Bounding entropies of hard squares and friends

How to pick a good vector

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The University of Queensland Australia

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INE YE OLDE DÆS

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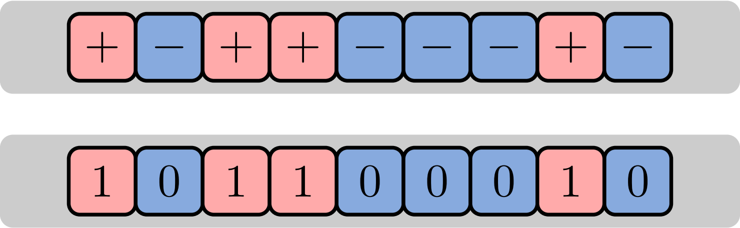
Data is stored along tape as magnetised regions.

Field up, field down, one and zero

Naive idea — store 1′s and 0′s as regions with field in different directions.



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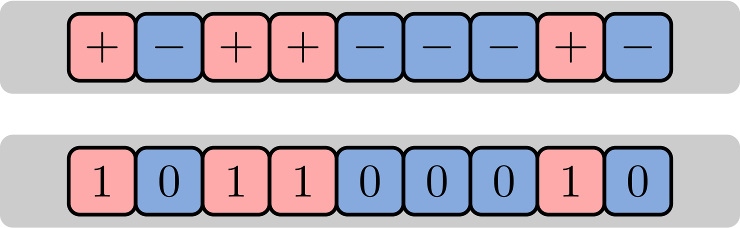

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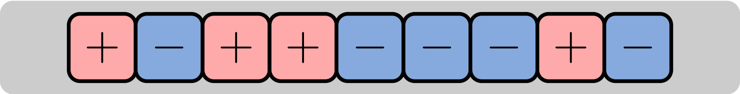

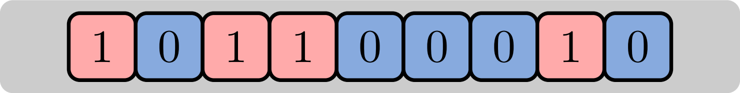

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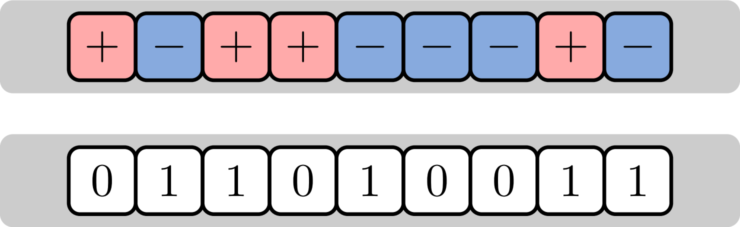
How much data can we store?

- n regions can store 2^n possible words.
- 1 bit per region.

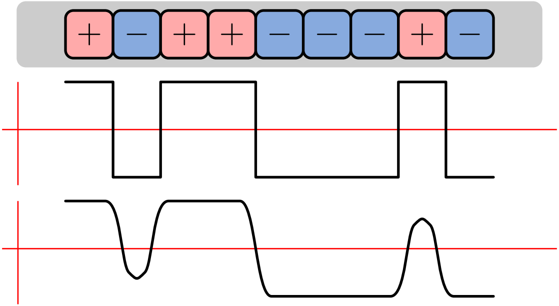
Real world gets in the way

The engineering is easier if we encode data as

- Store 0 as "field unchanged"
- Store 1 as "field changed"



Flip-flop problems



- The magnetic regions are not perfectly discrete
- The read mechanism might misread “change-change”.

Encode data differently

- Store data so that we forbid "change-change"
- Store words in $\{0, 1\}$ so that there is no "11" subword.

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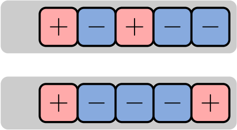
How many legal words are there?

COUNT LEGAL WORDS



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$\psi_N(\oplus)$

Let

- $\psi_n(\oplus)$ be # legal words ending in $\oplus$
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$$\psi_{n+1}(\oplus) = \psi_n(\ominus)$$
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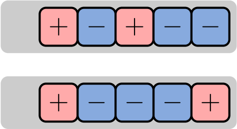

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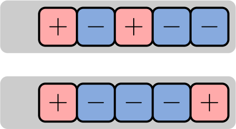

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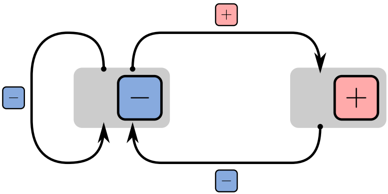
\psi_{n+1}(\ominus) &= \psi_n(\ominus) + \psi_{n-1}(\ominus) \\
\psi_n &= \psi_{n-1} + \psi_{n-2}
\end{aligned}$$

BUILD A TRANSFER MATRIX

More generally…



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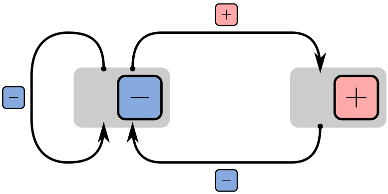

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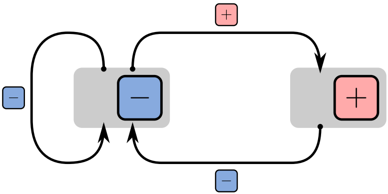

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$$= P^T \begin{pmatrix}\lambda_1^n & 0\\ 0 & \lambda_2^n\end{pmatrix} P \begin{bmatrix}1\\ 1\end{bmatrix}$$

Number of words $\sim n^{\text{th}}$ power of dominant eigenvalue

1D IS EASY

So for this "11"-forbidden model

$$\psi_n \sim \left(\frac{1+\sqrt{5}}{2}\right)^n$$

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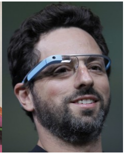
What about other models?

- Run-length limited (d, k)
  — forbid subwords $\{11, 101, 1001, \ldots 10^d1, 0^{k+1}\}$.
- Charge model (b)
  — cumulative charge lies between $\pm b$.
- Parity models
  — even # 0's between 1's.
  — odd # 0's between 1's.

Use same transfer matrix machinery.

BUT NOW WE LIVE IN THE FUTURE...



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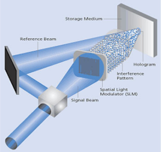

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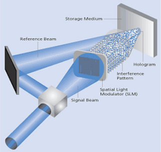

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A core question

How much data can we store in 2d?

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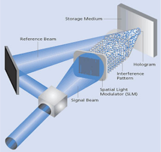

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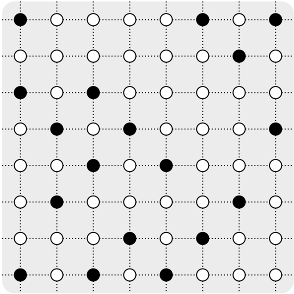
How many 2d words avoid 11 and $\begin{matrix}1\\1\end{matrix}$?

What does this look like?



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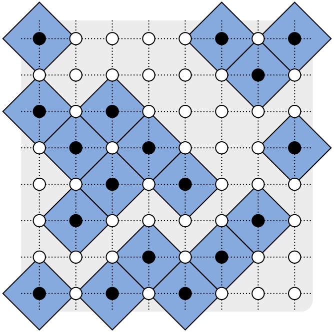

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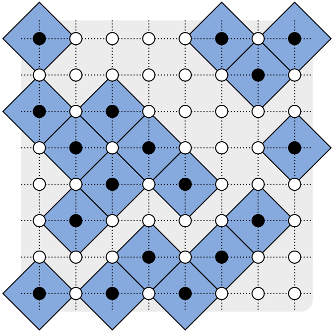

$$\begin{aligned}\text{2d coding problem} &= \text{hard square lattice gas}\\ &= \text{independent sets on } \mathbb{Z}^2\end{aligned}$$

WHAT DO WE WANT TO KNOW?

More generally…

2d shift of finite type

- Given a finite alphabet $\mathcal{A}$, and
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- Let $C_{n\times n}$ be the # valid $n \times n$ words.
- Entropy is $\log_2 \kappa = \lim_{n\to\infty} \frac{1}{n^2} \log_2 C_{n\times n}$

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- Algorithmically undecideable if there are any valid words

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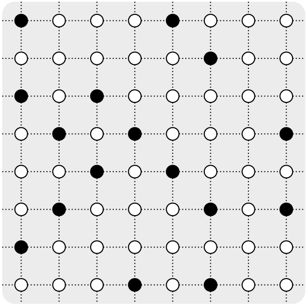
- In 2d and up, κ known exactly for very few SFTs

EXAMPLE OF EXACT

Odd constraint

Words in $\{0, 1\}$ so that between 1′s there are odd number of 0′s.
[Louidor & Marcus 2010] $\kappa = \sqrt{2}$.



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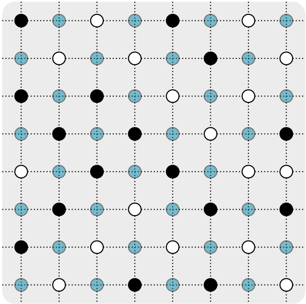

One sub-lattice fixed as 0′s and other is unconstrained.

BOUNDS

Back to hardsquares…

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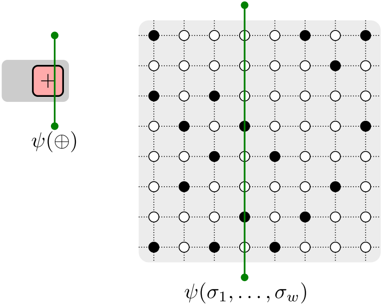
Most approaches based on transfer matrices



Big problem — # states grows exponentially with width

Transfer matrix

T_w = column-to-column TM for hard squares in strip of width w

	○○○	●○○	○●○	○○●	●○●
○○○	1	1	1	1	1
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$$\kappa = \lim_{w\to\infty} \Lambda_w^{1/w}$$ where Λ_w is dominant eigenvalue

Useful ideas from Linear Algebra 101

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Leverage these to get good bounds

[Engel 1990] and [Calkin & Wilf 1998]

Trace trick

Rewrite trace

$$\mathrm{Tr}\, V^{2k} = \sum V_{\psi_0,\psi_1} V_{\psi_1,\psi_2} \dots V_{\psi_{2k-1},\psi_0}$$

Sum is over all sequences of states, but only "legal" ones count

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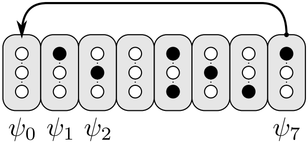

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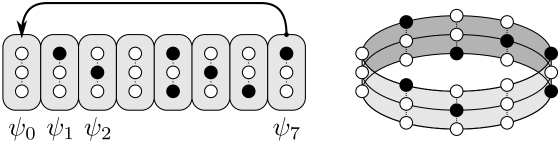

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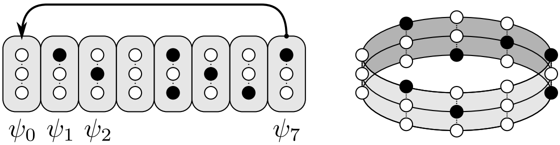

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Sneaky — "width" is now exponent.

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Raise to $1/w$ and let width $\to \infty$

$$\begin{array}{ccccc} \Lambda_w^{2k/w} & \leq & \left(\operatorname{Tr} T_w^{2k}\right)^{1/w} & = & \langle \mathbf{1} \,|\, B_{2k}^{w-1} \,|\, \mathbf{1} \rangle^{1/w} \\ \downarrow & & & & \downarrow \\ \kappa^{2k} & & & \leq & \xi_{2k} \end{array}$$

Upper bound

Let B_{2k} be the TM for system on ring of circumference $2k$, then

$$\kappa \leq \xi_{2k}^{1/2k}$$

where ξ_{2k} is dominant eigenvalue of B_{2k}.

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Huge transfer matrix — use symmetries to compress it.

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So the simplest idea — set $|x\rangle = |\mathbf{1}\rangle$.

Rayleigh quotients

Min-max theorem

$$\lambda_{min} \leq \frac{\langle x \,|\, V \,|\, x \rangle}{\langle x \,|\, x \rangle} \leq \lambda_{max}$$

So the simplest idea — set $|x\rangle = |\mathbf{1}\rangle$.

$$\Lambda_w \geq \frac{\langle \mathbf{1} \,|\, T_w \,|\, \mathbf{1} \rangle}{\langle \mathbf{1} \,|\, \mathbf{1} \rangle}$$

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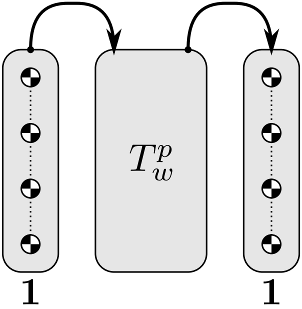
For fixed w this is silly — instead compute the eigenvalue by power method.
But if we can choose a better vector…

SNEAKY TRICKS AGAIN

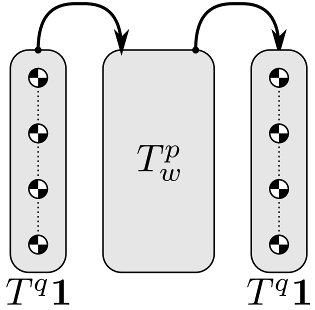
Vector $|\mathbf{1}\rangle$ a poor choice.



$$\Lambda_w^p \geq \frac{\langle \mathbf{1} \,|\, T_w^p \,|\, \mathbf{1} \rangle}{\langle \mathbf{1} \,|\, \mathbf{1} \rangle}$$

SNEAKY TRICKS AGAIN

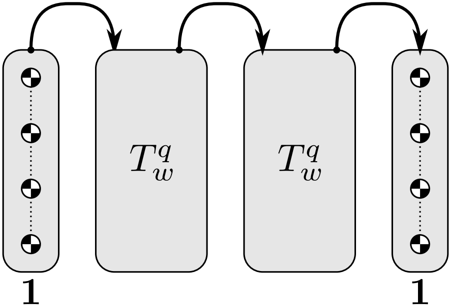
Power method — replace $|\mathbf{1}\rangle$ with $T_w^q\,|\mathbf{1}\rangle$.



$$\Lambda_w^p \geq \frac{\left\langle T_w^q\mathbf{1} \,\middle|\, T_w^p \,\middle|\, T_w^q\mathbf{1}\right\rangle}{\left\langle T_w^q\mathbf{1} \,\middle|\, T_w^q\mathbf{1}\right\rangle}$$

Sneaky tricks again

Massage denominator



$$\left\langle T_w^q \mathbf{1} \,\middle|\, T_w^q \mathbf{1} \right\rangle = \left\langle \mathbf{1} \,\middle|\, T_w^{2q} \,\middle|\, \mathbf{1} \right\rangle$$

Sneaky tricks again

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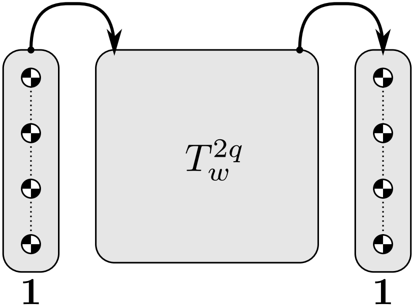

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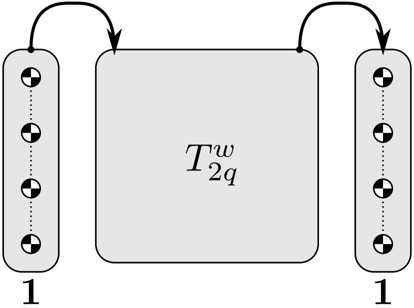
Sneaky tricks again

All configs in $w \times 2q$ rectangle = configs in $2q \times w$ rectangle

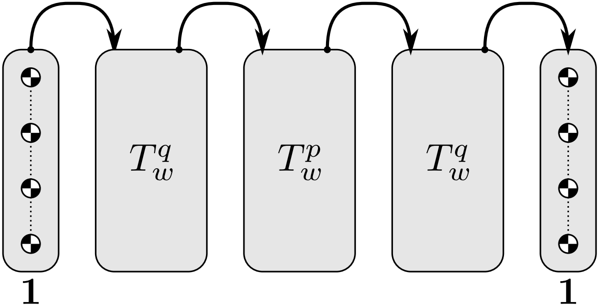


$$\langle T_w^q \mathbf{1} \mid T_w^q \mathbf{1} \rangle = \left\langle \mathbf{1} \,\middle|\, T_w^{2q} \,\middle|\, \mathbf{1} \right\rangle \quad = \langle \mathbf{1} \mid T_{2q}^w \mid \mathbf{1} \rangle$$

Sneaky — width becomes exponent

Sneaky tricks again

Look at numerator now



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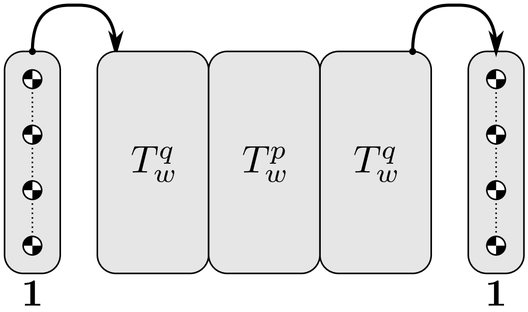
Sneaky tricks again

Massage things a little



$$\left\langle T_w^q \mathbf{1} \,\middle|\, T_w^p \,\middle|\, T_w^q \mathbf{1} \right\rangle = \left\langle \mathbf{1} \,\middle|\, T_w^{2q+p} \,\middle|\, \mathbf{1} \right\rangle$$

Sneaky tricks again

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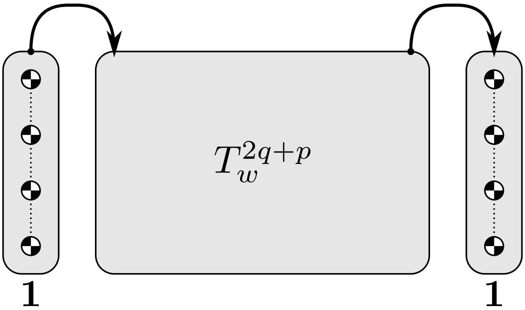

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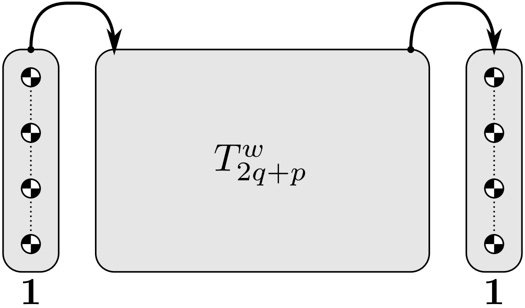
Sneaky tricks again

Again use the $x \leftrightarrow y$ symmetry



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Sneaky — width becomes exponent

RESULTS

Putting this together

$$\Lambda_w^p \geq \frac{\left\langle \mathbf{1} \,\middle|\, T_{2q+p}^w \,\middle|\, \mathbf{1} \right\rangle}{\left\langle \mathbf{1} \,\middle|\, T_{2q}^w \,\middle|\, \mathbf{1} \right\rangle}$$

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Lower bound [Calkin & Wilf 1998]

For any $p, q \geq 1$

$$\kappa^p \geq \frac{\Lambda_{2q+p}}{\Lambda_{2q}}$$

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- $\kappa \geq 1.50304768131466259\ldots (p = 3, q = 2)$ [Calkin & Wilf]
- $\kappa \geq 1.50304808247533226\ldots (p = 1, q = 13)$ [Friedland et al]

Pick a better vector

- We use corner transfer matrix formalism to pick a better vector.

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- Corner transfer matrices used to study lattice gas & magnet models [Baxter 1968]

PICK A BETTER VECTOR

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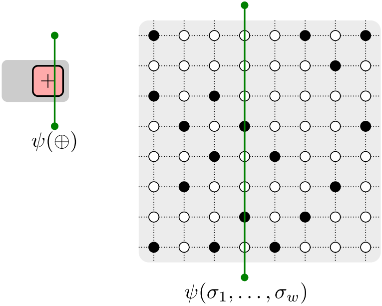
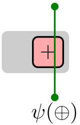
- Corner transfer matrices used to study lattice gas & magnet models **[Baxter 1968]**
- Very famously lead to solution of hard hexagons **[Baxter 1980]**

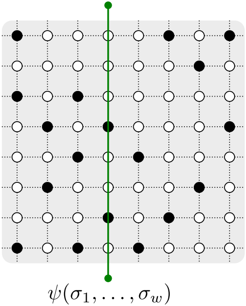
How to build a vector



Each entry of vector corresponds to a state along the cut

HOW TO BUILD A VECTOR





Each entry of vector corresponds to a state along the cut

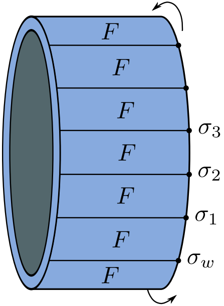
Baxter's Ansatz which extends [Kramers & Wannier 1941]

Build Rayleigh quotient with vector ψ

$$\psi(\sigma_1, \sigma_2, \ldots, \sigma_w) = \mathrm{Tr}\left[F(\sigma_1, \sigma_2)F(\sigma_2, \sigma_3)\ldots F(\sigma_w, \sigma_1)\right]$$

For some matrices $F(a, b)$.

WHAT DOES THIS LOOK LIKE?



$$= \psi(\sigma_1, \ldots, \sigma_w)$$

- Can think of *F* as a “literal” half-row transfer matrix.
  — but it can be almost any matrix.

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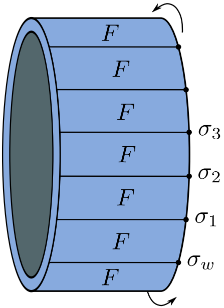

$$= \psi(\sigma_1, \ldots, \sigma_w)$$

- Can think of *F* as a “literal” half-row transfer matrix.
  — but it can be almost any matrix.
- Trace makes it a cylinder — doesn't change bound.

Rayleigh quotient → Traces

Rayleigh quotient

$$\Lambda_w \geq \frac{\langle \psi \mid T_w \mid \psi \rangle}{\langle \psi \mid \psi \rangle}$$

$$\langle \psi \mid T \mid \psi \rangle = \operatorname{Tr} S^w$$
$$\langle \psi \mid \psi \rangle = \operatorname{Tr} R^w$$

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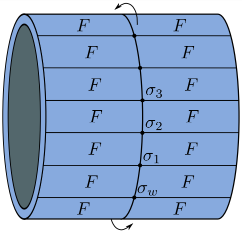
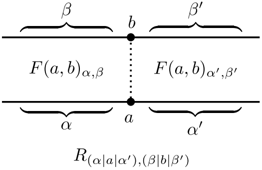


$= \langle\psi|\psi\rangle = \mathrm{Tr} R^w$



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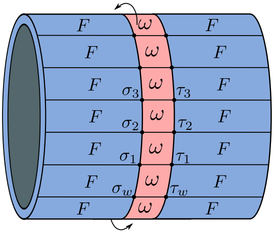

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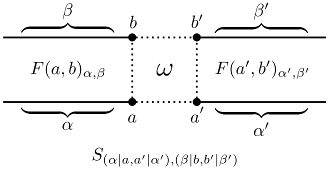

Where $\omega = 1$ if face valid else $\omega = 0$.

To get a bound

Lower bound

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where ξ, η are dominant eigenvalues of R and S.

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1. Pick matrices F — note dimension need not be related to w
2. Form matrices R and S
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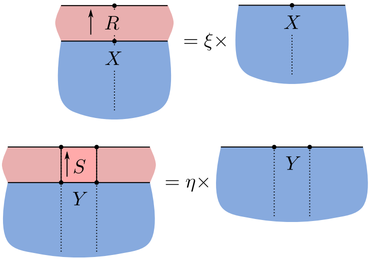
But how do we pick F?
And where are these infamous "corner transfer matrices"?

EIGENVECTORS ↦ EIGENMATRICES(?)

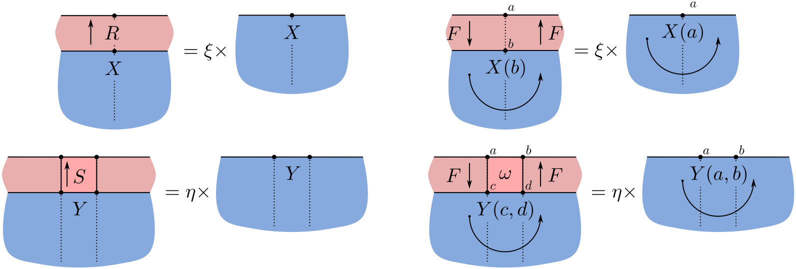


$$R\,|X\rangle = \xi\,|X\rangle$$

$$S\,|Y\rangle = \eta\,|Y\rangle$$

$|X\rangle\,,|Y\rangle$ eigenvectors of R and S.

EIGENVECTORS $\mapsto$ EIGENMATRICES(?)

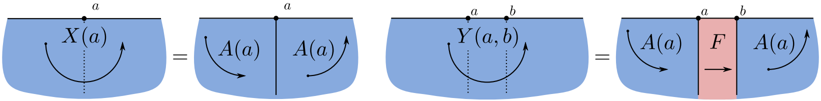


$$R\,|X\rangle = \xi\,|X\rangle \qquad \sum_b F(a,b)X(b)F(b,a) = \xi X(a)$$

$$S\,|Y\rangle = \eta\,|Y\rangle \qquad \sum_{c,d} \omega\begin{pmatrix} a & b \\ c & d \end{pmatrix} F(a,c)Y(c,d)F(d,b) = \eta Y(a,b)$$

$X(a), Y(a,b) \approx$ "half-plane transfer matrices"

TO MAXIMISE, PLANES $\mapsto$ CORNER×CORNER



Baxter showed that Rayleigh quotient stationary when

$$X(a) = A(a)^2 \qquad\qquad Y(a,b) = A(a)F(a,b)A(b)$$

where A is half of X — a "corner transfer matrix"
Baxter then carefully picked F to make things work.

Renormalise instead

- We have used “corner transfer matrix renormalisation group method” **[Nishino & Okunishi 1996]**
- Related to density matrix renormalisation group method **[White 1992]**

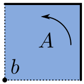
RENORMALISE INSTEAD

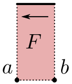
- We have used "corner transfer matrix renormalisation group method" **[Nishino & Okunishi 1996]**
- Related to density matrix renormalisation group method **[White 1992]**
- The central idea = only keep important parts of A.

BUILD RECURSIVELY

Start by building "literal" matrices. Let

- A be corner transfer matrix for a 2×2 grid
- F be the half-row / half-column transfer matrix for a 1×2 grid





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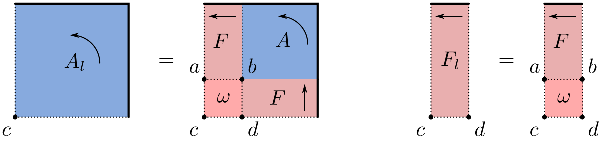

- Then build larger matrices by

$$A_l(c)|_{d,a} = \sum_d \omega\begin{pmatrix} a & b \\ c & d \end{pmatrix} F(c,d)A(b)F(b,a)$$

$$F(c,d)|_{b,a} = \omega\begin{pmatrix} a & b \\ c & d \end{pmatrix} F(b,a)$$

Build recursively

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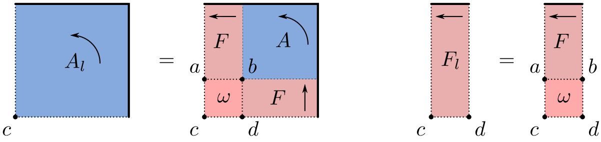

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- Iterate until A and F are huge — they are still "literal".

NOW ESTIMATE EIGENVALUES ξ, η

- Look at eigenvalue equation:

$$\xi \sum_{a} X(a) = \sum_{a,b} F(a,b) X(b) F(b,a)$$

NOW ESTIMATE EIGENVALUES ξ, η

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- Look at eigenvalue equation:

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Now estimate eigenvalues ξ, η

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- Invariant under similarity transform, so can diagonalise A.

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- Key idea: discard small eigenvalues
  Huge "literal" $A, F \mapsto$ small "aphysical" A, F.

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  Huge "literal" $A, F \mapsto$ small "aphysical" A, F.

Clever idea [Nishino & Okunishi 1996]

- Building huge literal A, F and then projecting it down is wasteful.
- Instead grow & project frequently until A, F converge.

Put it all together

1. Start with “reasonable” A, F.
2. Grow & project repeatedly until A, F converge.
3. Use this F to compute ξ, η and so lower bound for κ.
4. Grow A, F a little larger and repeat from #2.

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Lower bound [YBC & AR]

$$\kappa \geq 1.\ 503048082475332264322$$

Previous best lower bound [Friedland, Lundow & Markström 2010]

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Our lower bound

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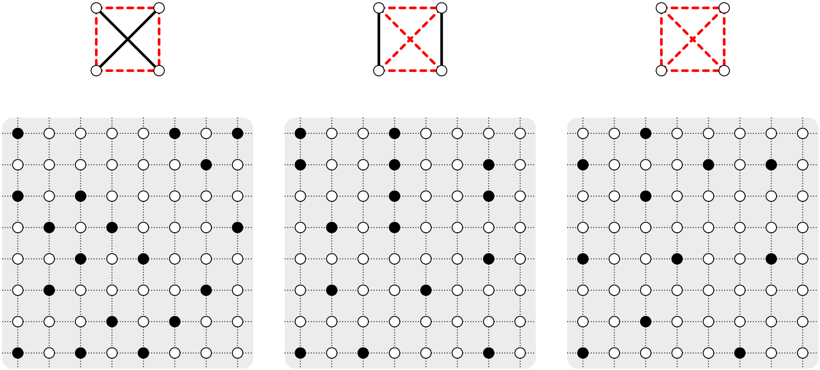
Previous best lower bound [Friedland, Lundow & Markström 2010]
Previous best estimate [Baxter 1999]
Our lower bound
Our best estimate same except last 2 digits.

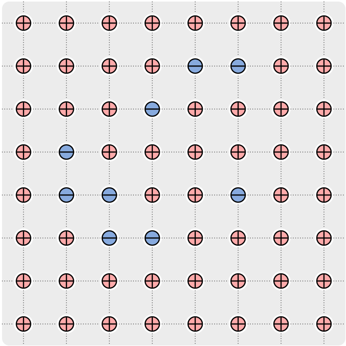
Other models

Hard squares, Read-write Isolated Memory and Non-Attacking Kings



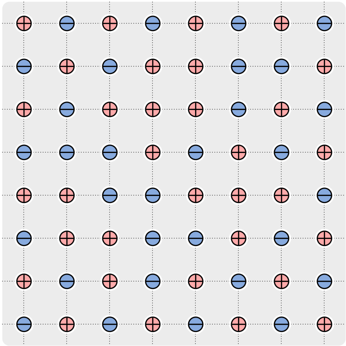
Other models

Even model



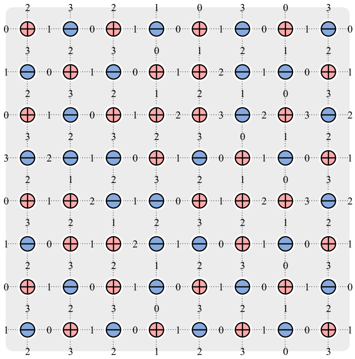
Other models

Charge 3



Other models

Charge 3



RESULTS

Substantial improvement of all previous lower bounds

Model	Matrix size	Lower bound on (and estimate of) κ
NAK	256	1.342 643 951 124 601 297 851 730 161 875 740 395 719 438 196 938 393 943 434 885 455 0 (1)
RWIM	128	1.448 957 371 775 608 489 872 231 406 108 136 686 434 371 (7)
Even	128	1.357 587 502 184 123 (5)
Charge(3)	74	1.357 587 50
4-Colouring	96	2.336 056 641 041 133 656 814 01 (4)
5-Colouring	64	3.250 404 923 167 119 143 819 73 (6)

- NAK, RWIM, Even, Charge(3) — [Louidor & Marcus (2010)]
- 4-Colouring and 5-colouring — [Lundow & Markström (2008)]

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Why are Even and Charge(3) the same?

Open questions

- What other models?

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Bounds due to [Collatz 1942]

If T is non-negative and x is any positive vector, then

$$\min_i \left| \frac{(Tx)_i}{x_i} \right| \leq \Lambda \leq \max_i \left| \frac{(Tx)_i}{x_i} \right|$$