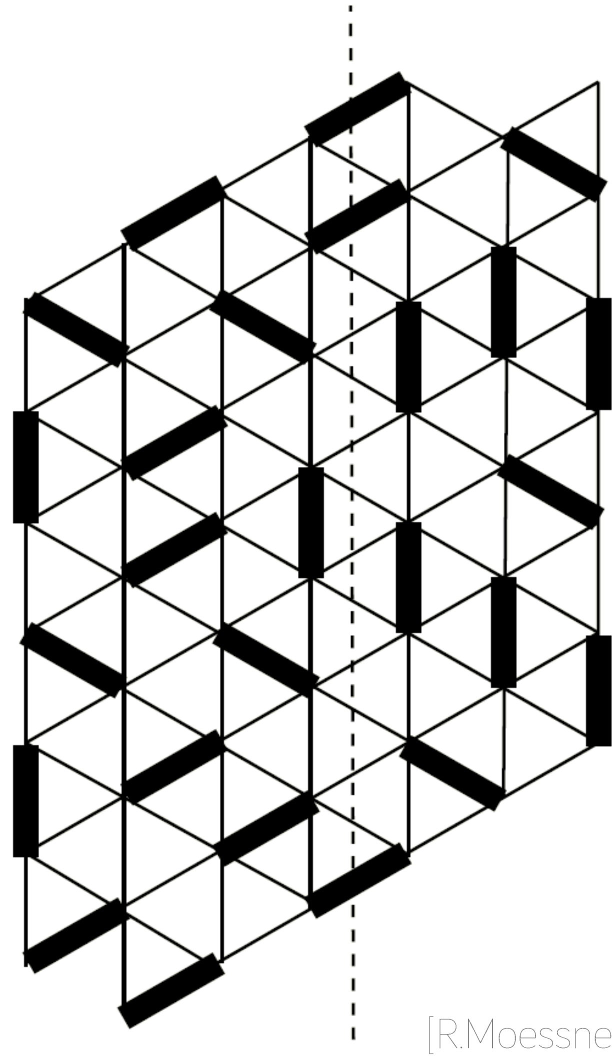
quantum dimers



[Linkopings U.]

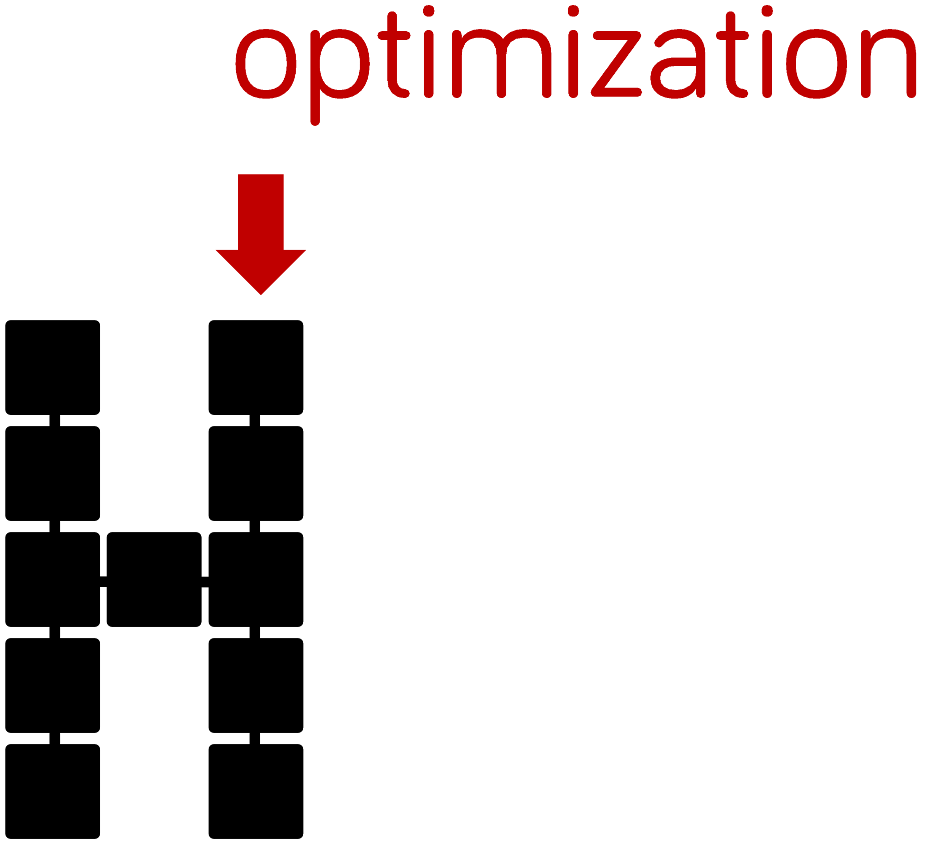


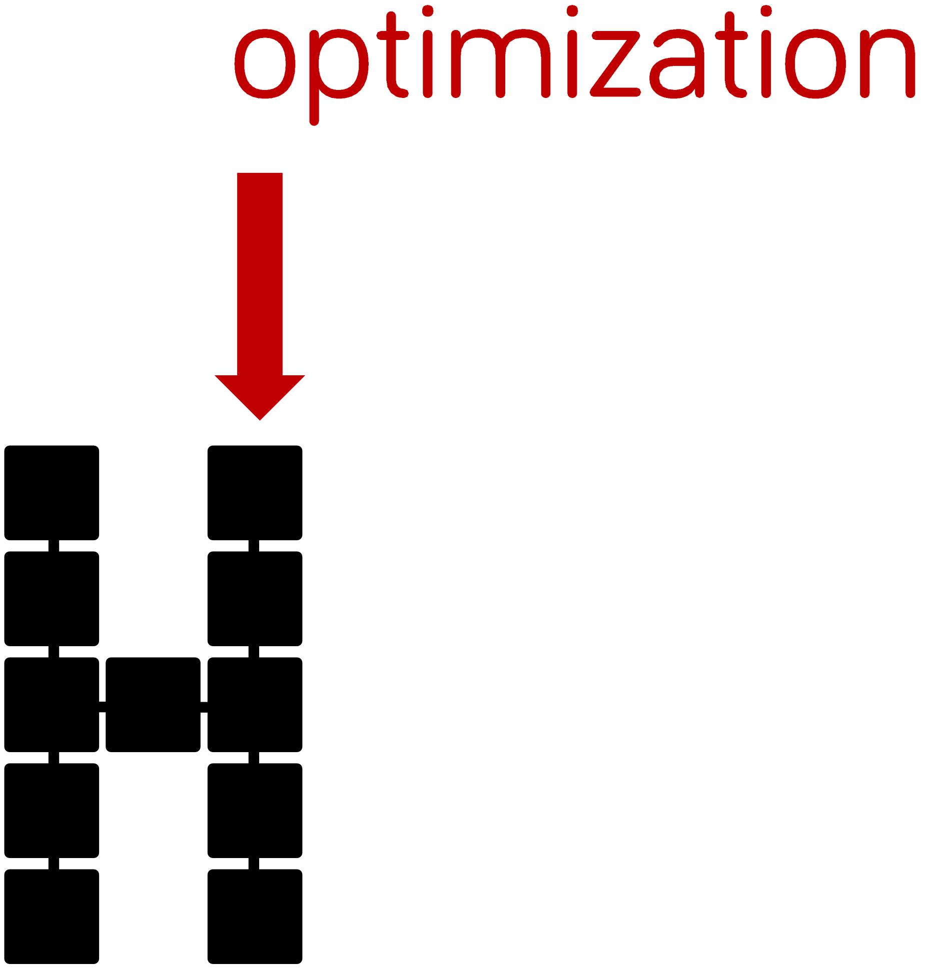
[A.Lauchli]

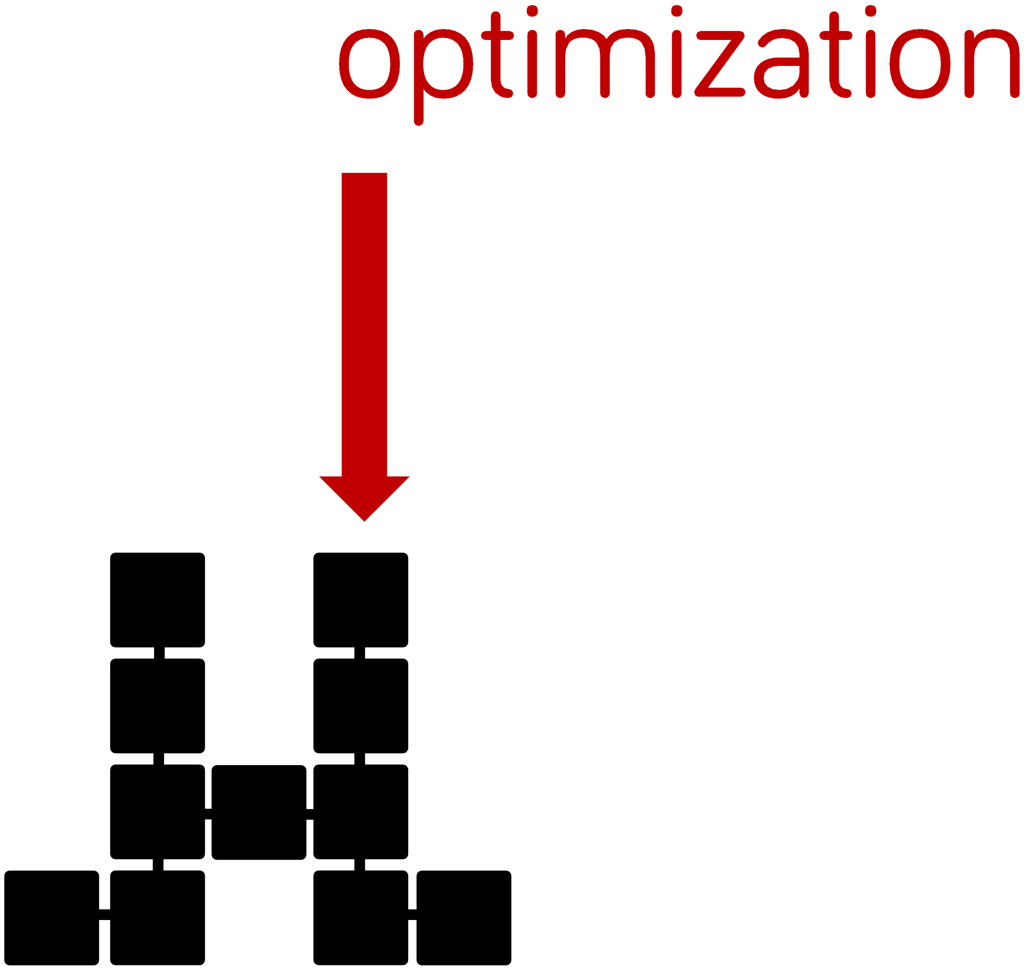


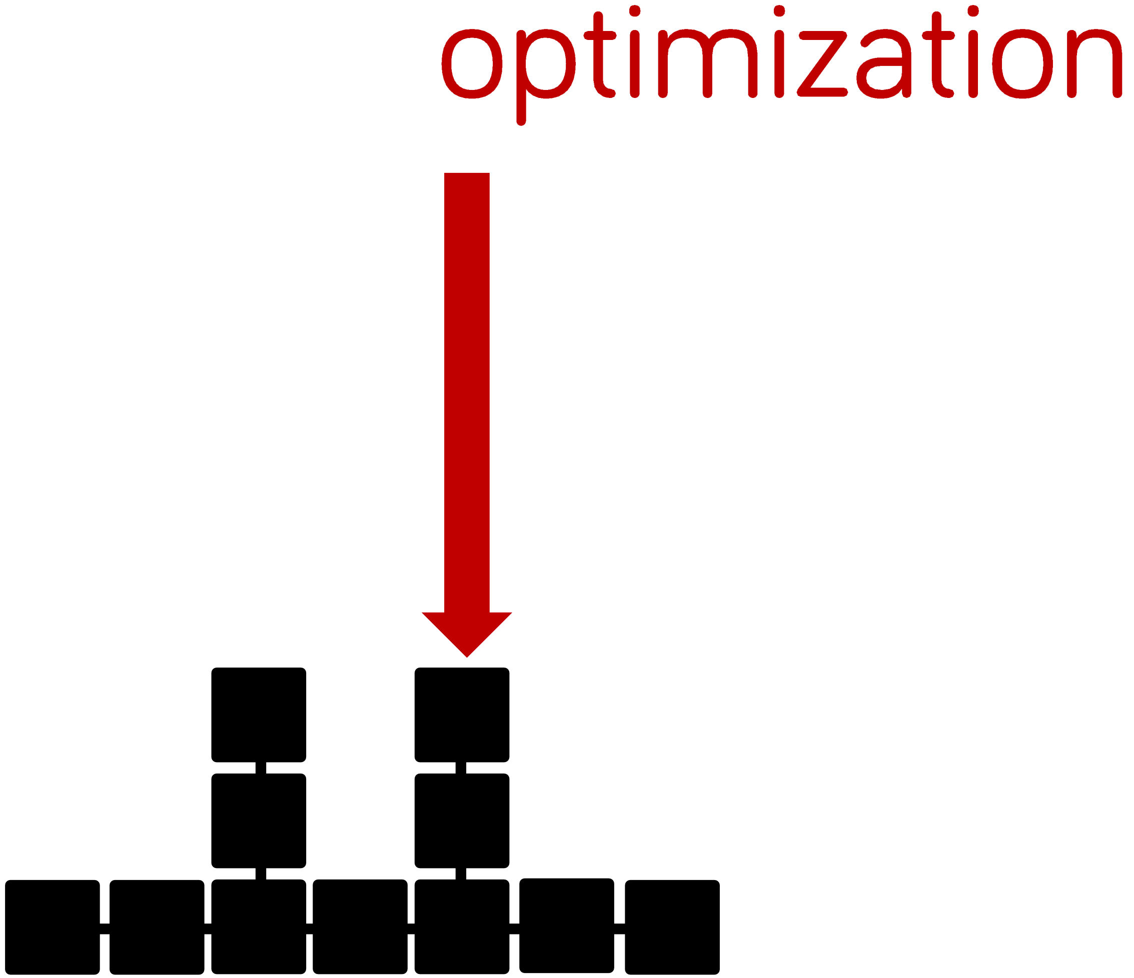
[R.Moessner]

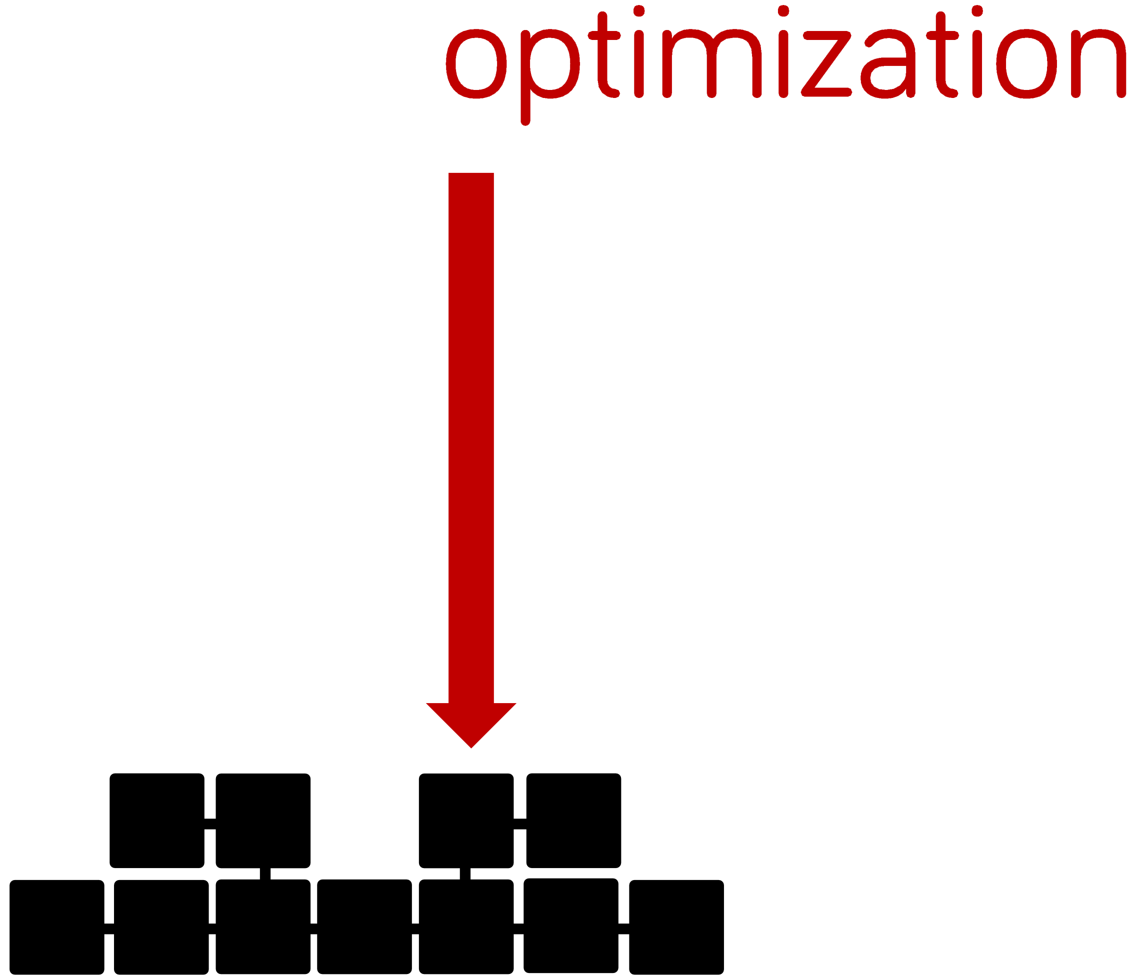
STATIC
the questions


optimization


optimization

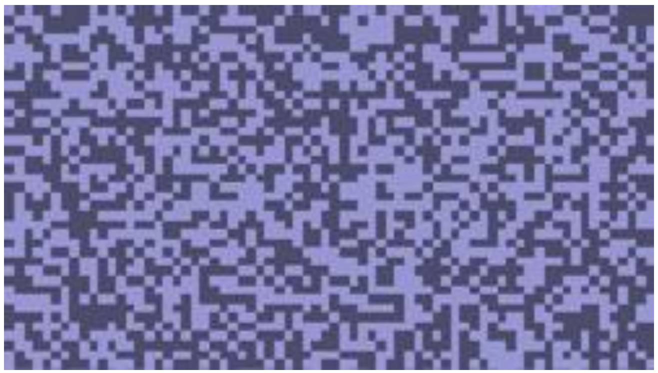

optimization


optimization

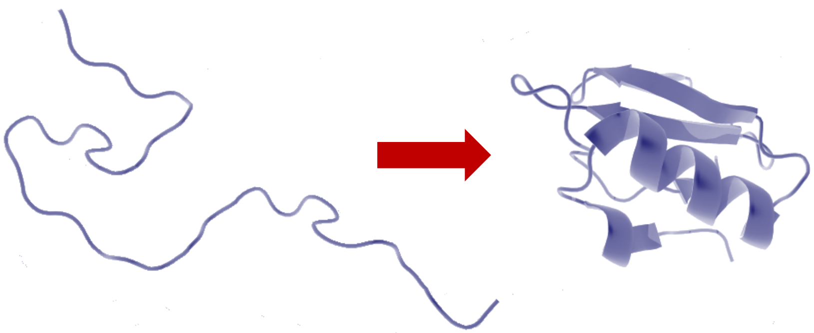

optimization

spin glasses

protein folding



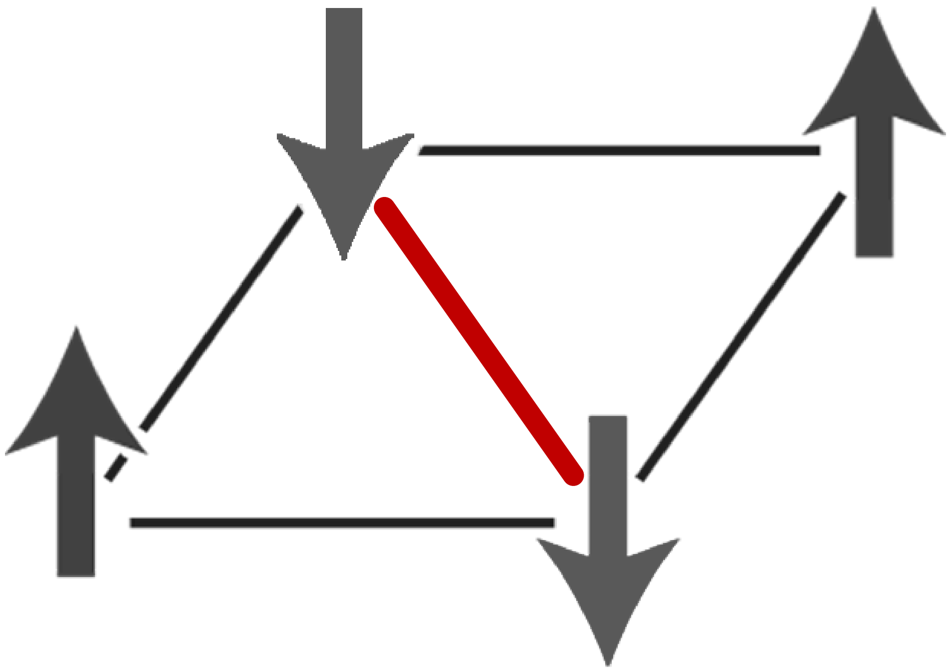
[uni-koeln.de]



[wikipedia]

local Hamiltonians

1 Frustration



a global
ground state

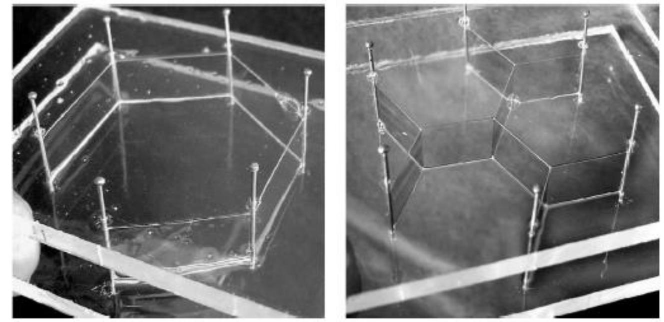
HARD?

finding it?
describing it?


frustrated
FRUST
RATED

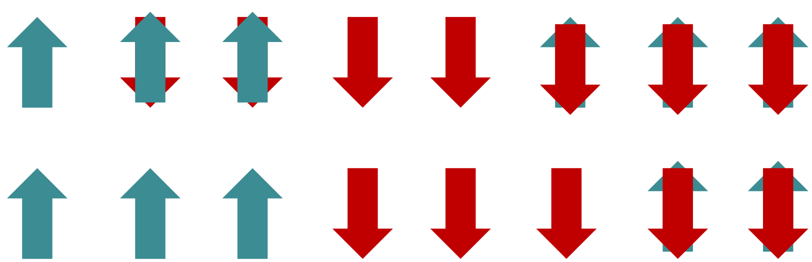
1 The ground state is cool

- doesn't nature find it?
  can't we cool the system?



[Dutta+, arXiv:0806.1340]

- simulated annealing:
  a nature-inspired heuristic



- optimization, CSP & spin glasses

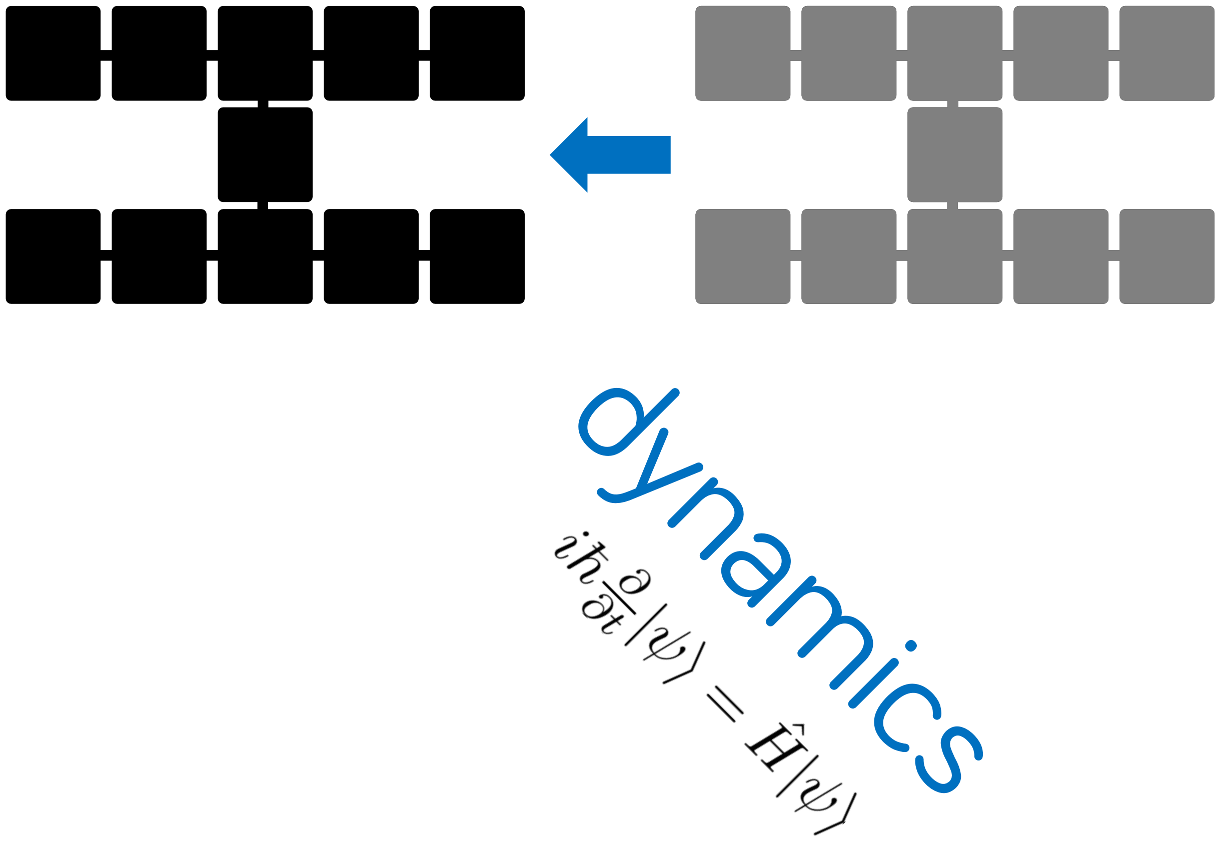
1 The questions we ask: static

- eigenstates?
  - ground state(s)
  - excitations
  - spectrum
- solvable? integrable?
  - symmetries
  - transformations
  - nature of states
- bulk properties?
  - phase transitions

[Oona Räisänen]

dynamical

the questions


dynamics
$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$

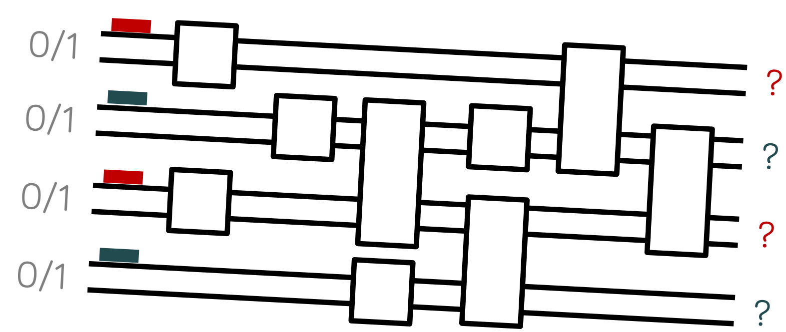

scattering
[fermilab]

scattering

Universal computation by multi-particle quantum walk

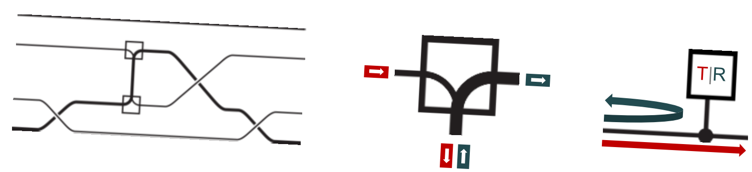
- dual-rail encoding
  N wavepackets

$$a_j^\dagger a_k + a_k^\dagger a_j$$



- CPHASE: interaction

$$a_j^\dagger a_k^\dagger a_j a_k$$



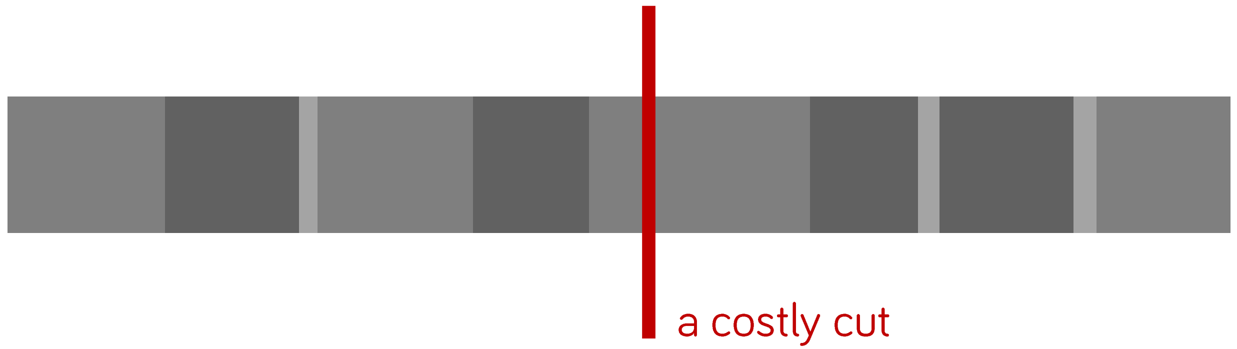
[Childs, Gosset, Webb, Science 339, 791 (2013)]

1 The questions we ask: *dynamic*

- simulating dynamics

trouble: states become more entangled

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

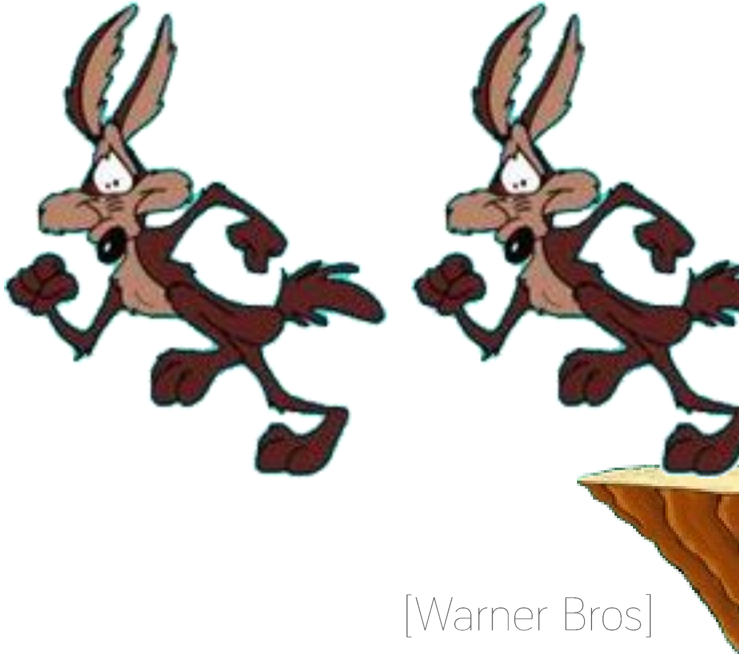


1 The questions we ask: *dynamic*

- simulating dynamics

  trouble: states become more entangled

- thermalization, quenching



[Warner Bros]

1 The questions we ask: *dynamic*

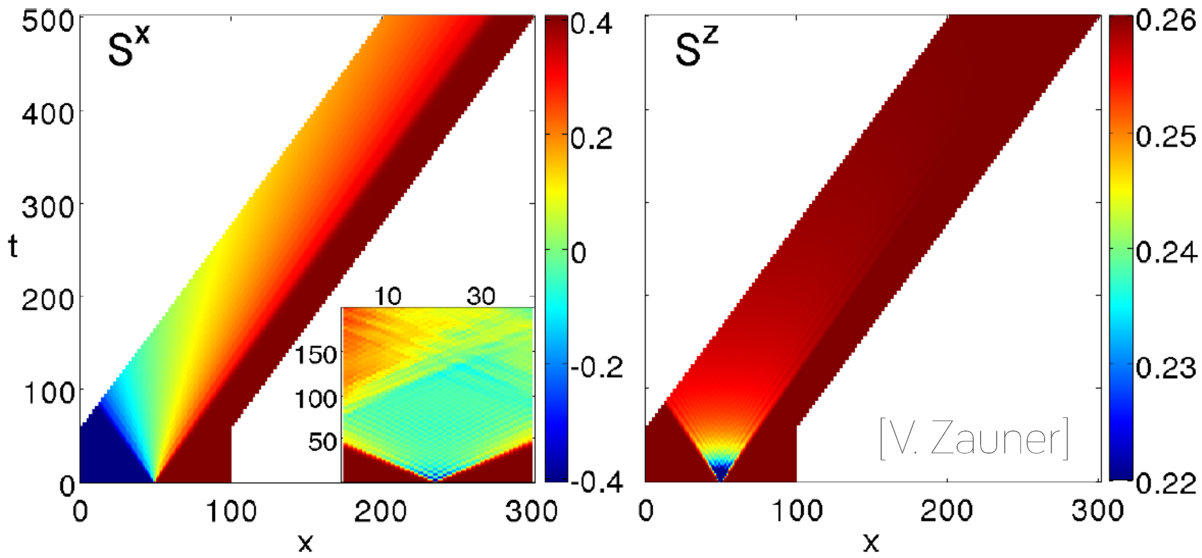
- simulating dynamics

  trouble: states become more entangled

- thermalization, quenching

  the behavior of correlations

  Lieb-Robinson bound $\|[A(t),B]\| \leq c\,\|A\|\,\|B\| \exp\left(-\mu(dist(X,Y) - v|t|)\right)$



1 The questions we ask: *dynamic*

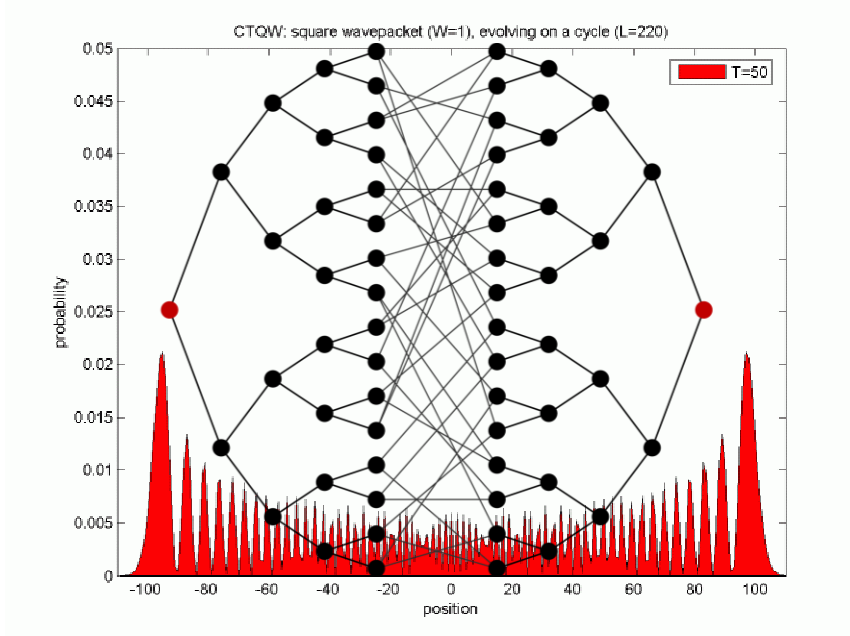
- simulating dynamics
- thermalization
- utilizing the dynamics

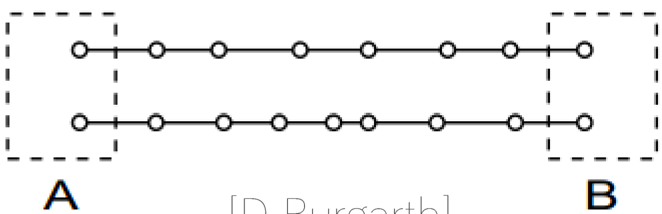
  control (state preparation)

  transport (signals, energy)

  simulation

  algorithms!





[D. Burgarth]

the questions

three questions

three questions

three questions

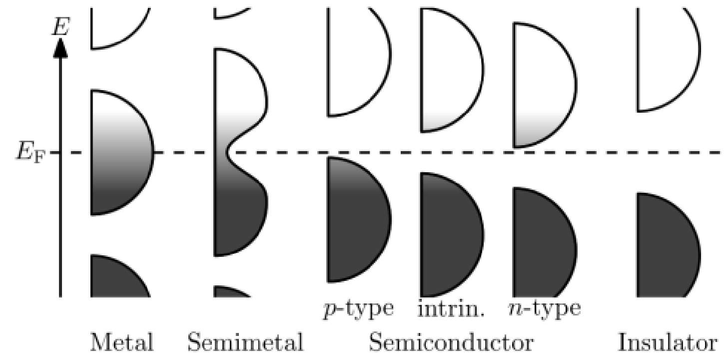
eigenstates & spectral properties

symmetries & solvability

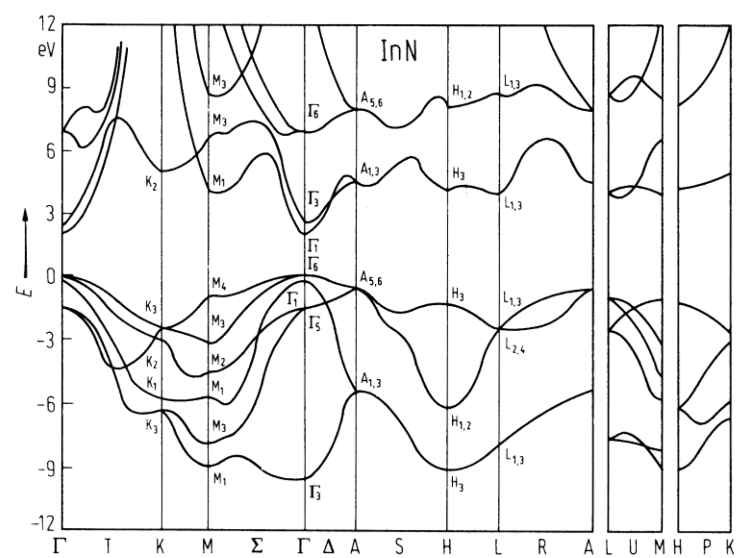
parameters & transitions

1 The spectrum of a system: band gaps

- a lattice + electrons
- orbitals... available levels filled with electrons
- conductors (metals) semiconductors insulators



[wikimedia: Nanite]



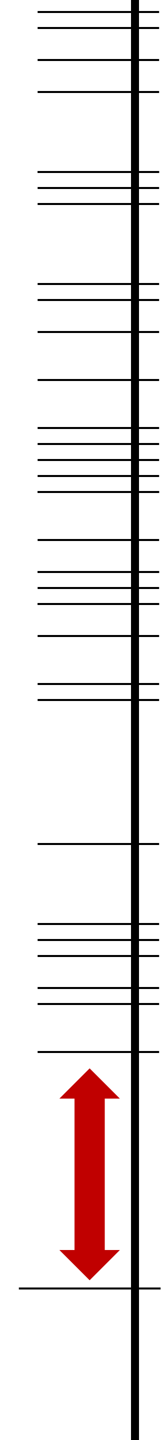
[Foley & Tansley]

1 The (ground state) gap in a system

$$N \to \infty$$

Are there states
close to the ground state
when we take the
thermodynamic limit?

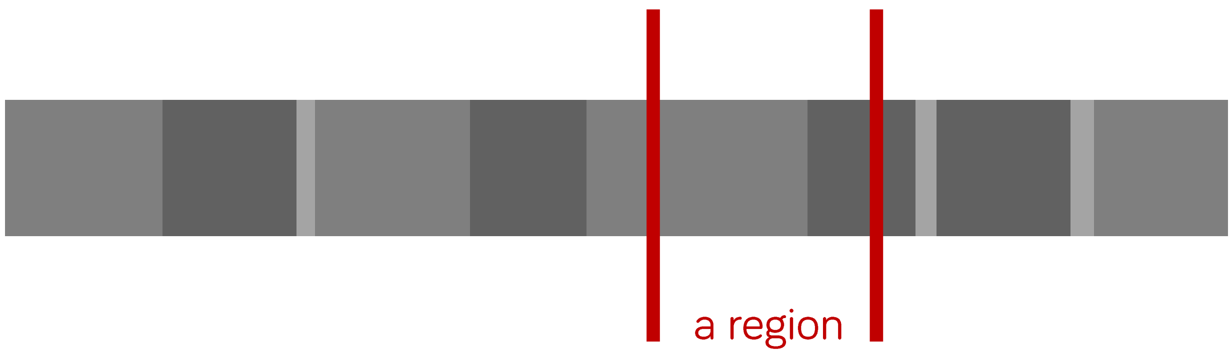
an inverse-poly gap? $\Delta = \frac{c}{N} \to 0$

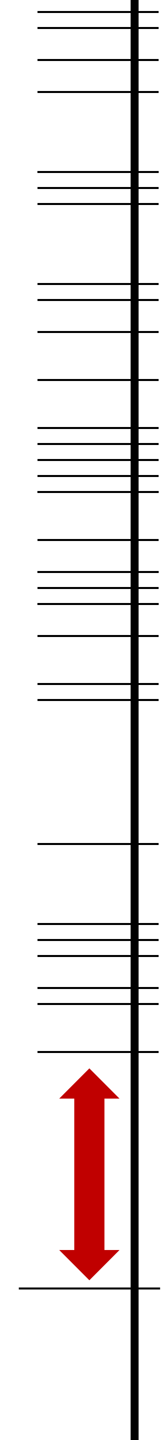


1 The (ground state) gap in a system

Do we have a gap?

- **YES?** area law – 1D [Hastings, Arad Landau Vazirani]
  inspired numerics (MPS, ...)





correlations fall off exponentially with distance

$$S(\rho) = -\mathrm{Tr}(\rho \log_2 \rho)$$

entropy from quantum correlations

1 The (ground state) gap in a system

Do we have a gap?

- **YES?** area law

  inspired numerics (MPS, …)

  imaginary time evolution

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

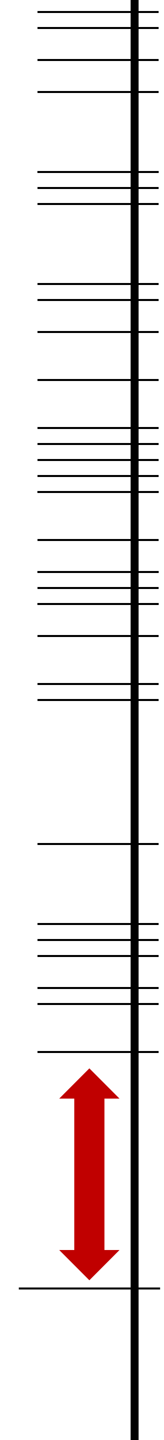
$$e^{-iH(-i\tau)}|\psi\rangle = e^{-H\tau}|\psi\rangle$$

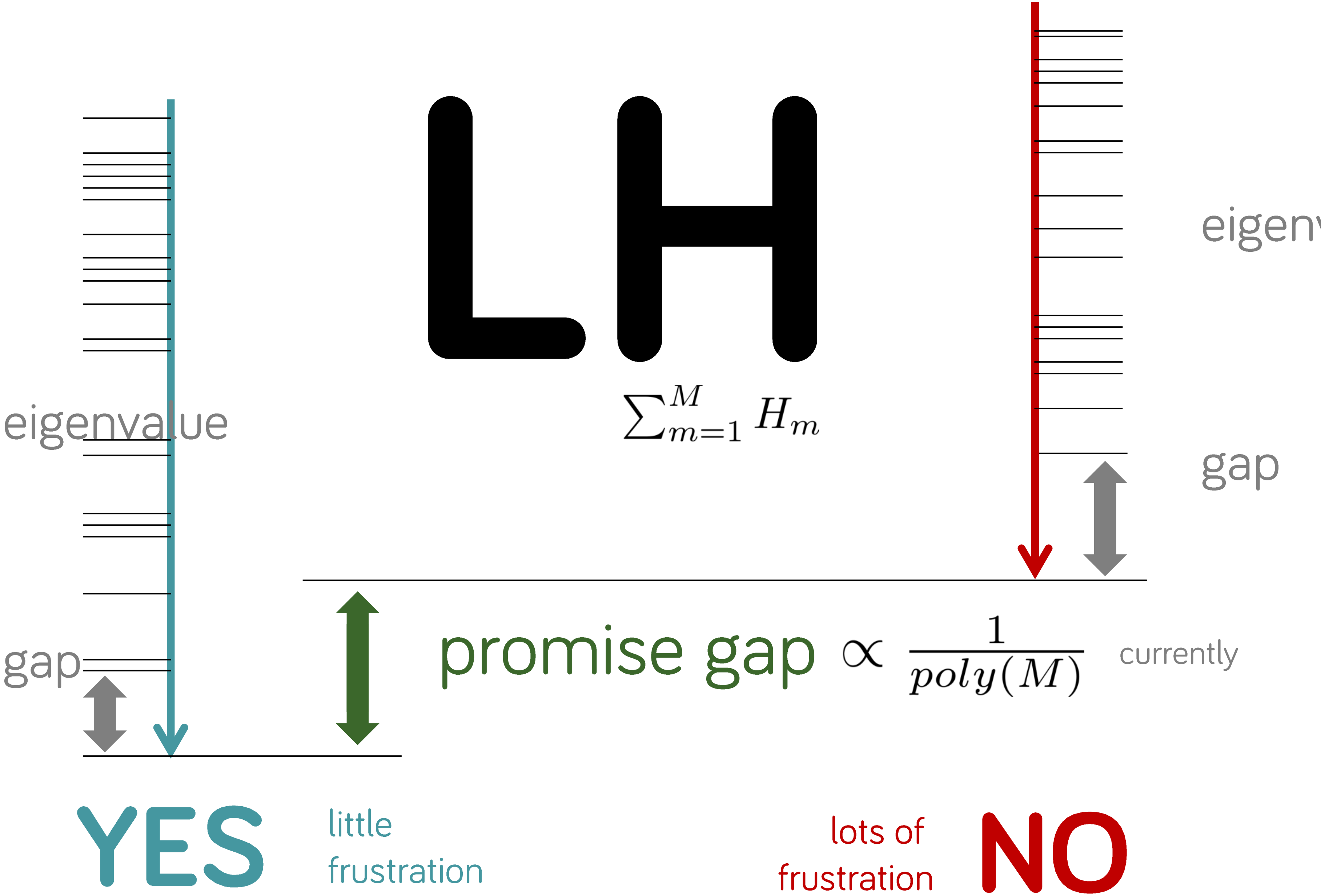
$$e^{-H\tau} \approx e^{-H_1\tau}e^{-H_2\tau}$$

- **NO?** what is nearby?

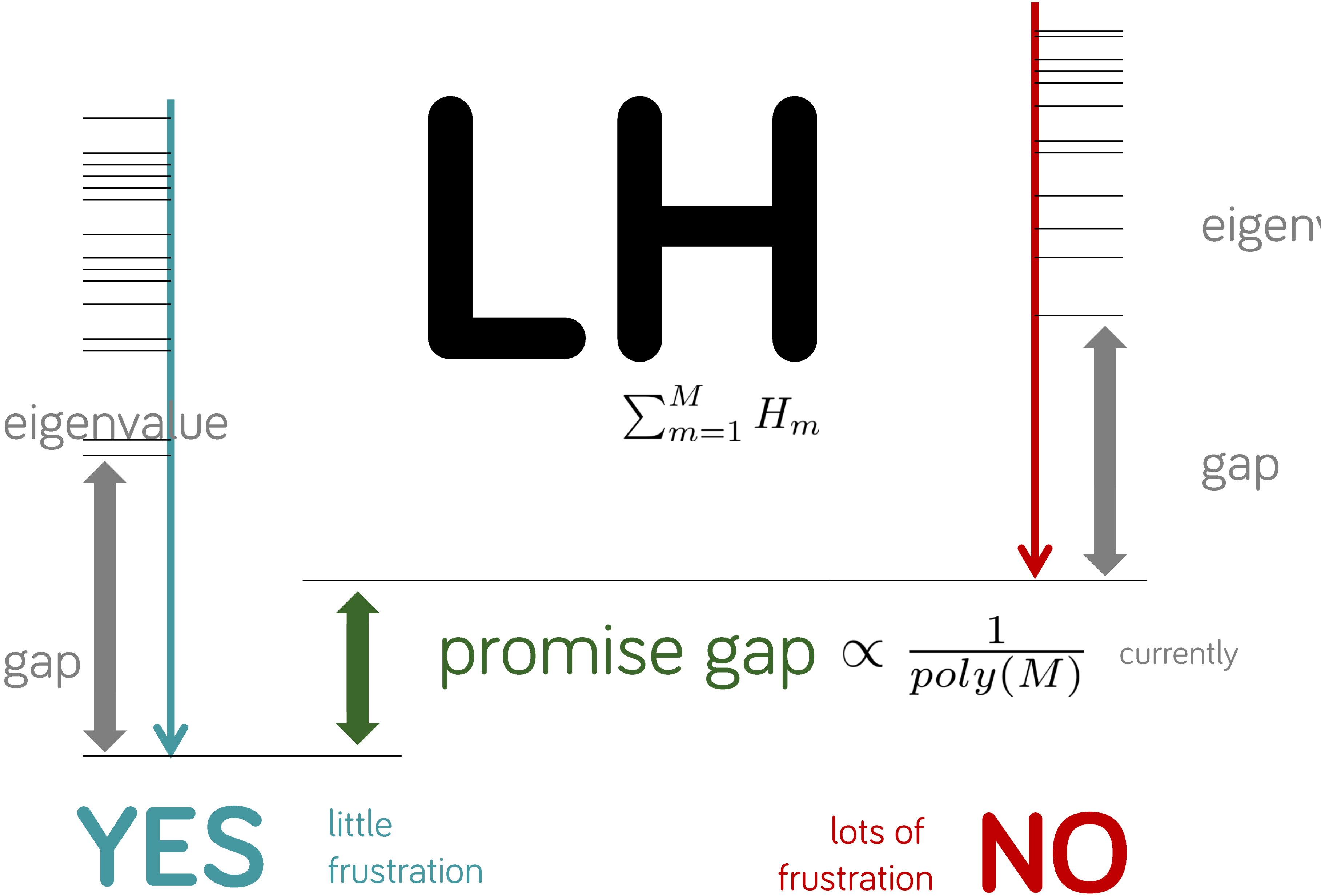
  qPCP, no trivial states [Hastings]

- **deciding it:** uncomputable [Cubitt Perez-Garcia Wolf]





LH
$\sum_{m=1}^{M} H_m$
eigenvalue
gap
eigenv
gap
promise gap $\propto \frac{1}{poly(M)}$
currently
YES
little
frustration
lots of
frustration
NO


LH
$\sum_{m=1}^{M} H_m$
eigenvalue
gap
eigenv
gap
promise gap $\propto \frac{1}{poly(M)}$
currently
YES
little
frustration
lots of
frustration
NO

1 "Solving" a system

- exactly solvable

the free energy/partition function

$$E(s) = \sum_j s_j s_{j+1} - h \sum_j s_j$$

- integrable systems

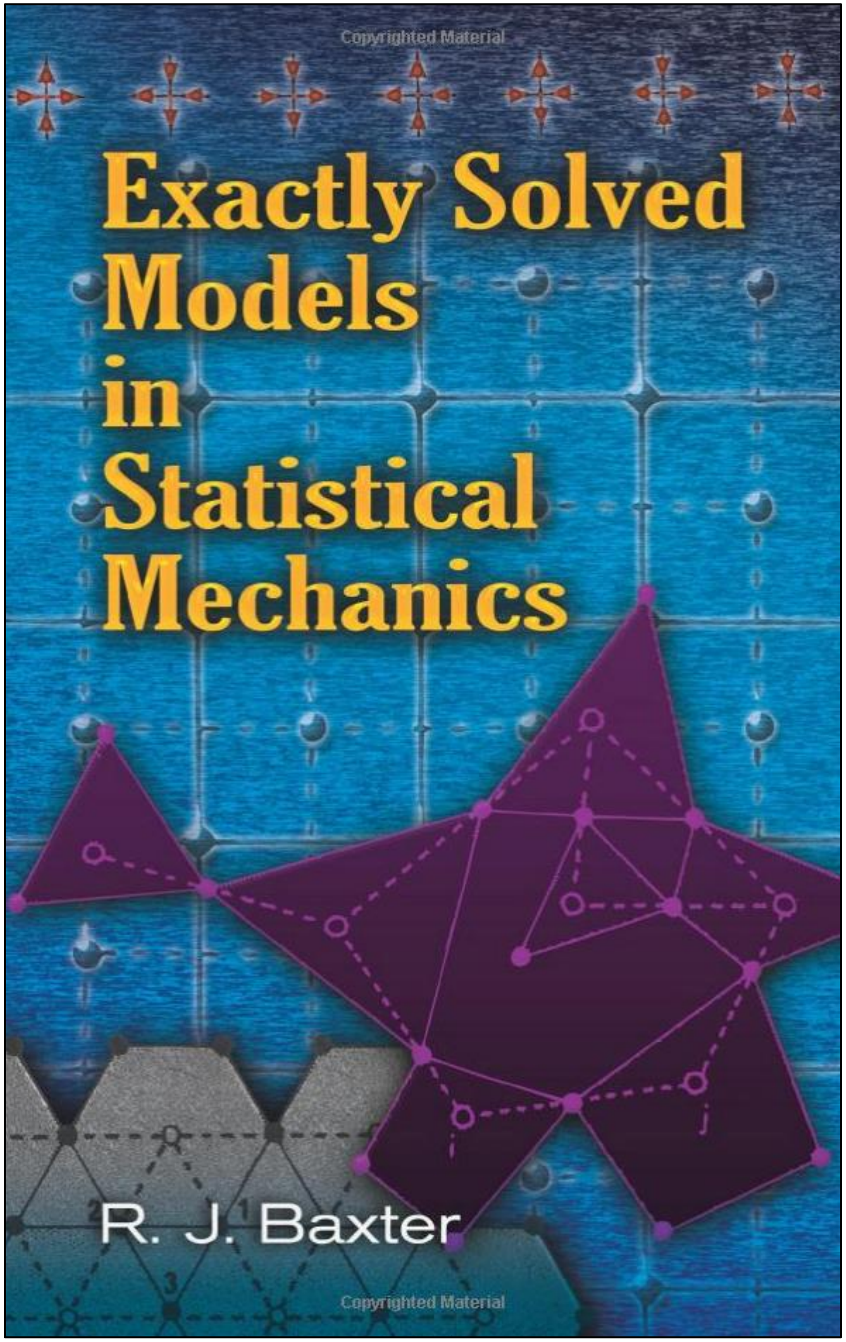
$$H = -J \sum_{n=1}^{N} \mathbf{S}_n \cdot \mathbf{S}_{n+1}$$

1D Heisenberg, conserved S_z

1- excitation waves

2-, 3-, … algebraic Bethe ansatz

… new equations & lots of work left!



1 What can we exactly diagonalize ... today?

- Spin S=1/2 models:
  40 spins square lattice, 39 sites triangular, 42 sites Honeycomb lattice
  48 sites kagome lattice
  64 spins or more in elevated magnetization sectors
  up to ~500 billion basis states

- Fractional quantum hall effect
  different filling fractions ν, up to 16-20 electrons
  up to 3.5 billion basis states

- Hubbard models (~ Full CI in Quantum Chemistry)
  20 sites square lattice at half filling, 21 sites triangular lattice
  24 sites honeycomb lattice
  up to 160 billion basis states

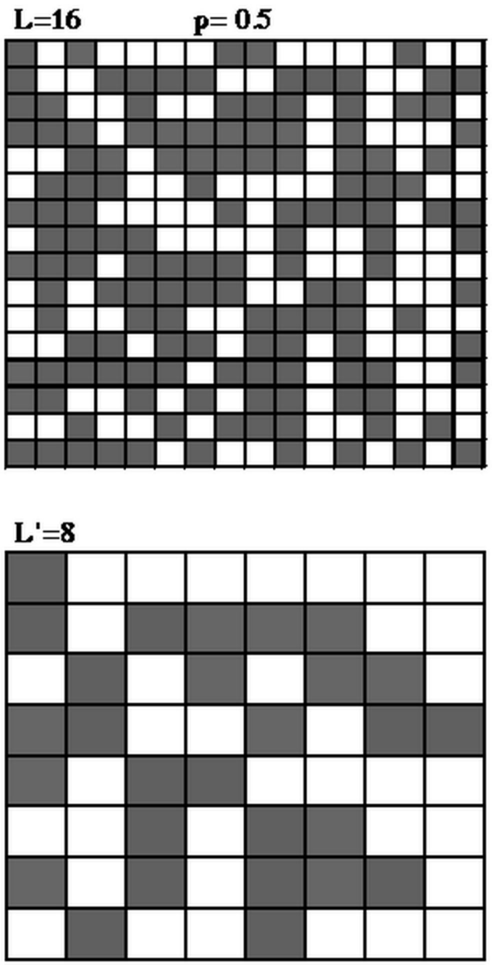
(low-lying states only)

[A.Lauchli]

1 Trying to understand a system

- exact diagonalization
- Monte Carlo sampling
- small clusters
- mean-field
  averaging over neighbors
- series expansions
- renormalization group
  relevant lengthscales
- replica trick $$\lim_{n\to 0} \frac{Z^n - 1}{n} = \ln Z$$

[D. Ceperley]



1 What's going on in a system

- varying parameters = varying nature?

  thermal fluctuations
  response functions

- phase transitions

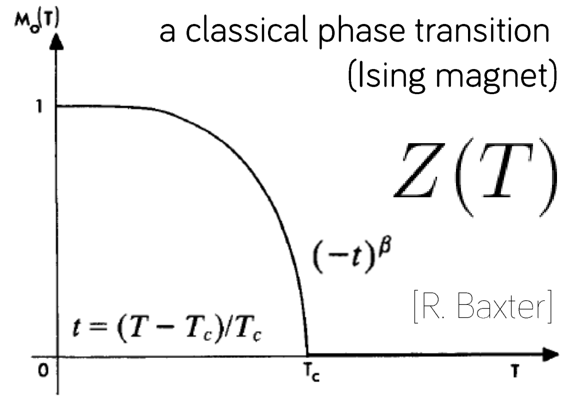
  order/disorder
  insulator/conductor
  power/exp correlation decay

- is there one? what is its type?

  scaling, critical exponents
  universality classes

a classical phase transition (Ising magnet)

$Z(T)$



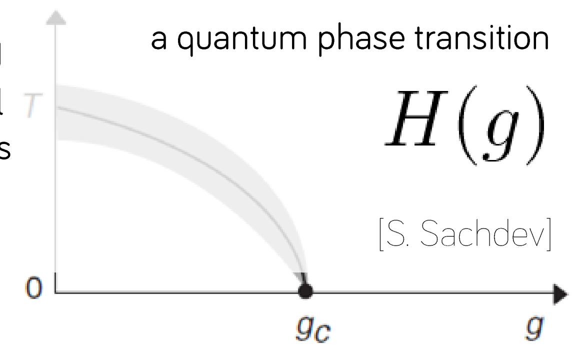
[R. Baxter]

varying T, discontinuity in M, X, C, ...

a quantum phase transition

$H(g)$

add thermal fluctuations



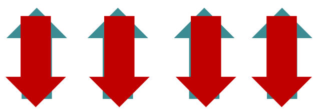
[S. Sachdev]

at T=0, discontinuity in E_0

what happens at T>0?

1 Phase transition in the quantum Ising chain

- in a transverse field $$H_I = -Jg \sum_i \hat{\sigma}_i^x - J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z$$



$g \ll 1$ $\qquad$ $g = g_c$ $\qquad$ $g \gg 1$

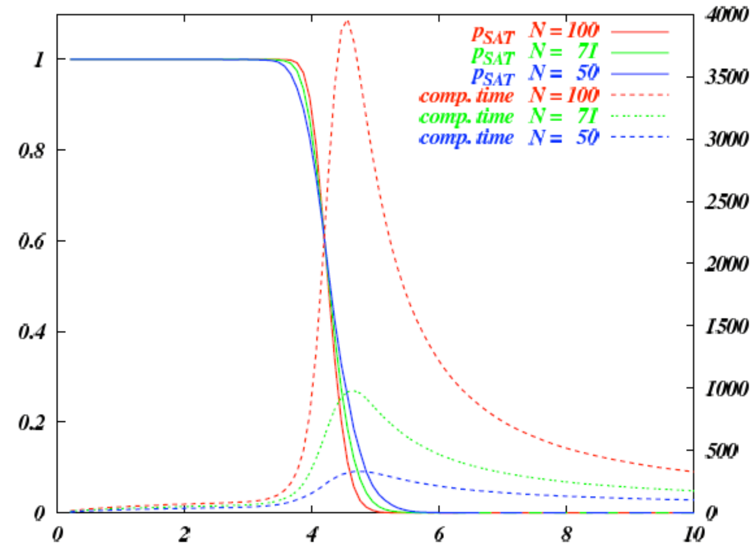
$$\langle 0 | \hat{\sigma}_i^z \hat{\sigma}_j^z | 0 \rangle \sim N_0^2 \qquad \sim \frac{1}{|x_i - x_j|^{d-2+\eta}} \qquad \sim e^{-|x_i - x_j|/\xi}$$

$$\langle 0 | \hat{\sigma}_i^z | 0 \rangle \sim N_0$$

- frustration, states get hard to describe
  correlations grow, area law corrections
  critical scaling, gap closes (finite-size: avoided crossing)

1 Phase transitions in CS

- the SAT/UNSAT transition in random SAT



[R. Zecchina]

solutions clustering

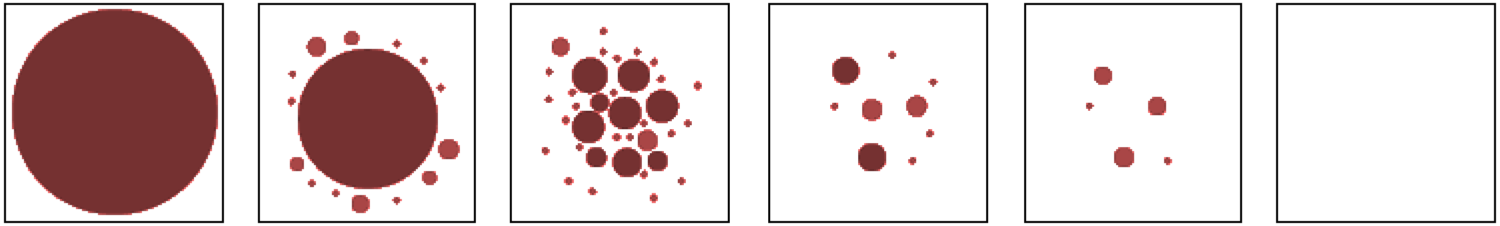
algorithms work/don't work

statistical physics analysis

... algorithms (cavity, belief, survey propagation)

[Parisi, Mezard, Zecchina, Monasson]

rigorous analysis [Coja-Oghlan]



[L. Zdeborová]

classifying

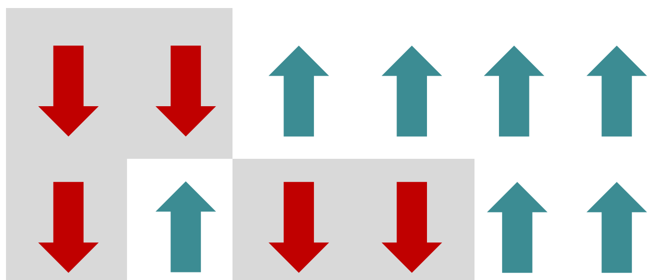
the difficulties

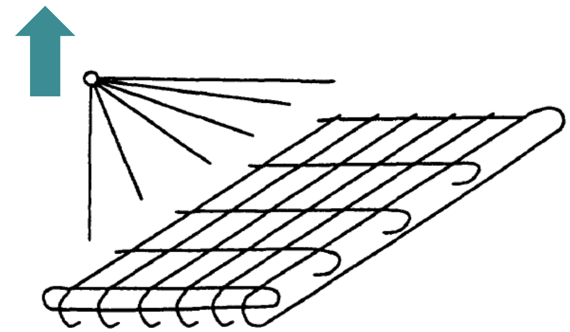
classical

2 The classical Ising spin glass can be hard (NP-C)

- 2D, varying couplings, external field [Barahona84]

$$E(s) = -\sum_{\langle i,j\rangle} J_{ij} s_i s_j - H \sum_i s_i$$



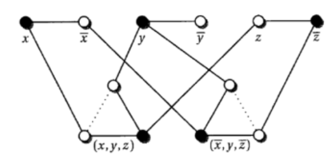


uniform *H*
varying *J*

$$= -\sum_{E} J_{ij} - HN + 2\sum_{E^{\pm}} J_{ij} + 2HF^{-}$$

$$= const. - \sum_{E^{\pm}} w_e$$

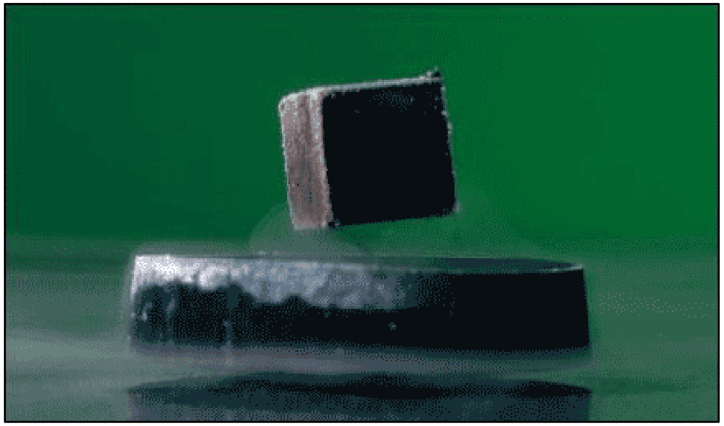
- MAX weighted CUT & finding E_0



[C. Moore, S. Mertens]

- OPTIMIZATION
  find the ground state

- UNDERSTANDING THE SYSTEM
  explain/predict expectation values



[northeastern.edu]

2 Partition function & counting

- all the properties of the system

  derivatives… properties
  responses, excitations

$$Z = \sum_s e^{-\beta E(s)}$$

$$p(s) = \frac{1}{Z} e^{-\frac{E(s)}{kT}}$$

- counting degeneracies

  Z dominated by the ground states at low T
  Ising, planar graphs: computing determinants [Kasteleyn, Fisher]
  nonplanar: #P complete (Potts, perf. matchings, permanents)

- sampling & approximation

  Markov Chain Monte Carlo
  [Jerrum Sinclair]

$$Z(T_n) = \frac{Z_n}{Z_{n-1}} \frac{Z_{n-1}}{Z_{n-2}} \cdots \frac{Z_1}{Z_0} Z_0$$

the quantumness

the quantum mess

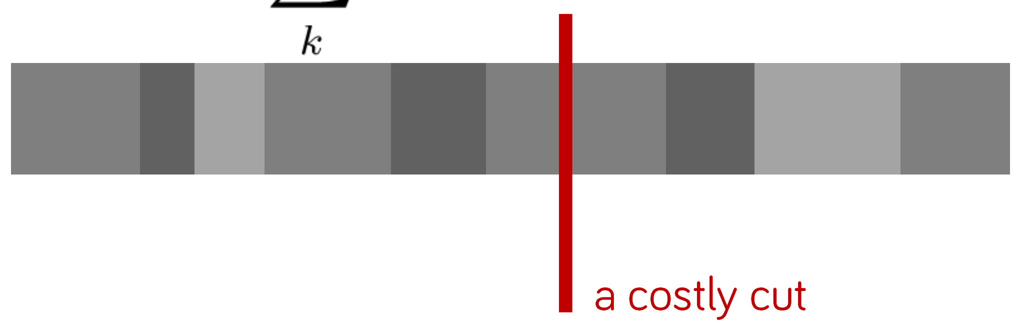
3 Quantum Many-Body Hamiltonians

- non-commuting terms $$H = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i^z\sigma_j^z - \sum B_i\sigma_i^x$$

entanglement (vs. products)

hard-to-find, hard-to describe ground states

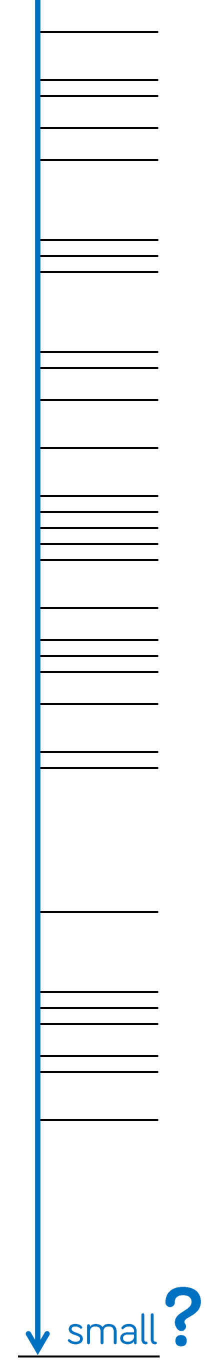
- Schmidt decomposition $$\sum_k \lambda_k |a_k\rangle \otimes |b_k\rangle$$



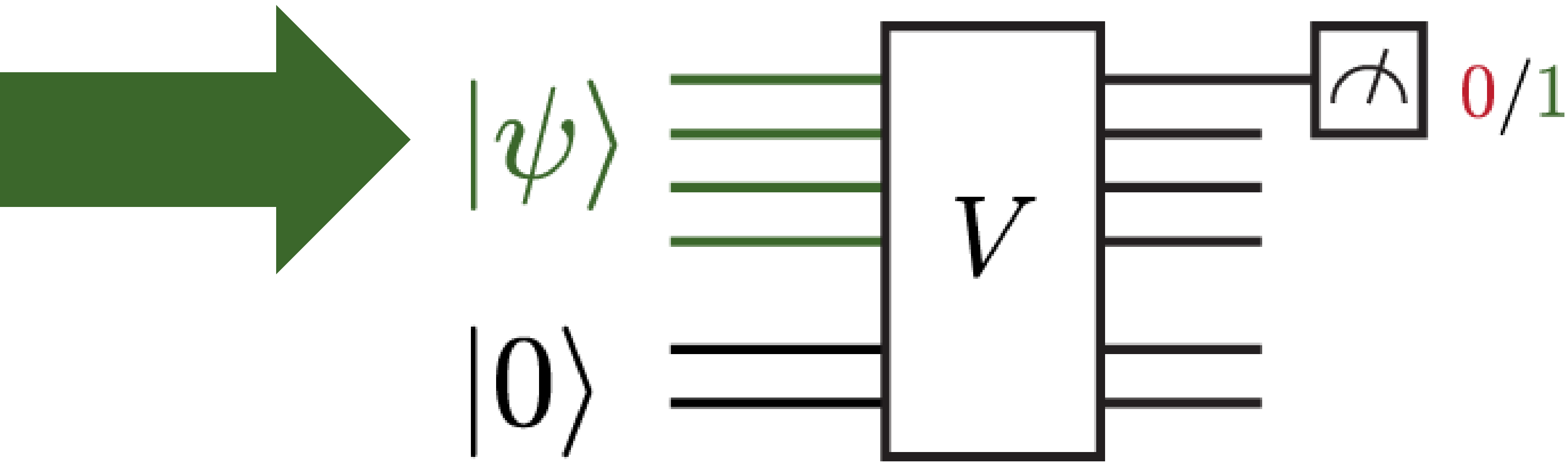
- the basic hard question: E_0

3 The Local Hamiltonian problem

Is the ground state energy of a **LH**

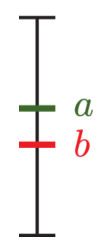


3 The QMA protocol



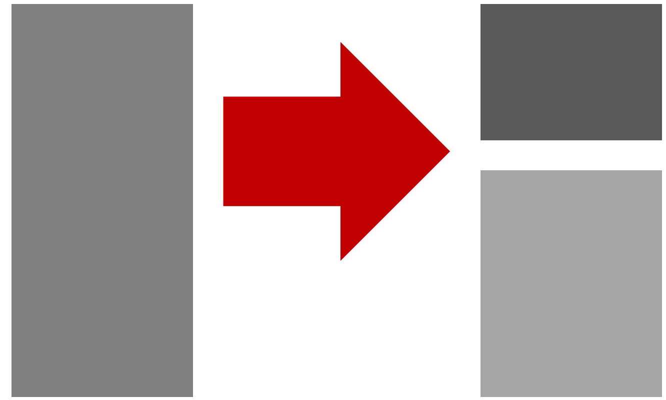
YES? Accept a good proof with $p > a$.

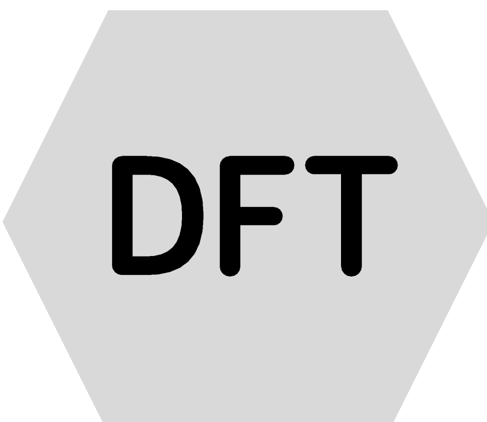
NO? Probability of accepting $p < b$.



3 Other QMA-complete problems

[Bookatz '13]

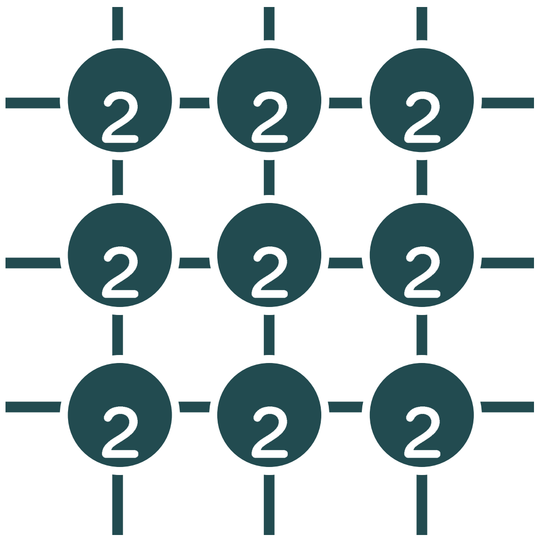




3 Other QMA-complete problems

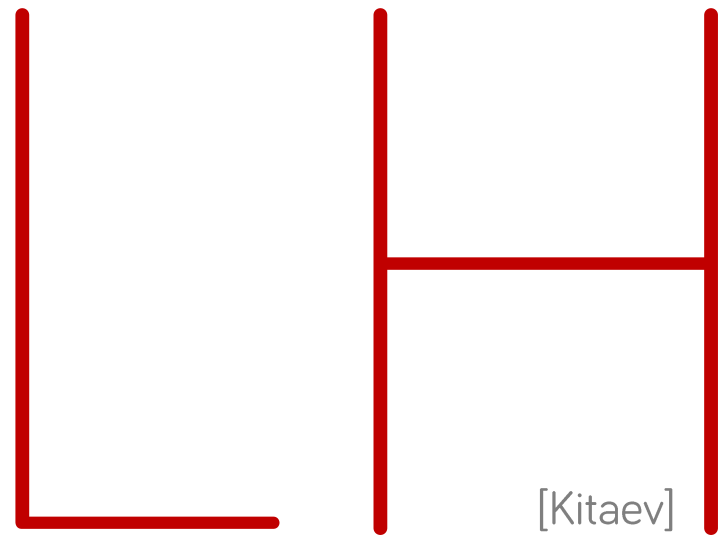
[Bookatz '13]

3 2-local Hamiltonian is QMA complete

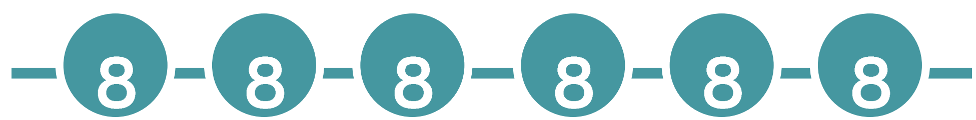


[Oliveira, Terhal '04]

a global minimum

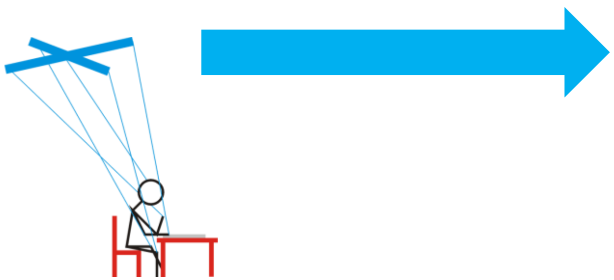


$$\sum H_{jk}$$



[Hallgren, N, Narayanaswami '13]

clock/work registers

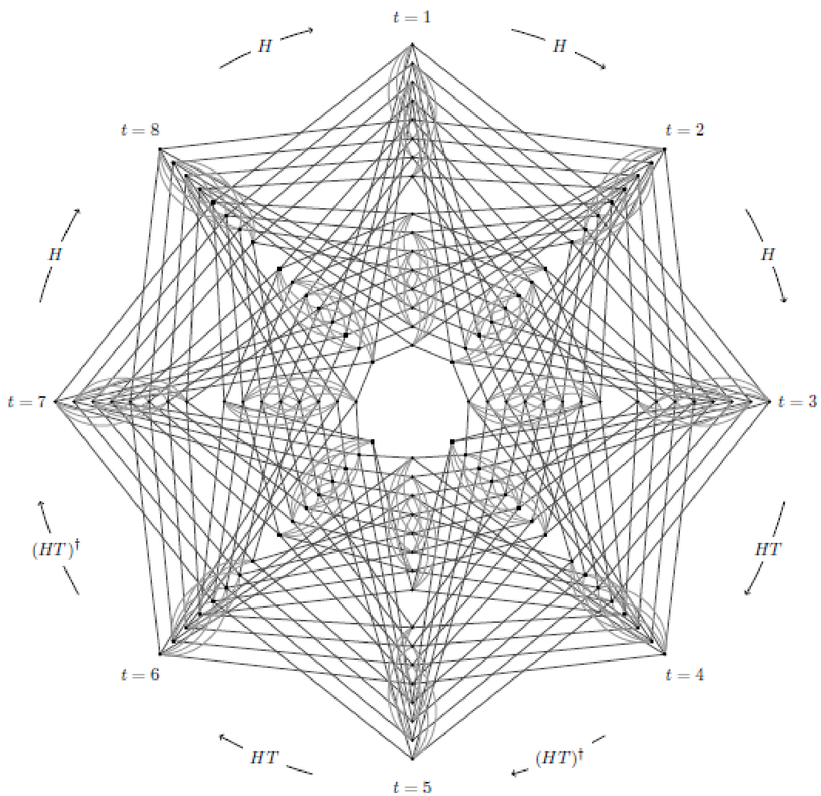


Can we get away from this?

QMA-complete problems that are more "natural"?

Problem 4 (Minimum Graph Eigenvalue). We are given a $D \times D$ symmetric 0-1 matrix A, specified by a classical deterministic circuit that takes as input a row $r \in [D]$ and computes the locations of the nonzero entries in that row. We are also given a real number a and a precision parameter $\epsilon = \frac{1}{N}$, where $N \in \mathbb{N}$ is specified in unary. We are promised that either the smallest eigenvalue of A is at most a (yes instance), or else it is at least $a + \epsilon$ (no instance), and asked to decide which is the case.

[Childs Gosset Webb 13]



Can we get away from this?

QMA-complete problems?

Universality & hardness?

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

[Childs Gosset Webb 13]

many-body physics & complexity 1

tough & interesting questions

classical

MODELS

quantum

4 Local Hamiltonians

Many local questions.

- What are they like?

  ground state (energy)

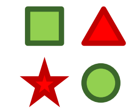
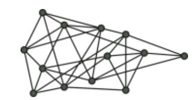
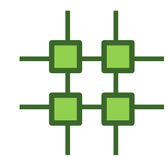
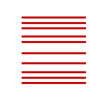
  QMA-complete problems

$$\sum_k H_k(t)$$

- What are they good for?

  control, transport, chemistry, making a (q) computer

  BQP universality

- local particle dimension 
- interaction geometry 
- time independence 
- translational invariance 
- promise and eigenvalue gaps 
- energy × time cost 

many-body physics & complexity 2

the problems & the tools

Daniel Nagaj

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