

(AN UNMATCHED LEFT PARENTHESIS
CREATES AN UNRESOLVED TENSION
THAT WILL STAY WITH YOU ALL DAY.

Criticality without Frustration

IQC Waterloo, 9/2012



Sergey Bravyi
IBM Watson

Libor Caha
Slovak Academy of Sciences

Ramis Movassagh
Northeastern University

Peter Shor
MIT

Daniel Nagaj



arXiv: 1203.5801

Thanks: IQC, QESSENCE, LPP QWAC

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1 finding ground states (1D)

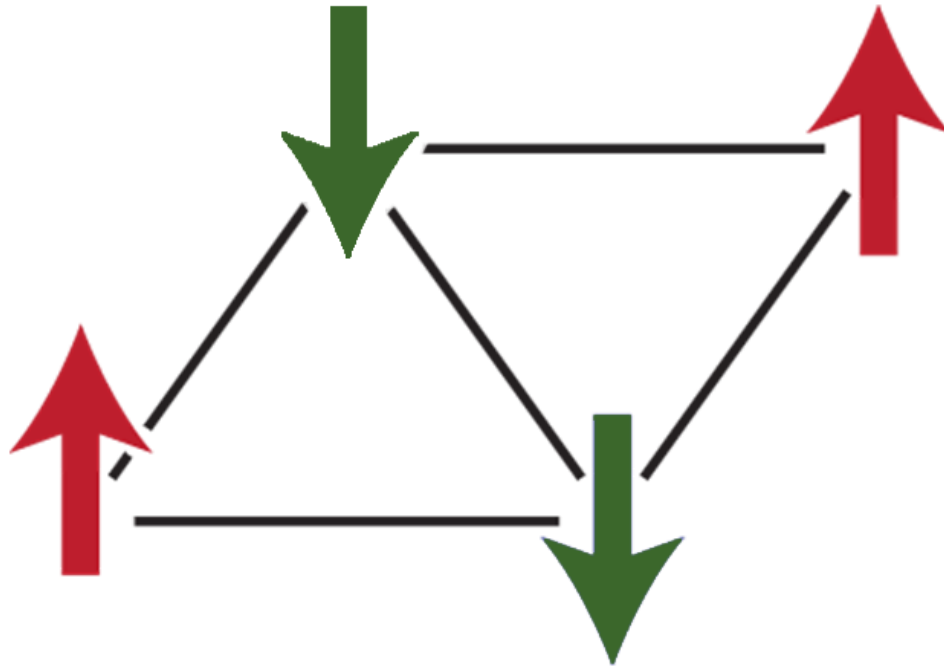
2 fun with qutrits

3 formidable calculations

4 frustration free future

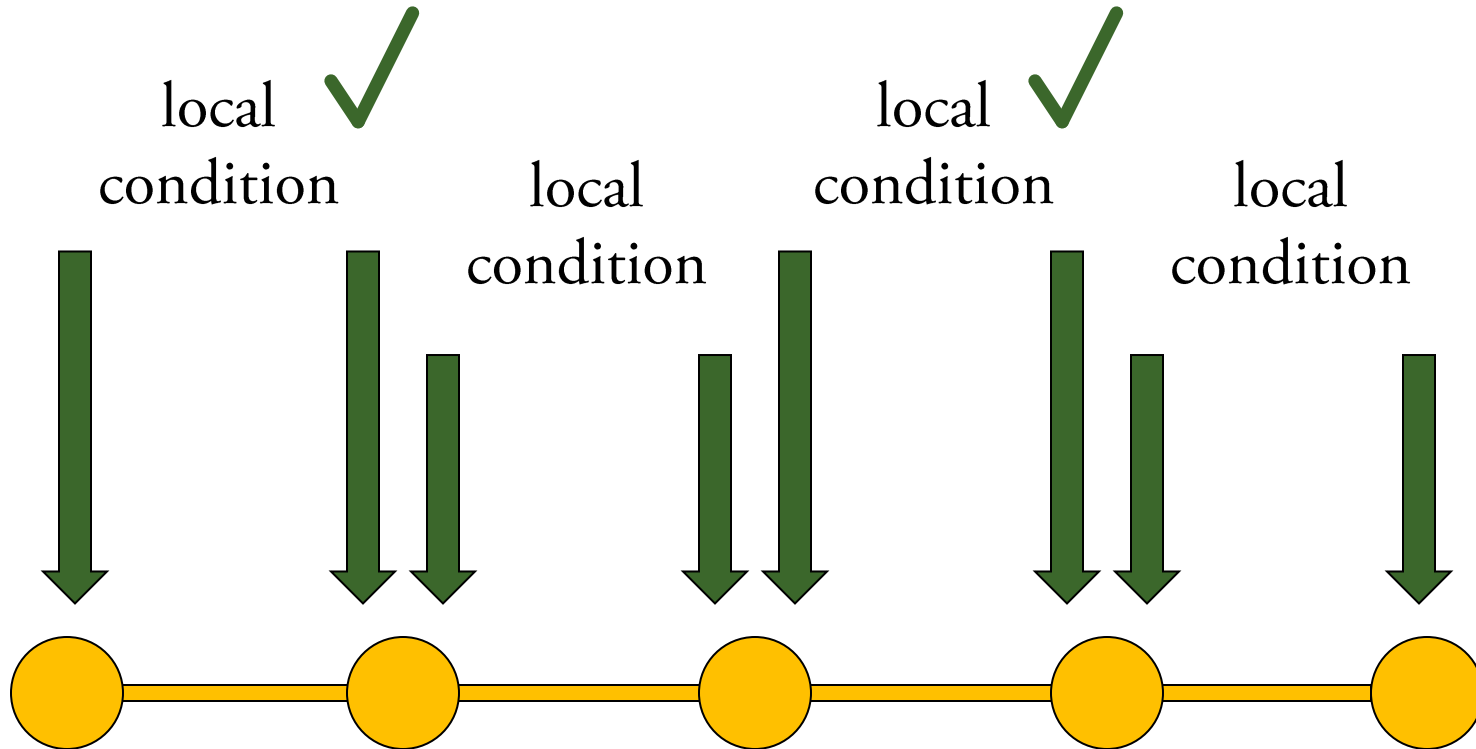
1 Frustrated systems

Sometimes you can't make everybody happy.



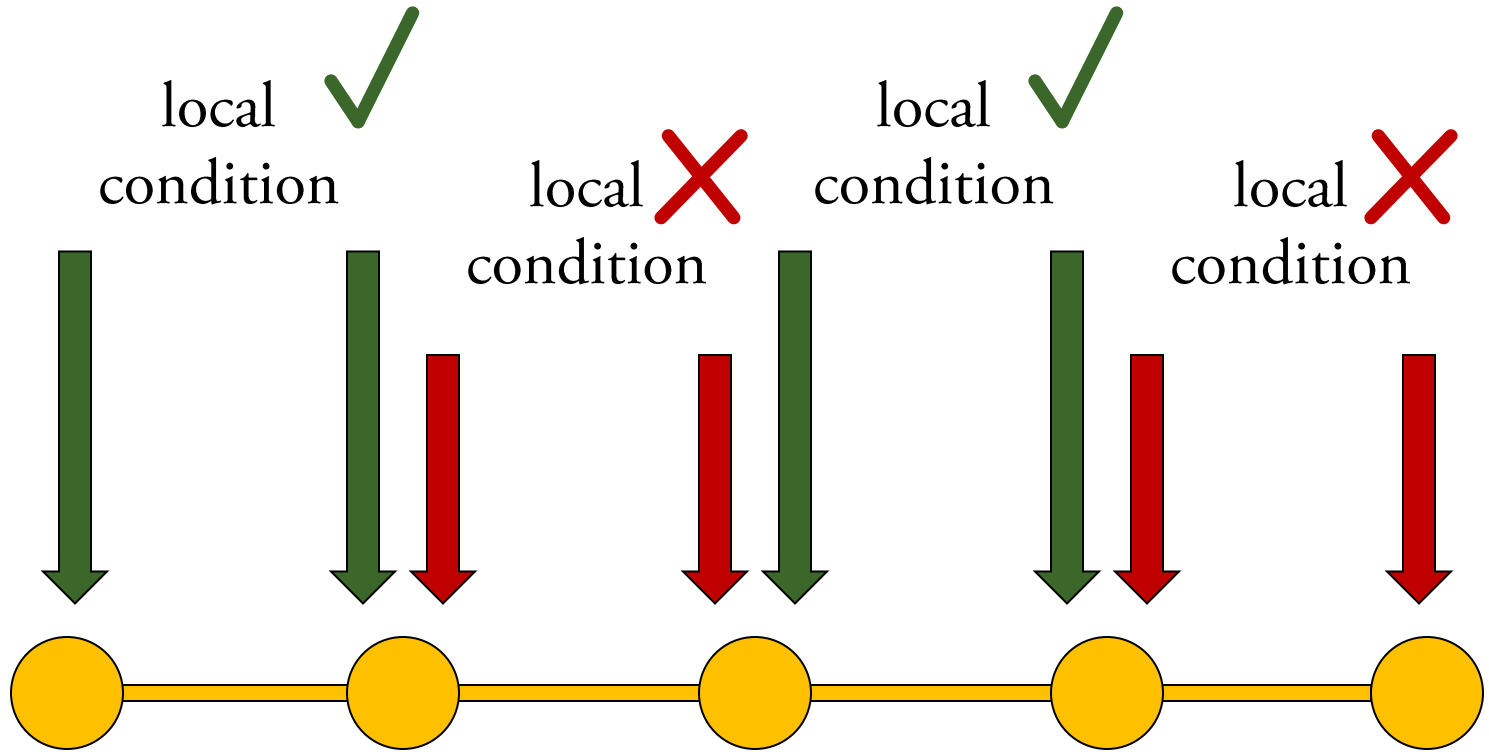
1 Frustrated ground states in 1D

Quantum chains with low d .



1 Frustrated ground states in 1D

Quantum chains with low d.



a global ground state

HARD?

find & describe it?
is it entangled?



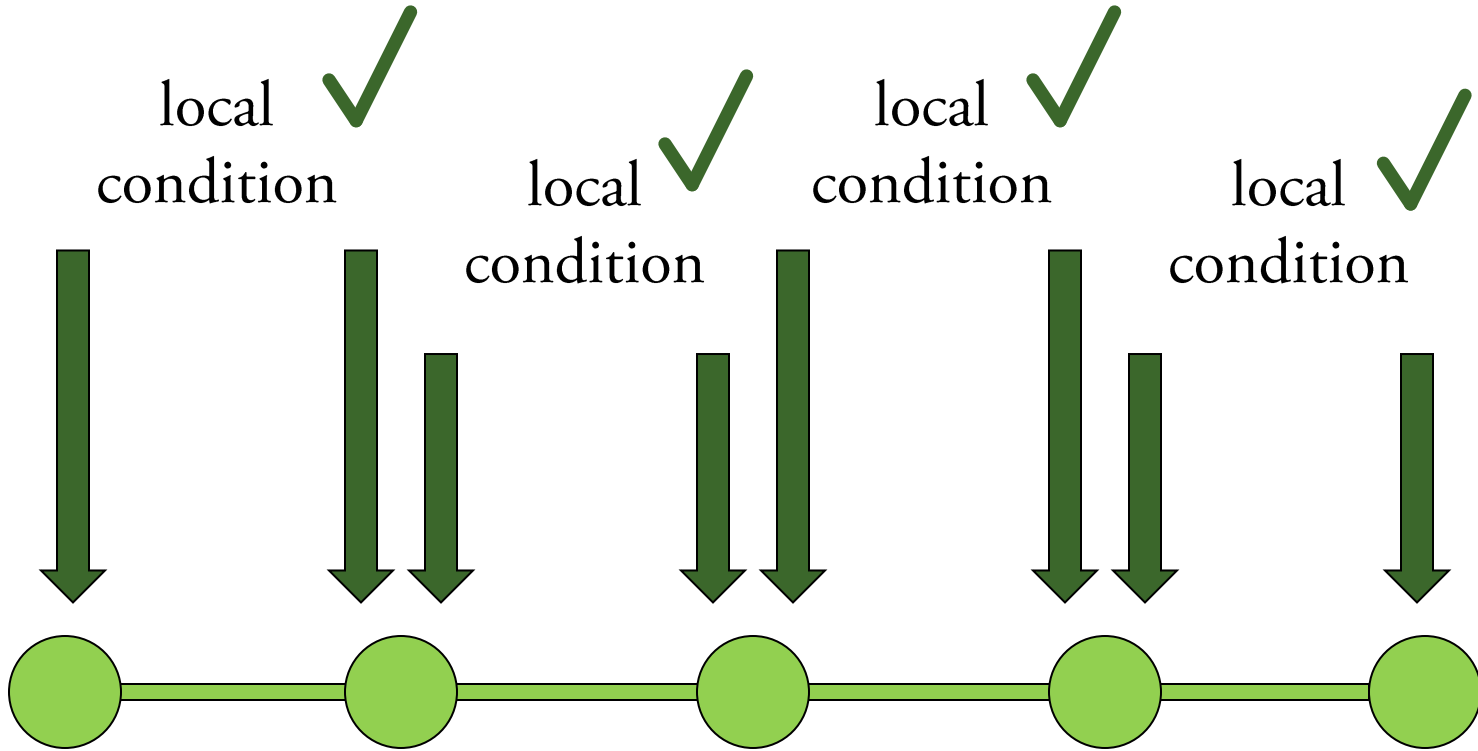
frustrated

FRUST
RATED

1

Unfrustrated ground states in 1D

Quantum chains with low d.



a global & local ground state

EASY?

find & describe it?
is it entangled?

1 Classical 1D: simple

Having higher dits doesn't add anything.

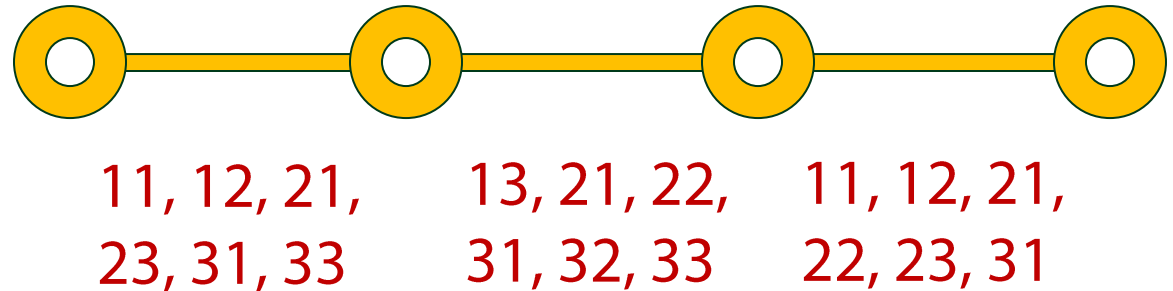
- unfrustrated ground states on a line?



1 Classical 1D: simple

Having higher dits doesn't add anything.

- unfrustrated ground states on a line?



- classical 2-SAT in 1D: a list of forbidden states

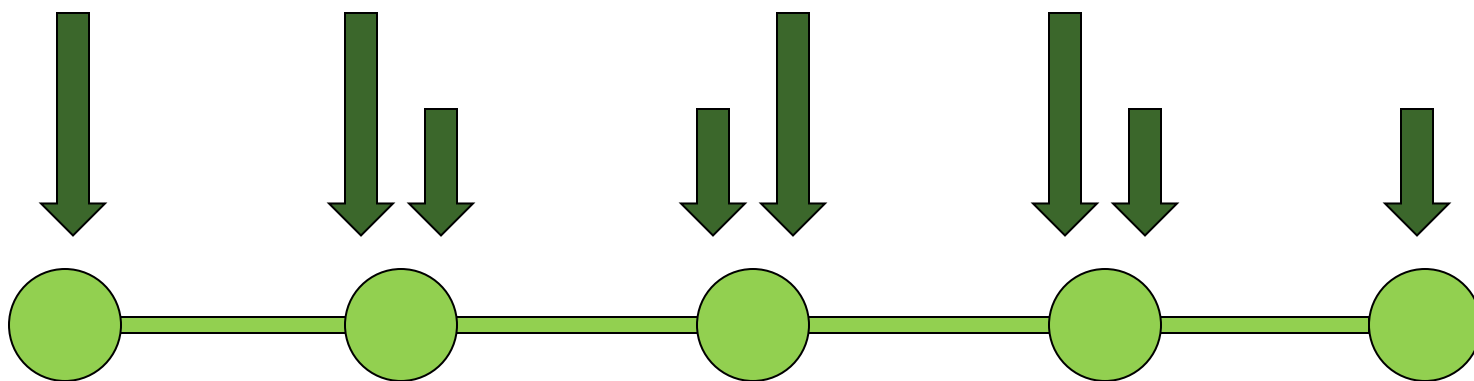
allowed pairs	13, 22, 32	11, 12, 23	13, 32, 33	
allowed states	1, 2, 3	2, 3	3	2, 3

the MAX-version is also solvable (dynamical programming)

1 Unfrustrated qubit chains in 1D

A quantum example.

$$H = \frac{1}{2} \sum_{k=1}^{L-1} |01 - 10\rangle\langle 01 - 10|_{k,k+1} \otimes \mathbb{I}$$



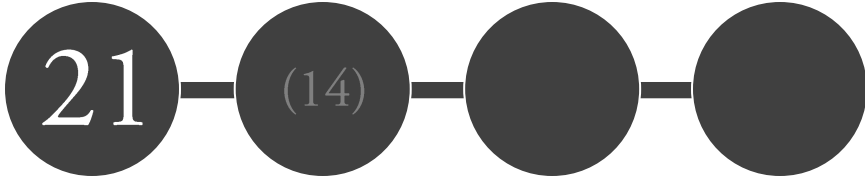
a simple product ground state $|11111\rangle$

1

Ground states in 1D

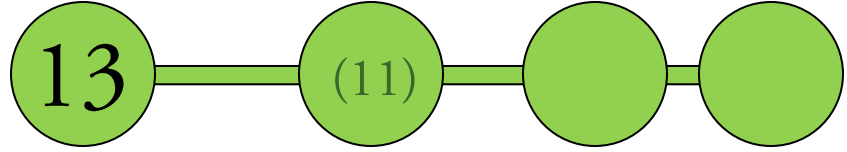
How hard is it to find/describe them?

entropy $\sim L$



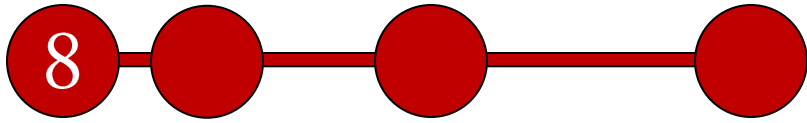
trans. invariant
[Irani]

QMA_1 -comp.



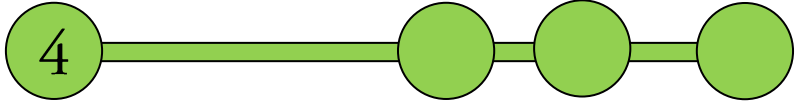
history state
[A+'06]

QMA -comp.



frustrated
[N+'12]

very entangled



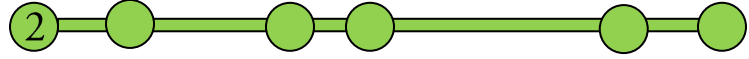
random projectors
[M+'10]

const. entropy



trans. invariant
AKLT model

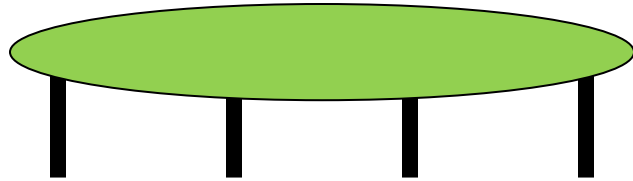
product states



Q 2-SAT in P
[Bravyi, C+]

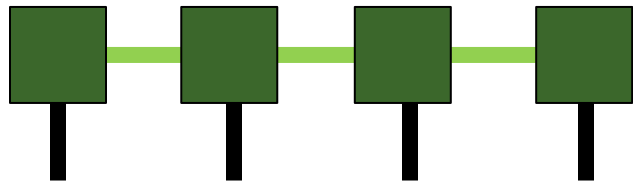
1 Finding 1D ground states

How to describe or approximate them?



$$|\psi\rangle = \sum_{s,t,u,v=0}^1 c_{stuv} |stuv\rangle$$

Schmidt decompositions \rightarrow a local description



$$c_{stuv} = \sum_{a,b,c=1}^{\chi} A_a^s B_{ab}^t C_{bc}^u D_c^v$$

■ Matrix Product States & DMRG

- ... low Schmidt rank ansatz
- ... local optimization
- ... matrix size \sim Schmidt rank

1 FF ground states in 1D

How hard is it to find/describe them?

- Are they hard to find?
- Can they be very entangled?

entanglement

qubits: NO

[Chen et al.]

qudits (high d): YES

[AGIK, Irani]

qubits

1 FF ground states in 1D

How hard is it to find/describe them?

- Are they hard to find?
- Can they be very entangled?

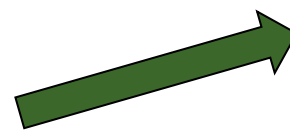
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qu3its?

1 FF ground states in 1D

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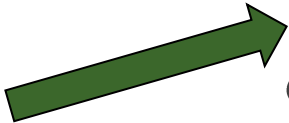
■ Are they hard to find?

entanglement

■ Can they be very entangled?

qubits: NO

[Chen et al.]



qudits (high d): YES

[AGIK, Irani]

■ Nice & surprising properties?

unique? gapped?

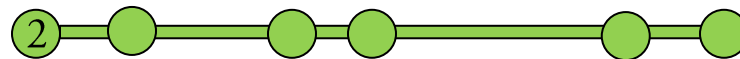
translationally invariant?

const. entropy



trans. invariant
AKLT model

product states



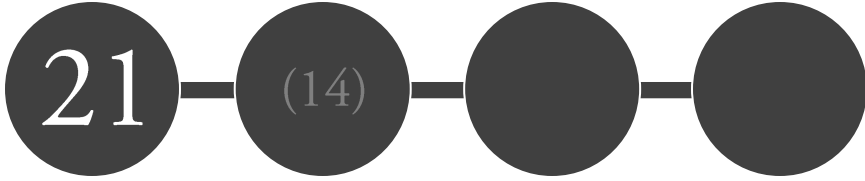
Q 2-SAT in P
[Bravyi, Chen]

1

Ground states in 1D

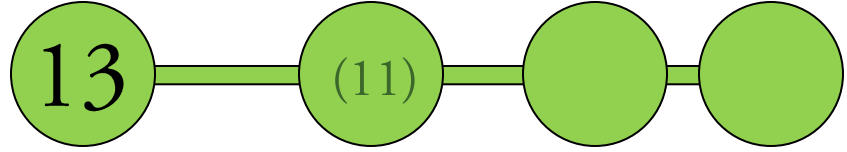
How hard is it to find/describe them?

entropy $\sim L$



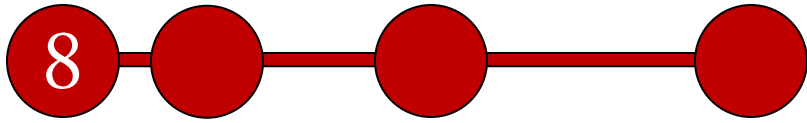
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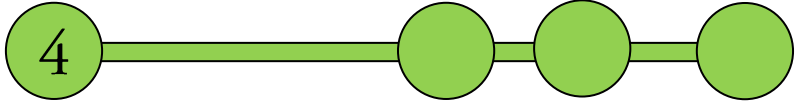
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very entangled



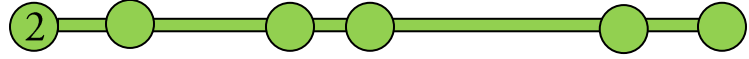
random projectors
[M+'10]

const. entropy



trans. invariant
AKLT model

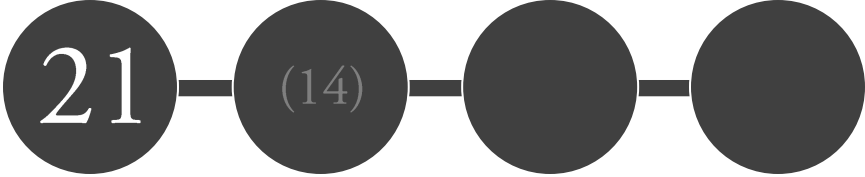
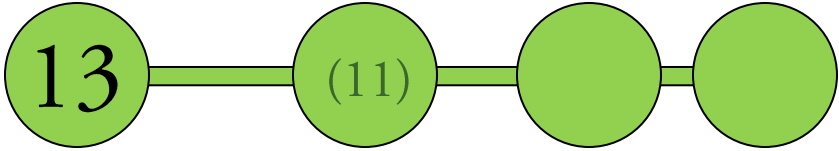
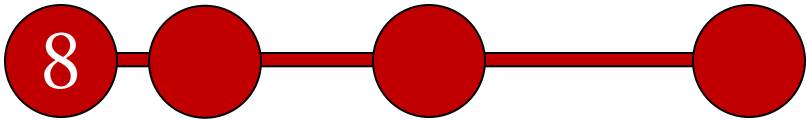
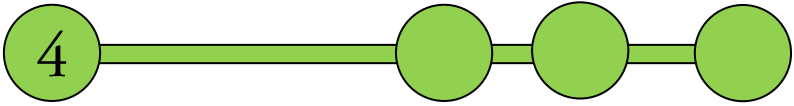


product states



Q 2-SAT in P
[Bravyi, C+]

1 Ground states in 1D

How hard is it to find/describe them?

entropy $\sim L$		trans. invariant [Irani]
QMA_1 -comp.		history state [A+'06]
QMA -comp.		frustrated [N+'12]
very entangled		random projectors [M+'10]
■ entropy $\sim \log L$		trans. invariant [B+'12]
product states		Q 2-SAT in P [Bravyi, C+]

2 Quantum + more dimensions: encode a computation

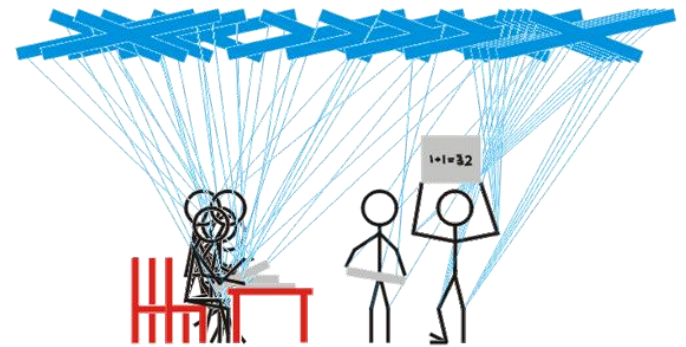
- Kitaev's Hamiltonian written in a local way

$$H_K = \frac{1}{2} \sum_{t=1}^T (|\psi_t\rangle - |\psi_{t-1}\rangle) (\langle\psi_t| - \langle\psi_{t-1}|)$$

- the history state

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

a global & local ground state



2 Quantum + more dimensions: encode a computation

- 2-locally checkable transitions

$$\frac{1}{2} (|ab\rangle - |cd\rangle) (\langle ab| - \langle cd|)$$

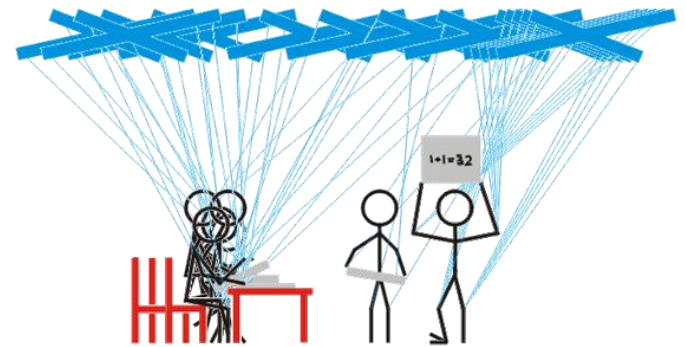
0-energy states

$$\begin{aligned} & \cdots |ab\rangle \cdots \\ & + \cdots |cd\rangle \cdots \end{aligned}$$

- the history state

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

a global & local ground state



high- d qubits
the data “moves”

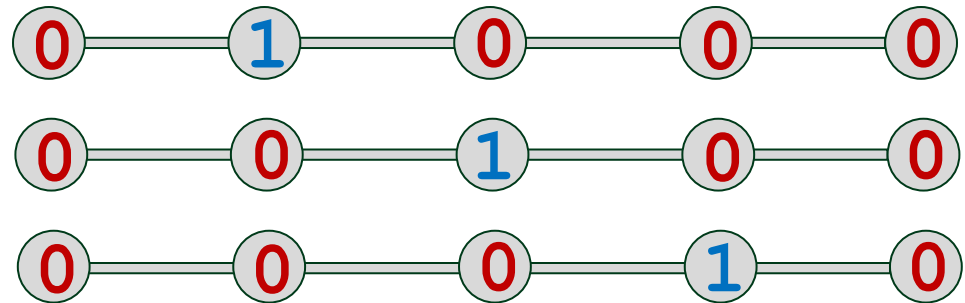


2 A less complicated task: moving qubits

Hopping on a line.

- allowed transitions

$$01 \leftrightarrow 10$$



- Hamiltonian: 2-local projectors

$$\frac{1}{2}(|01\rangle - |10\rangle)(\langle 01| - \langle 10|)$$

ground states: uniform superpositions

- invariant subspaces with different # of **1**'s
degenerate ground state (1 in each subspace)

cut down the deneneracy: rule out **11**

still a “dead” (product) ground state

1100
1010
1001
0110
0101
0011

0000

2 Surfing with qutrits

- the surfer construction
 $W, @, w$... a surfer riding a wave

transition rule $@w \leftrightarrow W@$

2-local projector to check the transition

$$\frac{1}{2} (|@w\rangle - |W@\rangle) (\langle @w| - \langle W@|)$$

ensure a single wave ... rule out

$wW, Ww, @@, w@, @W$
 + endpoint w/W

- a unique, entangled ground state
 quantum computation on a single qubit

Moving a domain wall.

$@wwwwwwwwww$
 $W@wwwwwwww$
 $WW@wwwwww$
 $WWW@wwww$
 $WWWW@www$
 $WWWWW@ww$
 $WWWWWW@w$
 $WWWWWWW@$

2 Surfing with qutrits

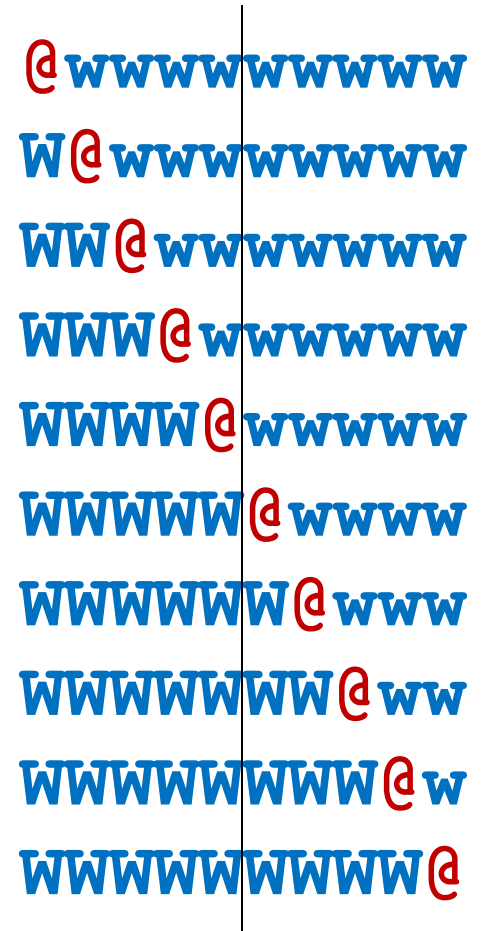
- is the surfer state entangled?

Schmidt decomposition

$$\sum_{j=1}^{\chi} \lambda_j |\phi_j\rangle_A \otimes |\psi_j\rangle_B$$

- constant MPS dimension $\chi = 2$
same as in the AKLT model

Moving a domain wall.

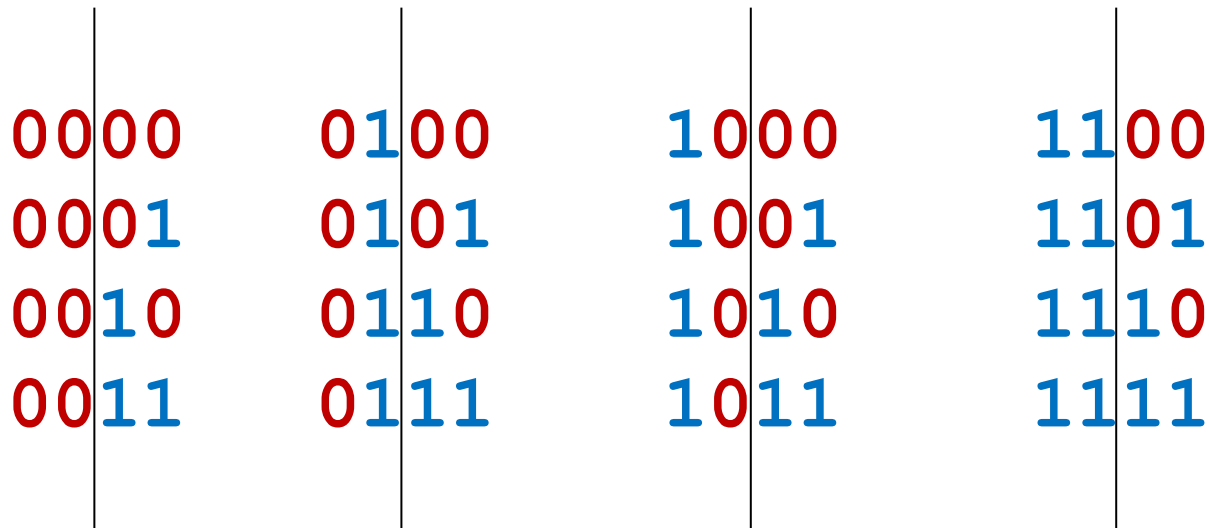


$$\begin{aligned}
 & (@www + W@www + \dots) \otimes wwwww \\
 & \quad + WWWW \otimes (@www + W@www + \dots)
 \end{aligned}$$

2 Entanglement and superpositions

Does one imply the other?

- a lot of terms in a superposition
not necessarily entangled



$$(0+1) (0+1) \otimes (0+1) (0+1)$$

2 Unique ground states

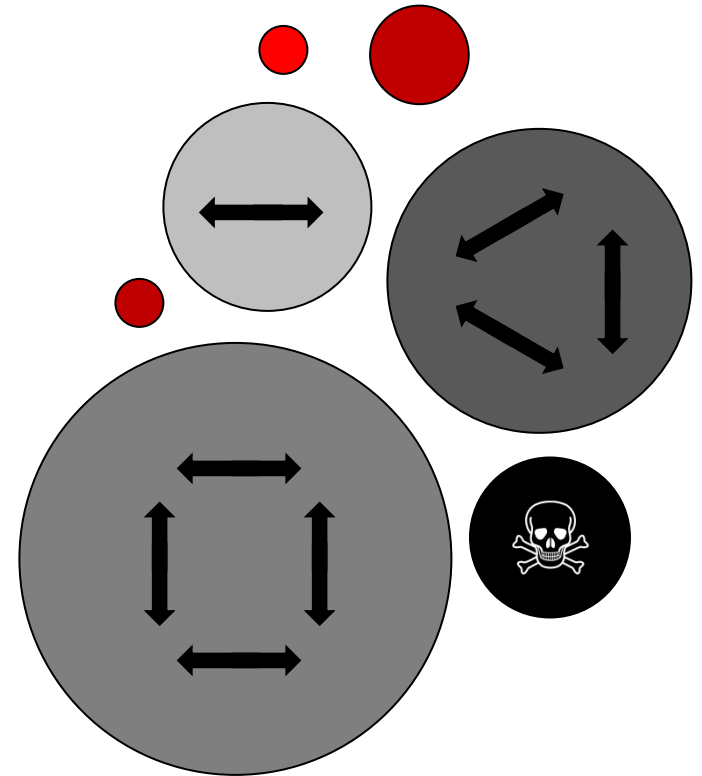
Invariant subspaces & killing all but one.

- interesting: lots of entanglement
large Schmidt number, ent. entropy

- build a superposition
history state-like?
transition rules
connected components

$$\frac{1}{\sqrt{C_N}} \sum_s |s\rangle$$

- make it unique
local rules (+ endpoints)



~~wwwww~~

W@wwww

WW@ww

WWWWWW~~X~~

2 The bracket construction

[[[Yes, this is it.]]]

- strings of 3 letters: [] -

transition rules -- ↔ []

[- ↔ - [

-] ↔] -

checkable by 2-local projectors

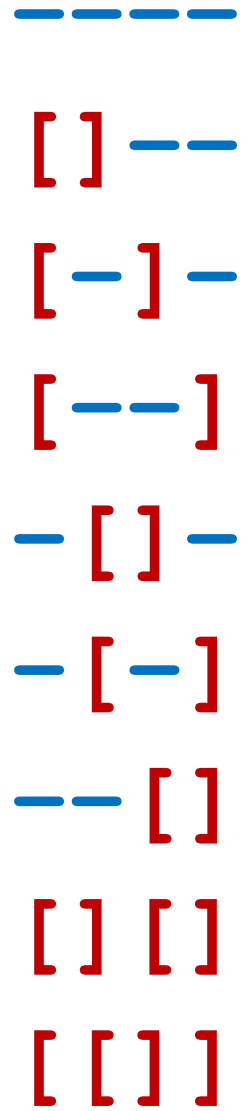
$$\frac{1}{2} (|ab\rangle - |cd\rangle) (\langle ab| - \langle cd|)$$

dislike bad brackets at the ends

] ... or ... [

- a unique ground state
well bracketed

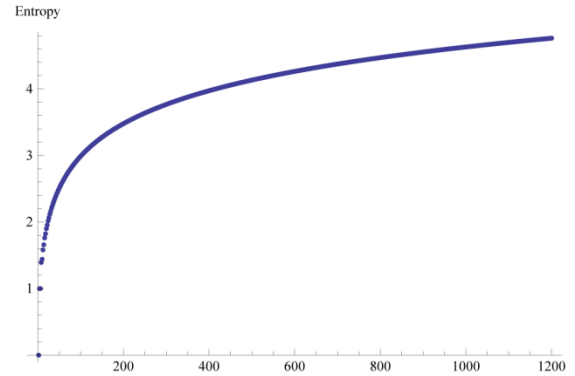
$$\frac{1}{\sqrt{M_n}} \sum_{s \in S_{0,0}^n} |s\rangle$$



3 Fantastic properties

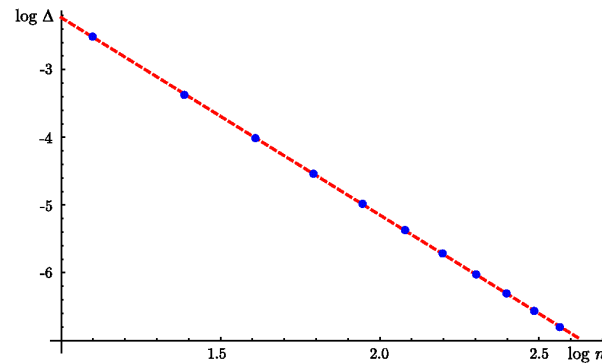
We will soon see this.

- logarithmic scaling of entanglement entropy



- a unique ground state of a frustration-free qutrit chain

- a polynomial Hamiltonian gap



3 Fantastic properties

We will soon see this.

- logarithmic scaling of entanglement entropy

CRITICALITY

- a unique ground state of a frustration-free qutrit chain

without frustration

- a polynomial Hamiltonian gap

[]--
[-]-
[--]
-[]-
-[-]
-- []
[] []
[[]]

3 Hilbert space structure

Making the ground state unique.

- allowed transitions

$$-- \leftrightarrow []$$

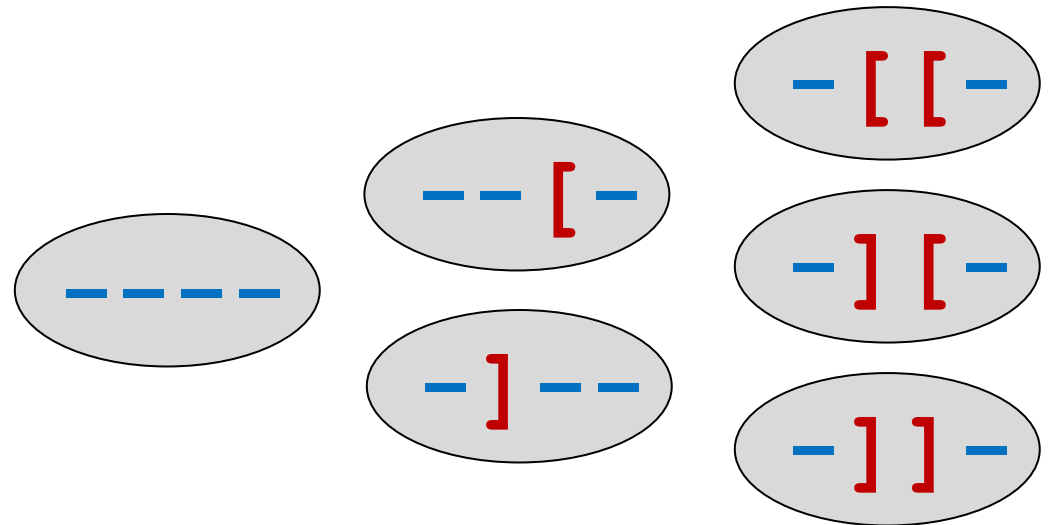
$$[- \leftrightarrow - [$$

$$-] \leftrightarrow] -$$

$H \geq 0$, a sum of projectors

$$\frac{1}{2} (|ab\rangle - |cd\rangle) (\langle ab| - \langle cd|)$$

- invariant subspaces:
(L,R) "bad" brackets



balanced

$$- [] - [- [-]]$$

$$[[-] [[-]]]$$

unbalanced

$$[- - []] - -] -$$

$$- [] - [] [[]]$$



3 Hilbert space structure

Making the ground state unique.

- allowed transitions

-- ↔ []

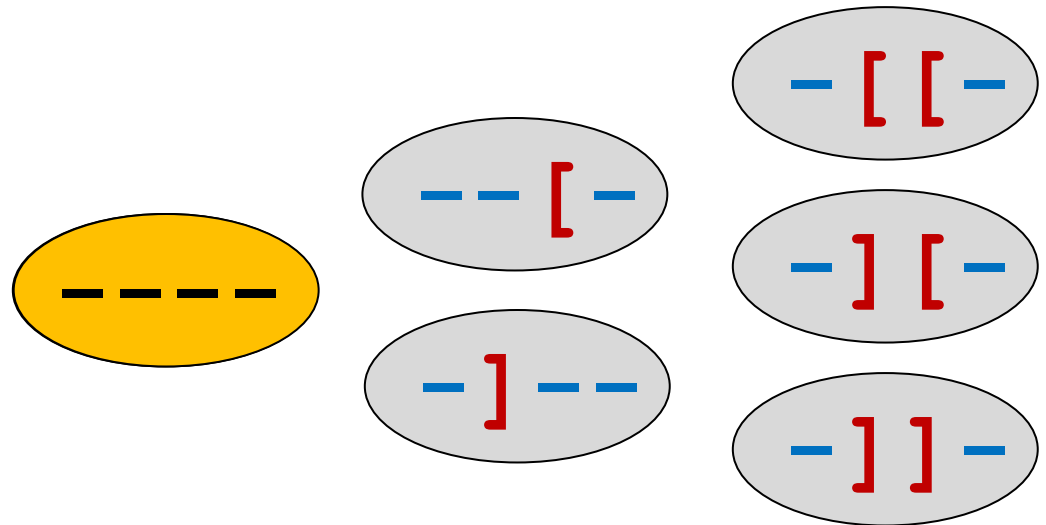
[- ↔ - [

-] ↔] -

$H \geq 0$, a sum of projectors

$$\frac{1}{2} (|ab\rangle - |cd\rangle) (\langle ab| - \langle cd|)$$

- invariant subspaces:
(L,R) “bad” brackets



- uniform superpositions within subspaces

- add endpoint projectors

a unique, unfrustrated ground state

3 The well-bracketed superposition

Matching brackets.

- the Motzkin state
uniform superposition

$$|\mathcal{M}_n\rangle = \frac{1}{\sqrt{M_n}} \sum_{s \in S_{0,0}^n} |s\rangle$$

[[]] - [] -- [- [-]] [-]
 - [- [] -- [-] - [-]] [-]

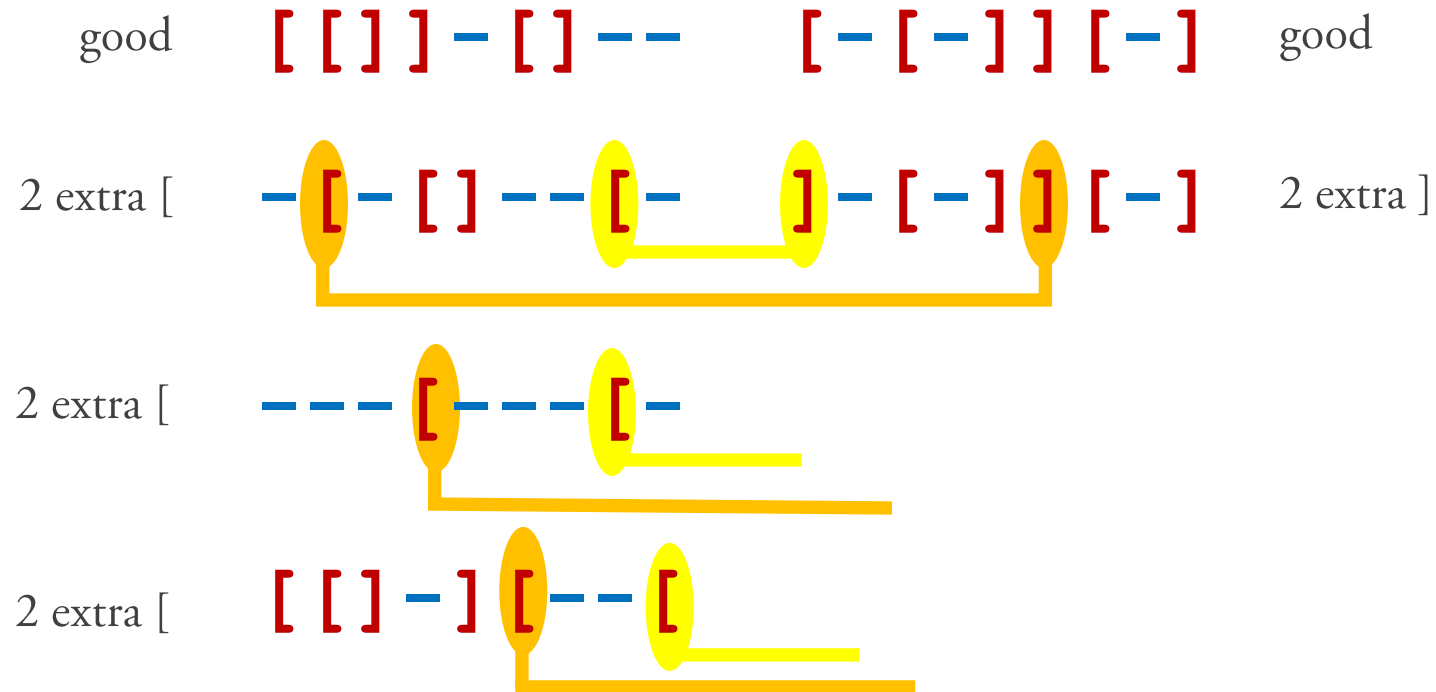
 [] --
 [-] -
 [- -]
 - [] -
 - [-]
 - - []
 [] []
 [[]]

3 Is the ground state entangled?

Cutting the ground state in half.

- the Motzkin state
uniform superposition

$$|\mathcal{M}_n\rangle = \frac{1}{\sqrt{M_n}} \sum_{s \in S_{0,0}^n} |s\rangle$$

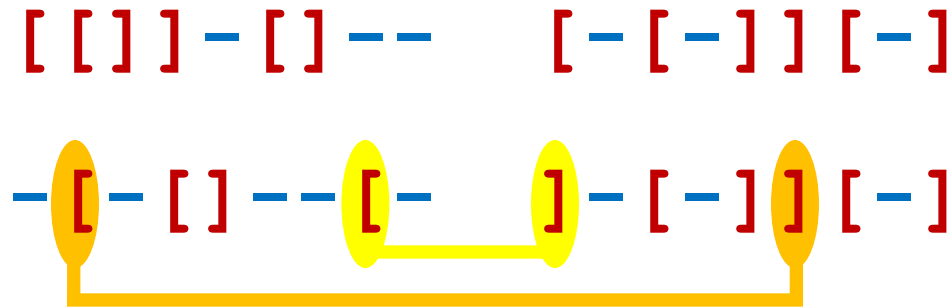


3 Is the ground state entangled?

Cutting the ground state in half.

- the Motzkin state

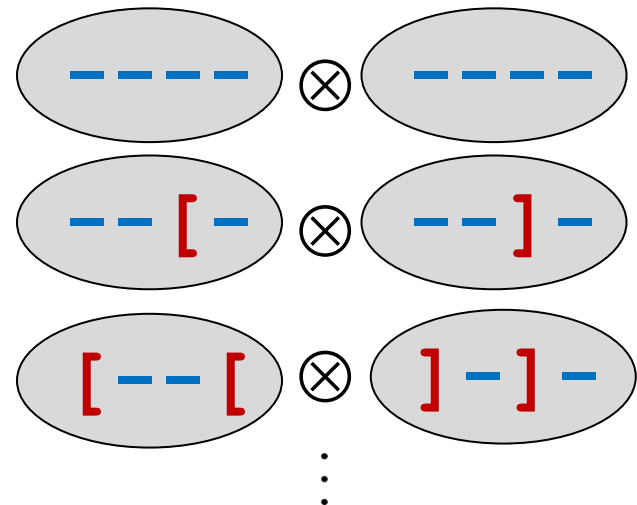
$$|\mathcal{M}_n\rangle = \frac{1}{\sqrt{M_n}} \sum_{s \in S_{0,0}^n} |s\rangle$$



- Schmidt decomposition

subspaces of length $n/2$
 m matching bad brackets

of terms: $\chi = n/2 + 1$



3 Is the ground state entangled?

Cutting the ground state in half.

- the Motzkin state

$$|\mathcal{M}_n\rangle = \frac{1}{\sqrt{M_n}} \sum_{s \in S_{0,0}^n} |s\rangle$$

$$\sum_{m=0}^{n/2} \sqrt{p_m} |\hat{C}_{0,m}\rangle_A \otimes |\hat{C}_{m,0}\rangle_B$$

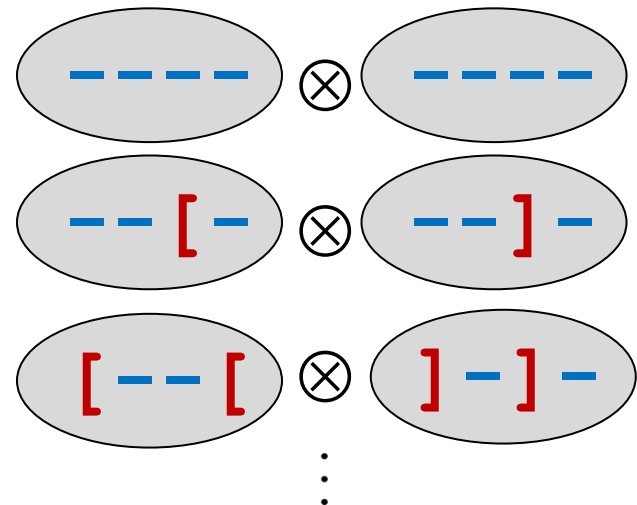
uniform superposition
length $n/2$, m extra left brackets

m extra
right brackets

- Schmidt decomposition

subspaces of length $n/2$
 m matching bad brackets

of terms: $\chi = n/2 + 1$

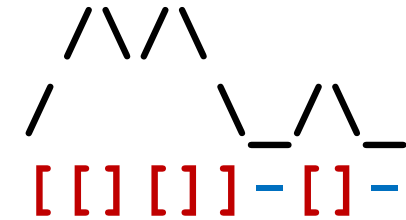
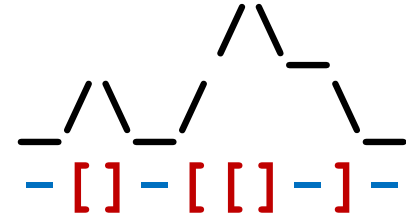


3 Quantifying entanglement

Required to compute the coefficients.

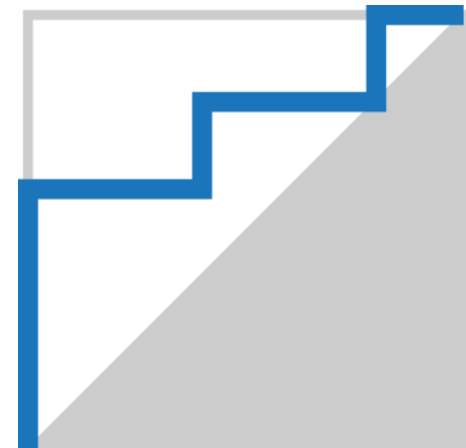
- Motzkin number M_n
of mountains of height $\leq n/2$

$$M_n = \sum_{k=1}^{\lfloor \frac{n}{2} \rfloor} C_k \binom{n}{2k}$$



- Catalan number C_k
of up/right paths above the diagonal on a $k \times k$ grid

$$C_k \propto \frac{4^n}{n^{3/2} \sqrt{\pi}}$$



3 Calculating the Catalan numbers

A neat trick.

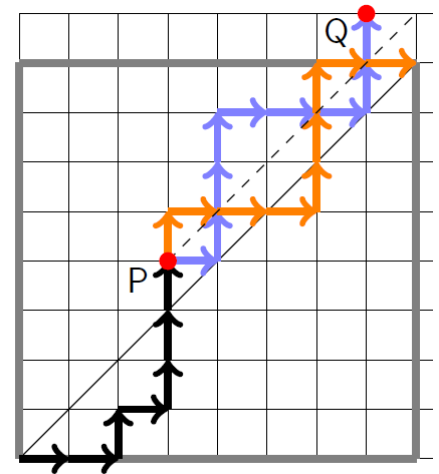
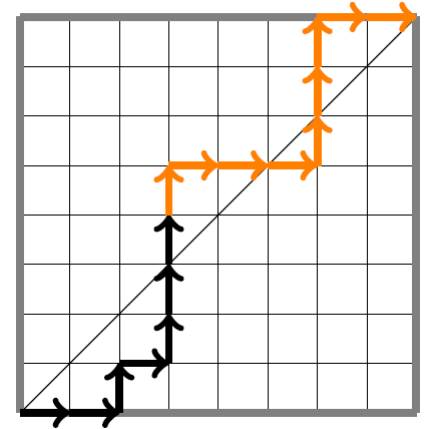
- André's reflection method

count all paths

subtract paths
crossing the diagonal

reflect after the first crossing
... paths on a $(k - 1) \times (k + 1)$ grid

$$C_k = \binom{2k}{k} - \binom{2k}{k+1}$$



3 Entanglement Entropy

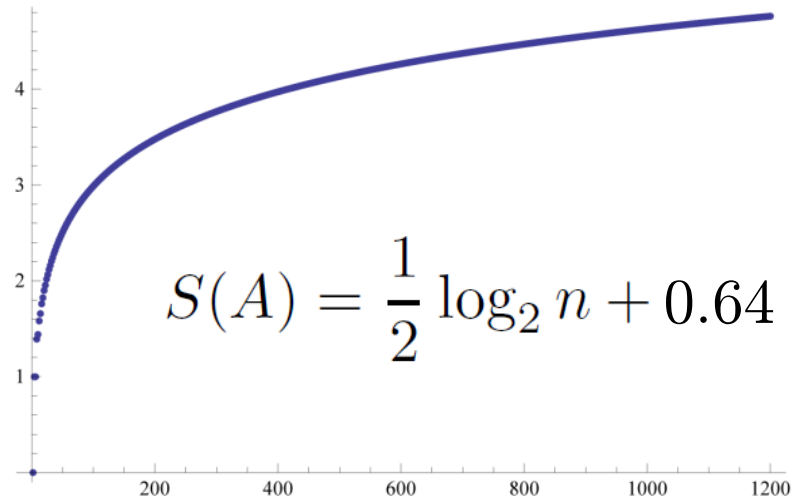
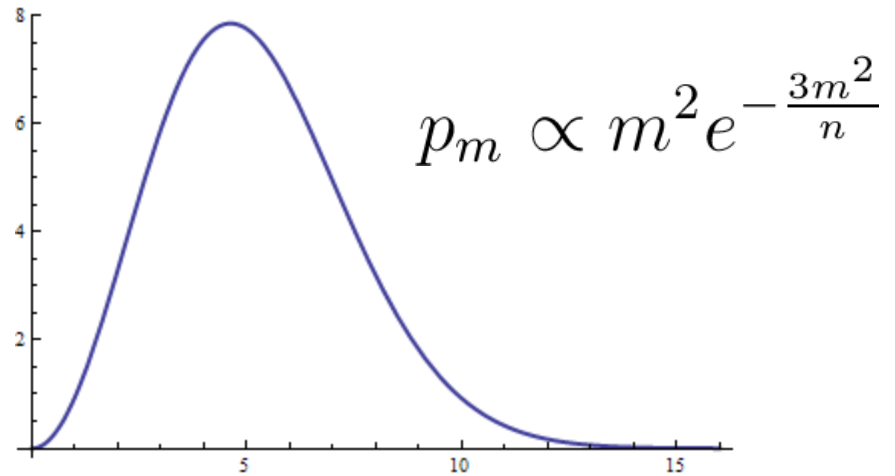
A cut through the middle.

- many significant Schmidt coefficients

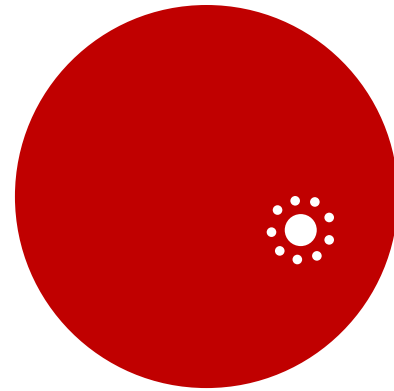
$$\sum_{m=0}^{n/2} \sqrt{p_m} |\hat{C}_{0,m}\rangle_A \otimes |\hat{C}_{m,0}\rangle_B$$

- logarithmic entanglement entropy

$$S(A) = -\text{Tr} \rho_A \log_2 \rho_A$$



a unique entangled ground state




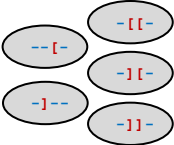
3 Bounding the energy gap

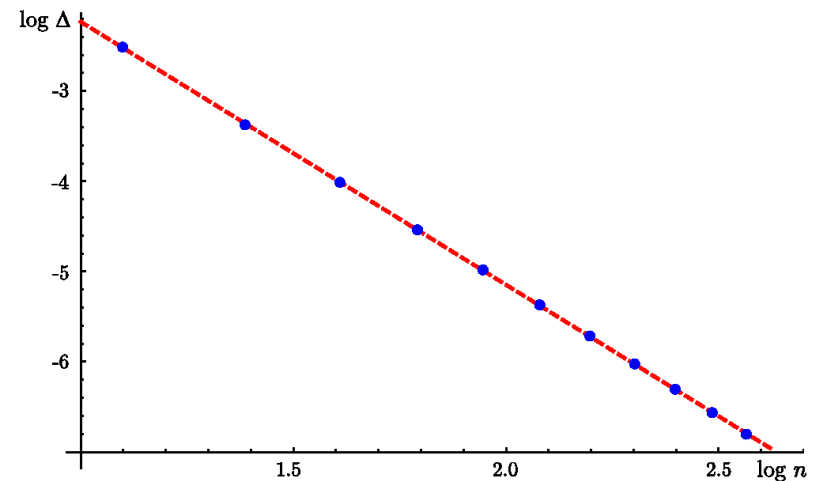
A prelude to a long story.

- frustration-free
ground state: $E=0$

$$H = H_{move} + H_{create} + H_{end}$$

- well-bracketed subspace 
... second eigenvalue?

- unbalanced subspaces 
... lowest energy?



$$\log \Delta = -0.68 - 2.91 \cdot \log n$$

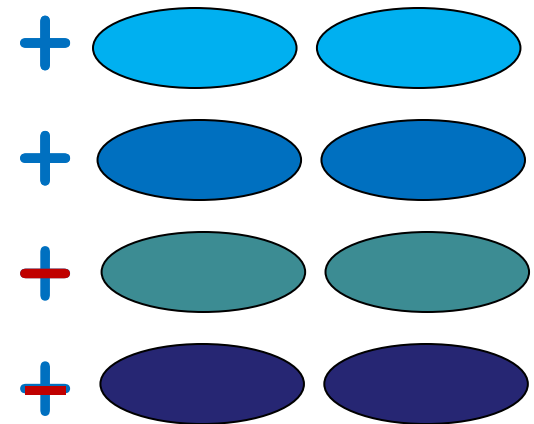
3 Is the gap small at all?

Test: twist the ground state.

- ground state: uniform

$$\sum_{m=0}^{n/2} \sqrt{p_m} |\hat{C}_{0,m}\rangle_A \otimes |\hat{C}_{m,0}\rangle_B$$

- an almost orthogonal state
from some k on use $-\sqrt{p_m}$



- caught by only a few terms
an upper bound on the gap

$$\Delta \leq O\left(\frac{1}{\sqrt{n}}\right)$$

3 Lower bounding the good subspace gap

A long story.

- [[] - [[]] - Hamiltonian
on Motzkin paths

effective
Hamiltonian
on Dyck paths



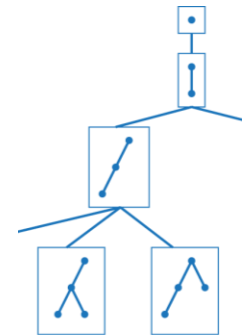
$P_{x,y}$ Markov chain
on Dyck paths

graph congestion
bounds the gap



congestion from
canonical paths

canonical paths
from fractional matchings



3 The projection lemma

Combining HUGE and tiny Hamiltonians.

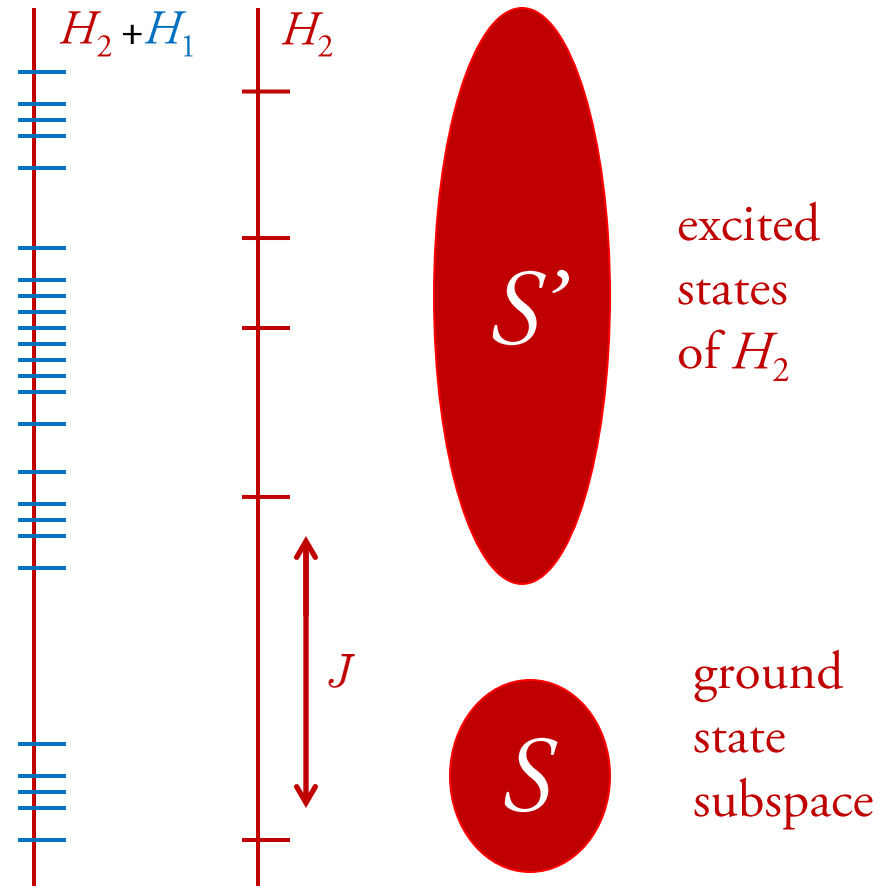
$$H_2 + H_1$$

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

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

- estimate the small eigenvalues of $H_2 + H_1$ by an effective Hamiltonian

$$H_1|_S$$



3 Projection lemma, “good” subspace

Lower bounding λ_2 .

- full Hamiltonian

$$H = H_{move} + H_{create} + H_{end}$$

$-- \leftrightarrow []$
 $[- \leftrightarrow - [$
 $-] \leftrightarrow]-$

3 Projection lemma, “good” subspace

Lower bounding λ_2 .

- full Hamiltonian

-- ↔ []

$$H|_{good} = H_{move} + H_{create}$$

- pretend the “create” part is small

$$H_\epsilon = H_{move}^{\blacksquare\blacksquare} + \epsilon H_{create}^{\blacksquare\blacksquare}$$

ferromagnetic
Heisenberg
spin $\frac{1}{2}$ chain
gap $O(n^2)$



excited
states
of H_{move}

- low spectrum

$$H_{create}|_S$$

well-bracketed words
uniformly spread



ground
states
of H_{move}

3 From Motzkin paths to Dyck Paths

Good-bye, spaces!

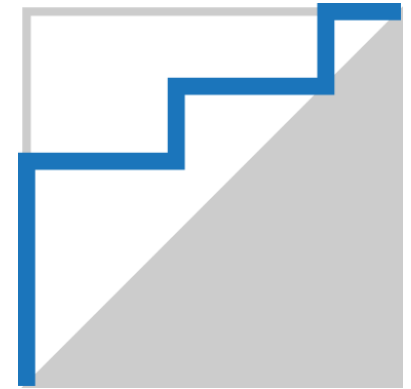
- a new basis

$$\begin{array}{c} \wedge _ \\ [] - \end{array} + \begin{array}{c} _ \\ / \ \backslash \\ [-] \end{array} + \begin{array}{c} _ \\ - \ / \ \backslash \\ - [] \end{array}$$

superpositions of Motzkin paths
with the same Dyck path

[]

labeled by
Dyck paths



[[[]] []] []

- low spectrum

$H_{create} | S$

well-bracketed words
uniformly spread



ground
states
of H_{move}

3 From Motzkin paths to Dyck Paths

Good-bye, spaces!

- a new basis

$$\begin{array}{c} \wedge _ \\ [] - \end{array} + \begin{array}{c} _ \\ / \ \backslash \\ [-] \end{array} + \begin{array}{c} _ \\ - \ / \ \backslash \\ - [] \end{array}$$

superpositions of Motzkin paths
with the same Dyck path

[]

labeled by
Dyck paths



- low spectrum

$H_{create} | S$

well-bracketed words
uniformly spread



ground
states
of H_{move}

3 From Motzkin paths to Dyck Paths

Good-bye, spaces!

- a new basis

$$\begin{array}{c} \wedge \backslash _ \\ \color{red}[] - \end{array} + \begin{array}{c} _ \\ \color{red}[-] \end{array} + \begin{array}{c} _ \\ - \color{red}[] \end{array}$$

superpositions of Motzkin paths
with the same Dyck path



labeled by
Dyck paths



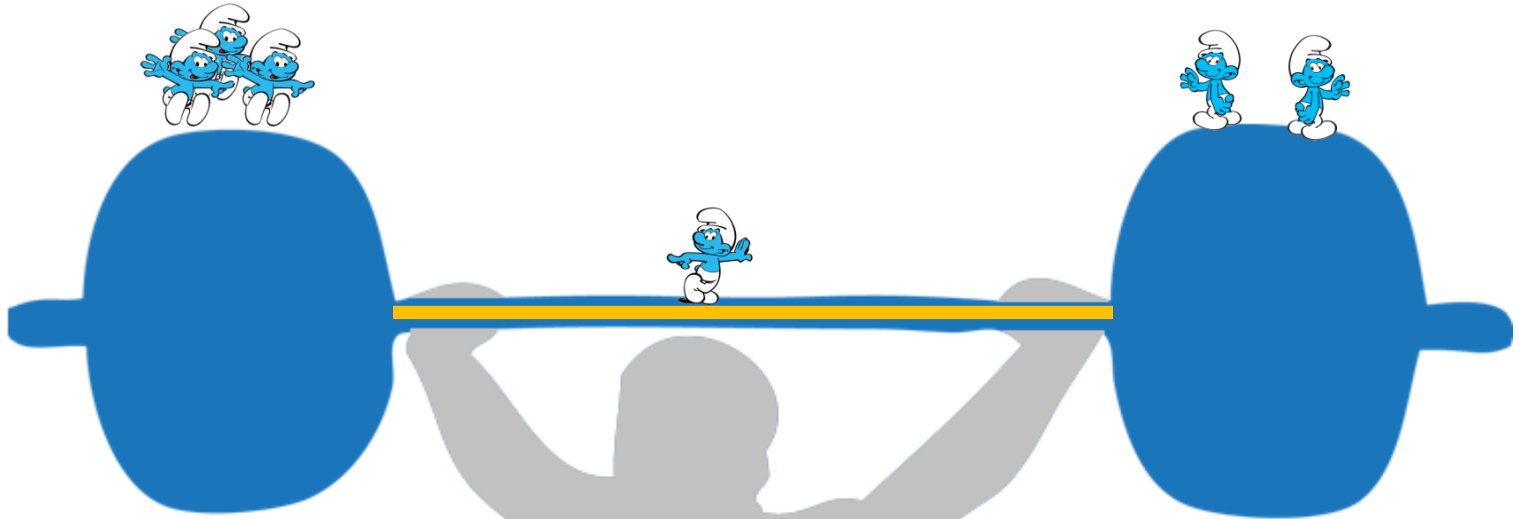
- effective Hamiltonian: a random walk on Dyck paths



- connections: erosion / eruption

3 Congestion in a graph

Is any edge overworked?

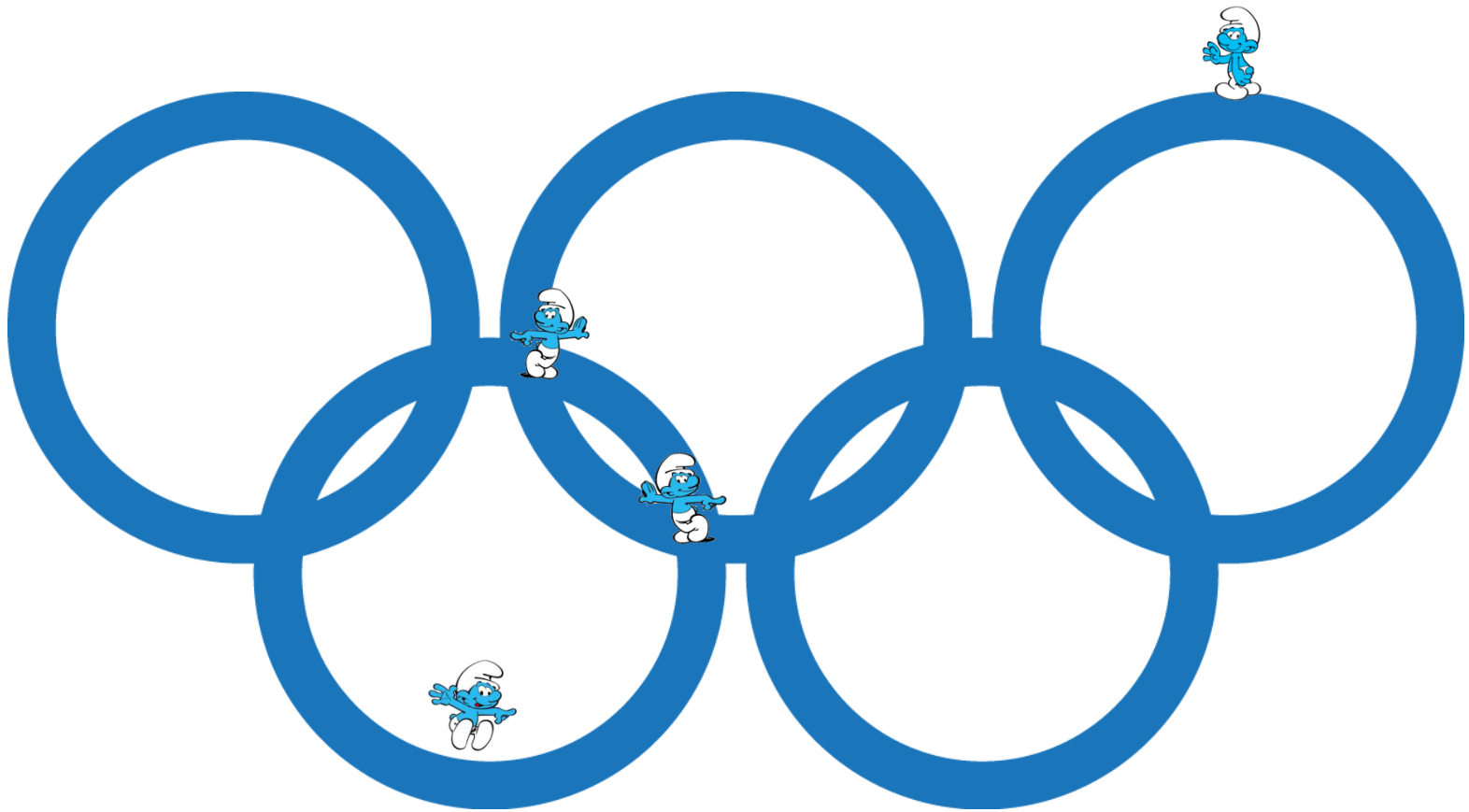


canonical paths
[Sinclair'92]

$$1 - \lambda_2(P) \geq \frac{1}{\rho l}$$

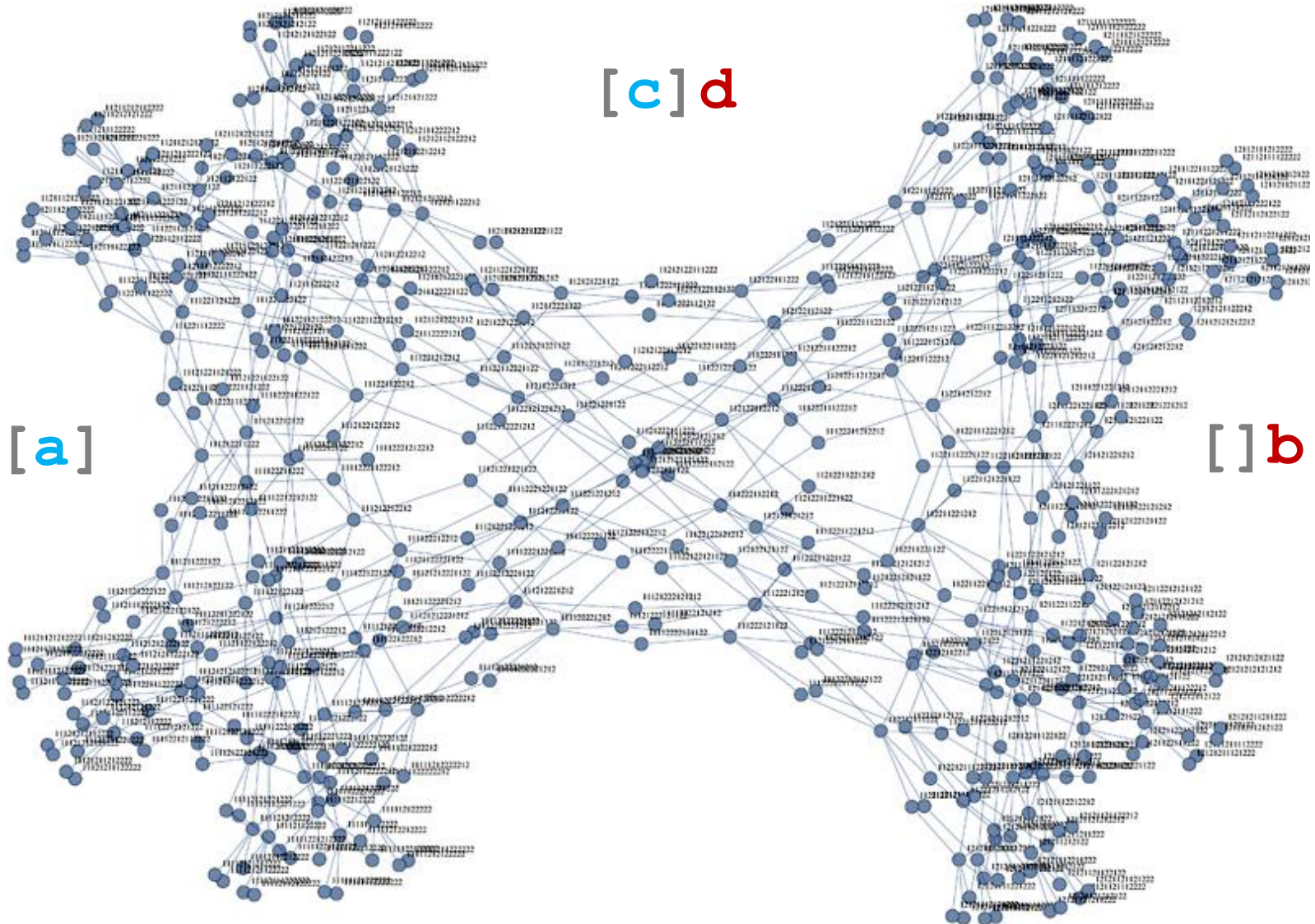
3 Congestion in a graph

Is any vertex overworked?



3 Connecting Dyck paths

It looks well connected. How to prove it?

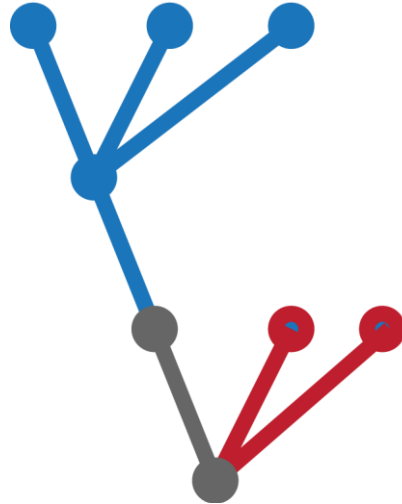


3 Pruning and growing subtrees

The lesson: be careful!

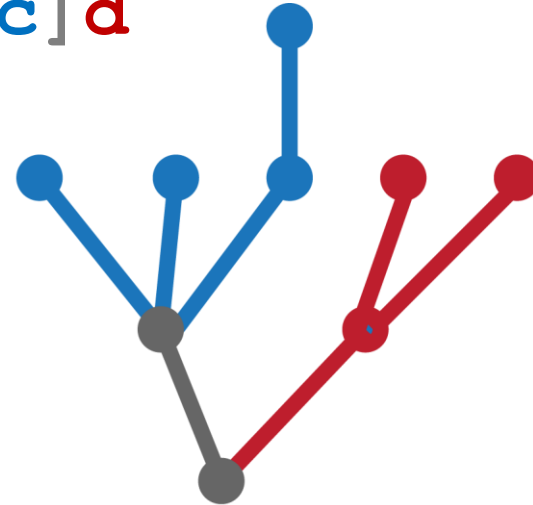
[[[] [] []]] [[] []]

[a] b

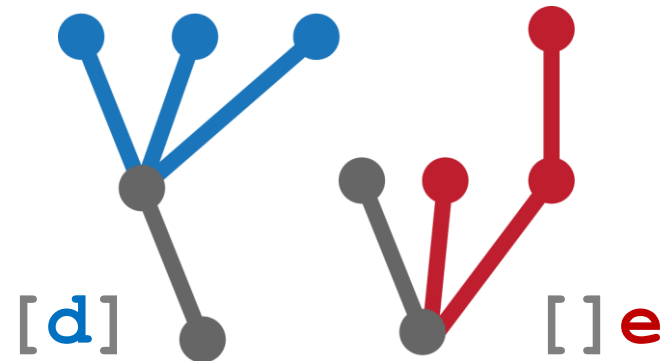


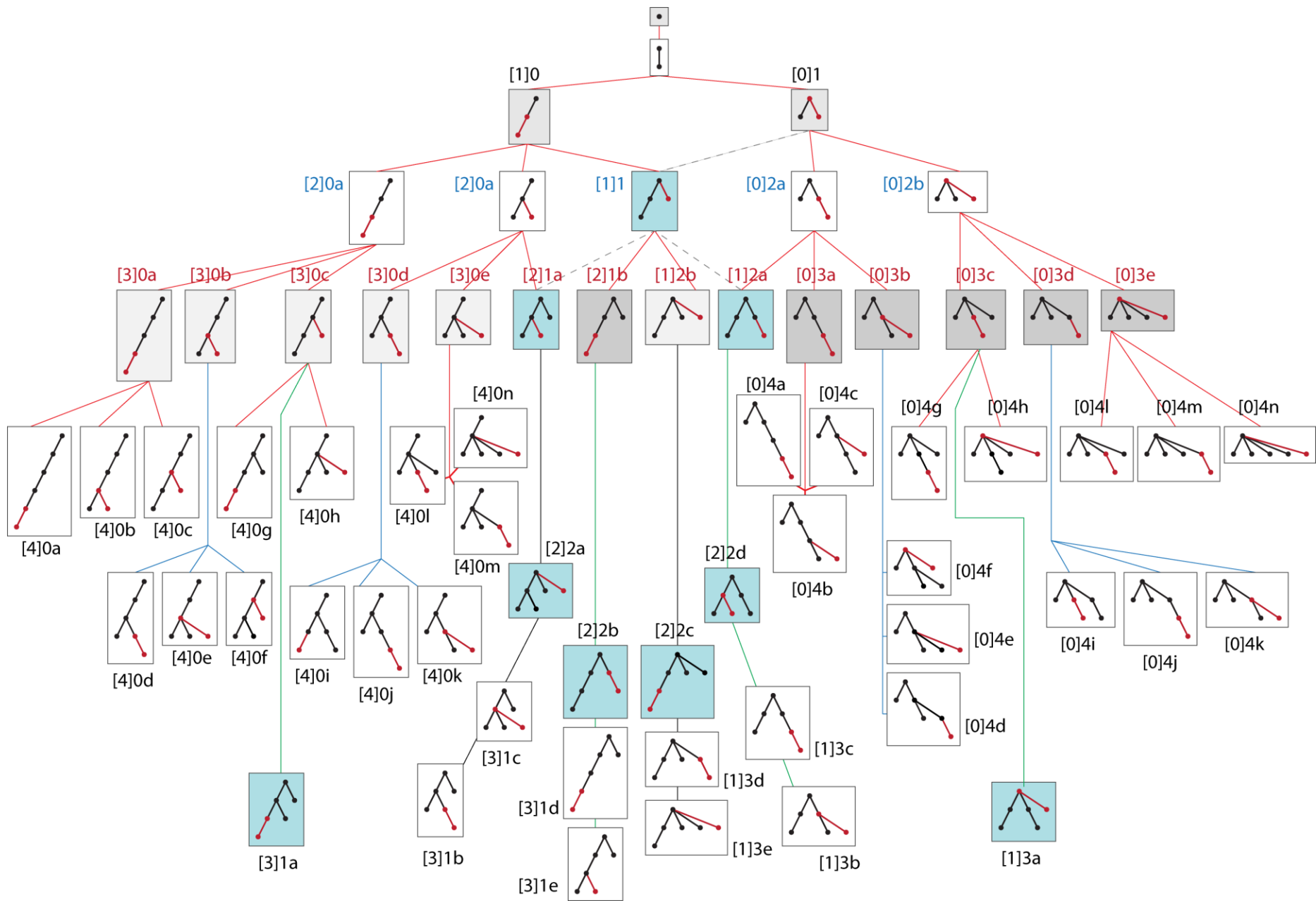
[[[] [] []]] [[] []]

[c] d



- transform subtrees
- cut first, grow later: **NO**
- cut/grow/cut/grow: **YES**



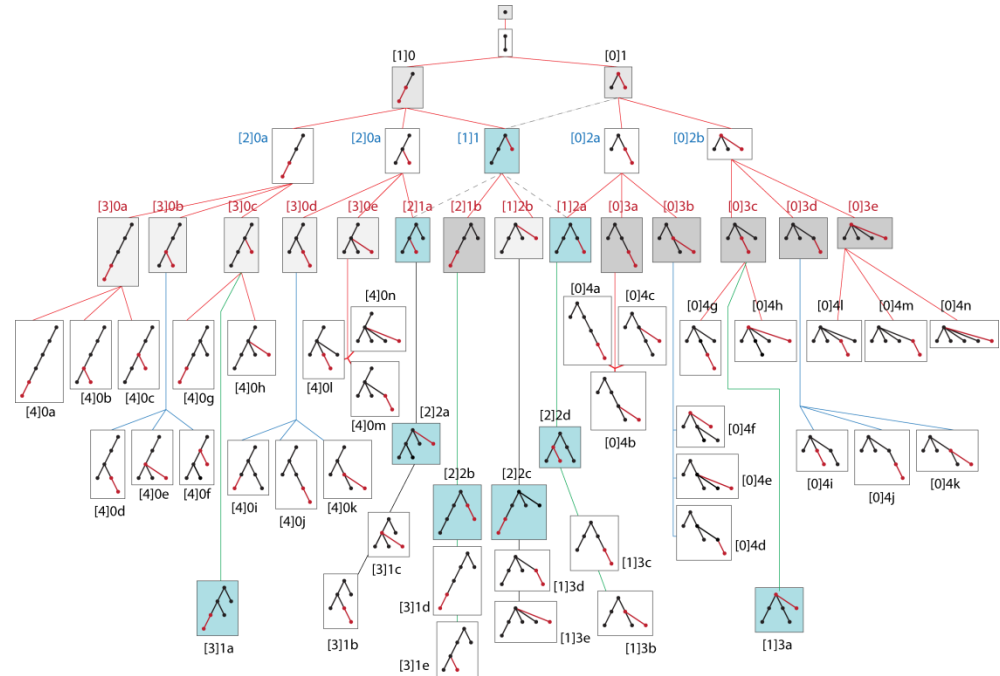


3 Growing trees: at most 4 children

Balance as well as possible.

- canonical growing initial steps

- cut & grow a left/right balanced randomized strategy



- proof of existence fractional matchings

$$\lambda_{2,good} = O(n^{-c})$$

3 Eigenvalues from bad subspaces

- unbalanced brackets don't mix

$$H' = H_{rest} + H_{moveX}$$

- projection lemma 1: move the \mathbf{X} 's

$$H'_\epsilon = H_{rest} + \epsilon H_{moveX}$$

a new effective subspace

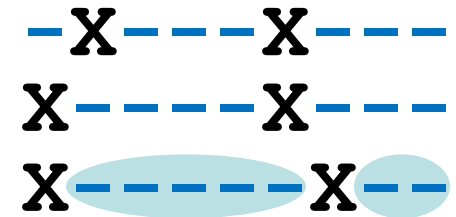
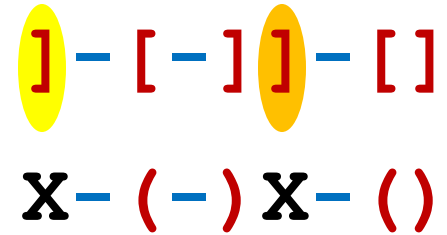
calculate the coefficients

- projection lemma 2: watch the ends

$$H'' = H_{moveX} + \delta H_{end}$$

in the g. subspace of H_{moveX}

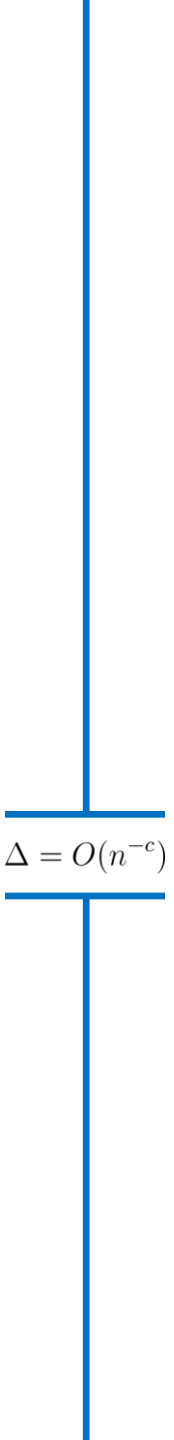
We'll catch them at the end.



a well-bracketed
superposition

$$\lambda_{1,bad} = O(n^{-c})$$

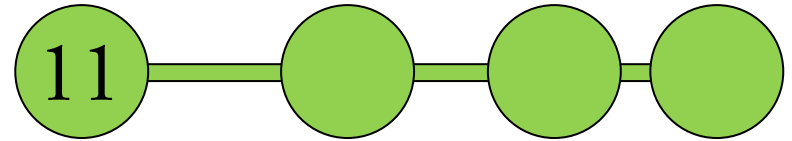
a polynomially small gap


$$\Delta = O(n^{-c})$$

4 Criticality without frustration in 1D

Conclusions.

- even happy chains can be difficult and fun

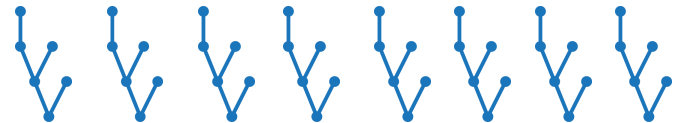


- brackets are way cooler than surfers

- [[] - [] - []] -

A unique, entangled, frustration-free ground state of a translationally-invariant qutrit chain with a polynomial gap.

- the tools we have used



Schmidt decomposition, Catalan numbers, Motzkin & Dyck paths, random walks, projection lemma, canonical paths, fractional matchings

4 Is the future frustration-free?

Where next?

- optimal entropy scaling?
- a class of problems?
- pushdown automata?

WWWW@wwwwww
WWWWW@wwwwww
WWWWW@wwww

- more bracket types [M'12]

-AB-AB-AB-AB

- thermodynamic limit?
- do we need boundaries?
- connections to CFT's?

- [- - [] - -] [] -
- [- [- -] -] - - -
- [-] - - [-] - - -
- [- - [] [- -]] -

frustrated

FRUST
RATED

((()))

□ □ □



enlightened

Criticality without Frustration

IQC Waterloo, 9/2012



Sergey Bravyi
IBM Watson

Libor Caha
Slovak Academy of Sciences

Ramis Movassagh
Northeastern University

Peter Shor
MIT

Daniel Nagaj



arXiv: 1203.5801

Thanks: IQC, QESSENCE, LPP QWAC

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