Shannon entropies in low-dimensional quantum magnets

Workshop on « Recent Progress in Low-Dimensional Quantum Magnetism »
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Outline

- What is the « Shannon entropy » of a wave-function ?
  - definition
  - some examples (spin models)
  - volume law
  - Shannon entropy *vs* von Neumann (entanglement) entropy

- What can we learn using Shannon-Rényi entropies ?
  - Look for (universal) subleading terms
  - Application to Luttinger liquids ($D = 1$)
  - Systems with Goldstone modes in $D = 2$ $\leftarrow$ GM, Pasquier & Oshikawa, arXiv:1607.02465

What is « Shannon entropy » of a wave-function ?

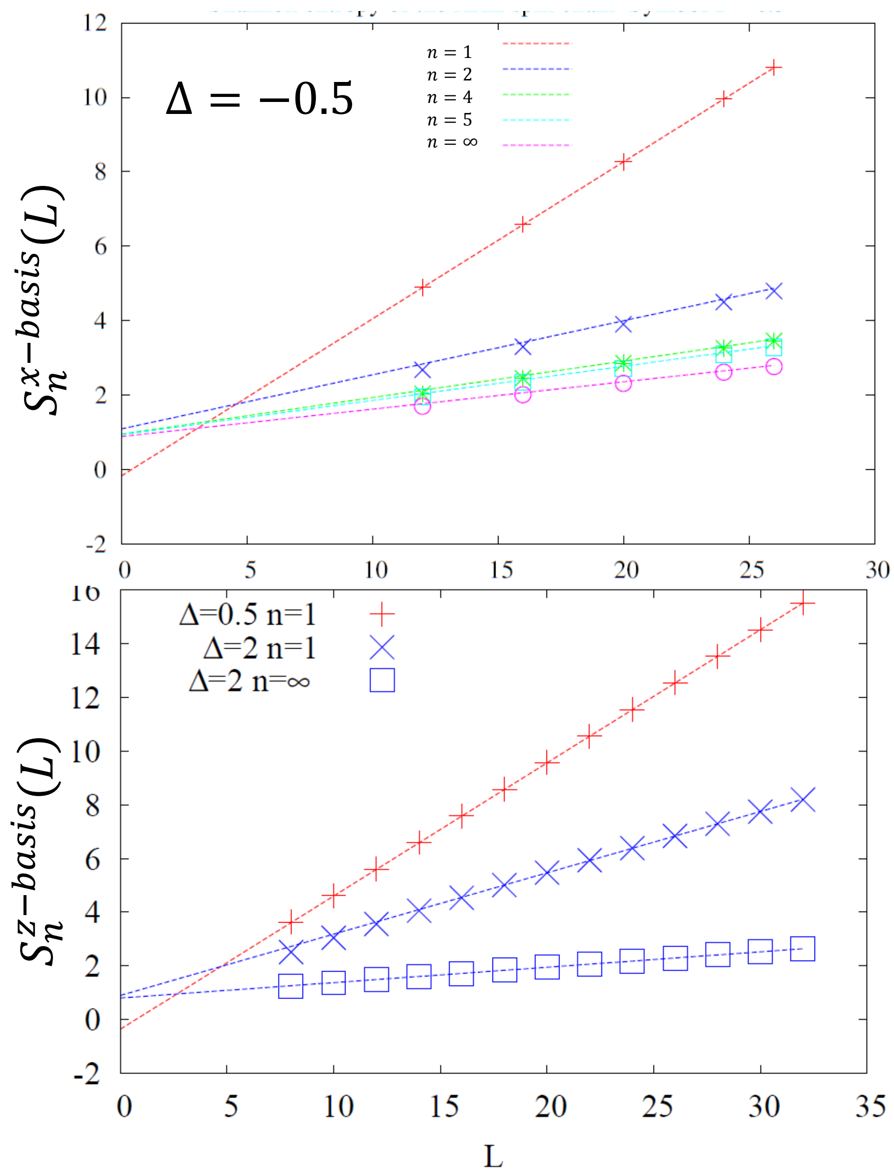
Shannon-Rényi entropy

- Definitions
  - Lattice quantum many-body Hamiltonian: H
  - $|\psi\rangle$ ground state of H (finite system size)
  - Preferential basis $\{|i\rangle\}$
  - Probabilities: $p_i = |\langle\psi|i\rangle|^2$ $\quad \sum_i p_i = 1$
  - Shannon entropy $S_{n=1} = -\sum_i p_i \log p_i$
  - Measures how *localized* is a state in a given basis
  - Rényi entropy $S_n = \frac{1}{1-n}\log\sum_i (p_i)^n$
  - $S_{n\to\infty} = -\log p_{max}$
- Example in $D = 1$:

  XXZ spin chain

  $$H = \sum_j \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z\right)$$

  2 'natural' basis: S^z & S^y
- 'Volume' law: $S_n(L) \sim a_n\, L^D + \ \ldots$



Shannon-Rényi entropy

- Many-body ground-state: $|\psi\rangle$ Large Hilbert space dimension $\sim a^N$
- Preferential basis $\{|i\rangle\}$
- Probabilities: $p_i = |\langle\psi|i\rangle|^2$
- Rényi entropy $S_n = \frac{1}{1-n}\log Z(n)$ $Z(n) = \sum_i (p_i)^n$

Miscellaneous remarks:

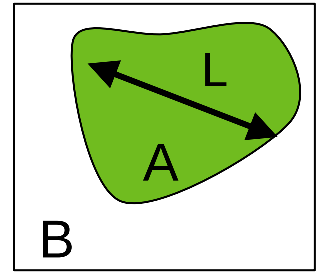
- ❑ $Z(n)$: partition function for some fictitious stat.-mech. model
- ❑ Varying n is like changing the (inverse) 'temperature' of that model
  $\rightarrow$ natural way to probe a many-body state
- ❑ Relation with 1-body problems & inverse participation ratios
  Natural basis: $\{|r\rangle\}$ (localized in real space)

$$\int d^D r\, |\psi(r)|^{2n} = Z(n) \sim \begin{cases} \mathcal{O}(1) \text{ localized state} \\ \mathcal{O}(L^{-D(n-1)}) \text{ delocalized state} \end{cases}$$

Shannon entropy
versus
Entanglement (von Neumann) entropy

Shannon & Von Neumann

- Starting point: lattice quantum many-body wave-function $|\psi\rangle$



- Input:
  - Subsystem A → trace out B → ρ_A→ von Neumann entropy

$$\rho = |\psi\rangle\langle\psi|$$
$$\rho_A = \mathrm{Tr}_B[\rho] = \mathrm{Tr}_B[|\psi\rangle\langle\psi|]$$
$$S_A^{vN} = -\mathrm{Tr}_A[\rho_A \log \rho_A]$$

  - Basis $\{|i\rangle\}$ → probabilities → Shannon entropy $S_{basis\,\{|i\rangle\}}^{Shannon}$

NB: one can also study the Shannon entropy of a subsystem, in a given basis. See for instance [J.-M Stéphan, PRB 2014]

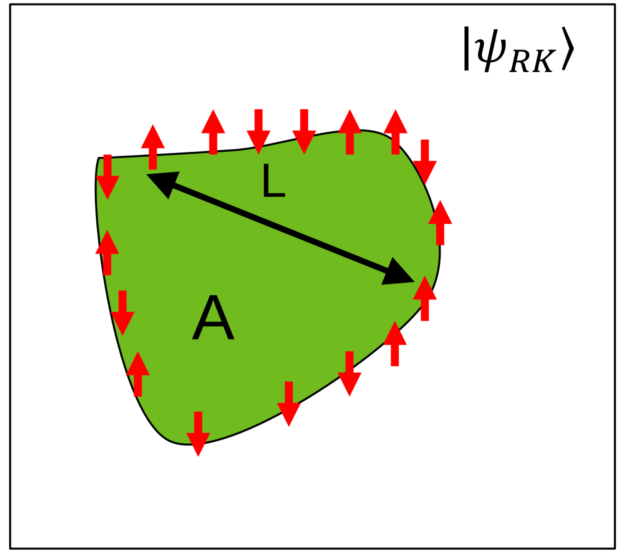
- Scaling
  - Area law $S_A^{vN}(L) \sim L^{D-1}$ ('generic' behavior for low-energy states of local Hamiltonians)
  - Volume law $S_{basis\,\{|i\rangle\}}^{Shannon}(L) \sim L^D$
- Both can provide some important information about the system:
  - spontaneous symmetry breaking (discrete & continuous)
  - criticality
  - topological order

...

Shannon & von Neumann & Rokhsar-Kivelson

- Classical stat-mech model:
  - configurations c
  - local Boltzmann weights $e^{-E(c)}$
  - partition function $Z = \sum_c e^{-E(c)}$
- Define a quantum state:
  - Hilbert space with $\{|c\rangle\}$ as an orthonormal basis
  - $|\psi_{RK}\rangle = \frac{1}{\sqrt{Z}} \sum_c e^{-\frac{1}{2}E(c)} |c\rangle$
- Subsystem A and configuration c
  - boundary configurations i: configuration c restricted to ∂A, the boundary of A
  - marginal probability $p_i = \frac{1}{Z} \sum_{c\,/\,\partial A = i} e^{-E(c)}$
- Define a quantum state $|\psi\rangle$, living at the boundary of A:

$$|\psi\rangle = \sum_i \sqrt{p_i} |i\rangle$$



- Result : $\boxed{S_A^{\mathrm{vN},|\psi_{RK}\rangle} = S^{\mathrm{Shannon},|\psi\rangle}_{\mathrm{basis}\{|i\rangle\}}} = \sum_i p_i \log p_i \sim L^{D-1}$

Furukawa & GM, Phys Rev B 2007; Stéphan, Furukawa, GM, Pasquier, PRB 2009

What can we learn using Shannon entropies ?

i) critical spin chains

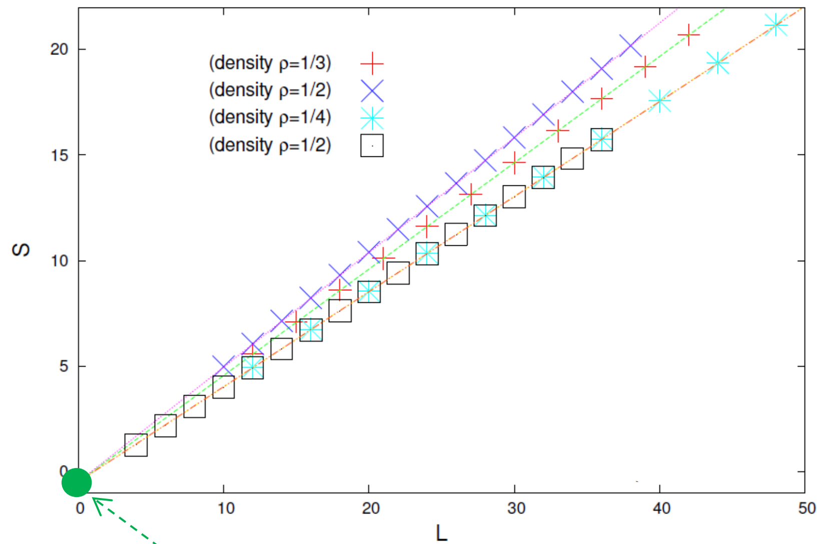
Universal terms in Shannon entropies

Stéphan, Furukawa, GM, Pasquier, PRB 2009; Oshikawa arXiv 2010;
Stéphan, GM, Pasquier, PRB 2010; PRB 2011

- Subleading terms are universal:

$$S_n = \frac{1}{1-n} \log \sum_i (p_i)^n$$

$$\simeq \begin{cases} \alpha_n L + s_n + \cdots \text{ (translation invariant system)} \\ \alpha_n L + l_n \log(L) + \cdots \text{ (open chains)} \end{cases}$$



- Example 1: periodic XXZ chain & z-basis

$$s_{n<4/R} = \log R - \frac{\log n}{2(n-1)}$$

$$s_{n>4/R} = \frac{1}{1-n}(-n \log R + \log 2)$$

$$R = \text{compactification radius} = \mathrm{K}^{-\frac{1}{2}} = \sqrt{2 - \frac{2}{\pi} \arccos \Delta}$$

Free-fermion states in the same « universality class » ($R = 1$) → same subleading constant $s_1 = -\frac{1}{2}$.

(boundary) Phase transition as a function of n: $n_c = 4/R$

- Example 2: Critical Ising chain in transverse field. $s_1 = 0.254395(5) = ???$

- Example 3: XXZ chain, in the x –basis → several phase transitions !

GM & Oshikawa, work in progress… (boundary CFT approach & numerics)

What can we learn using Shannon entropies ?

ii) D=2: Goldstone modes

Nambu-Goldstone modes & entropies

❑ Entanglement entropy

N_{NG} Nambu-Goldstone modes → $\log$ terms in the entanglement entropy:

$$S^{\text{von Neumann}} \simeq \mathcal{O}(L^{D-1}) + \frac{N_{NG}}{2}\log L^{D-1}$$

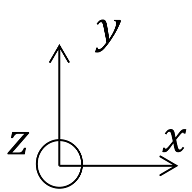
Kallin *et al.* 2011; Metlitsky-Grover 2011; Kulchytskyy *et al.* 2015; Laflorencie *et al.* 2015; Rademaker 2015; …

❑ What about the Shannon entropy ? Similar !

QMC results by Luitz, Alet & Laflorencie (PRL 2014) :

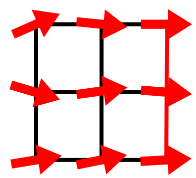
$D = 2$, XY model, $S = \frac{1}{2}$, square lattice: $S^{\text{Shannon}}_{n=2,x-\text{basis}} \simeq \mathcal{O}(N) + 0.585(6)\log N$

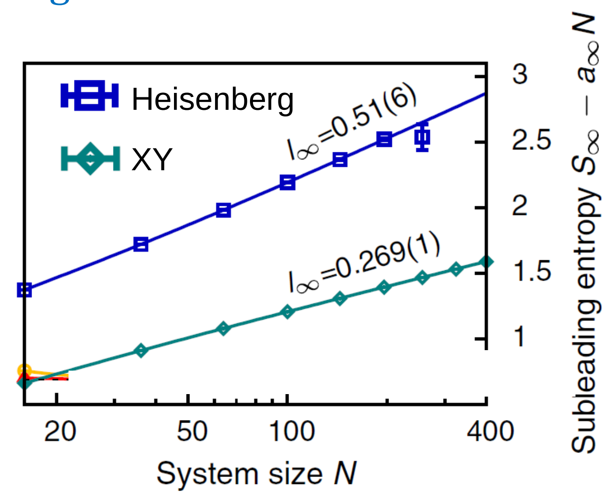
$$S^{\text{Shannon}}_{n=\infty,x-\text{basis}} \simeq \mathcal{O}(N) + 0.269(1)\log N$$



$$H = -\sum_{\langle i,j\rangle} \sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y$$

$U(1)$ symmetry:
rotations about the z axis





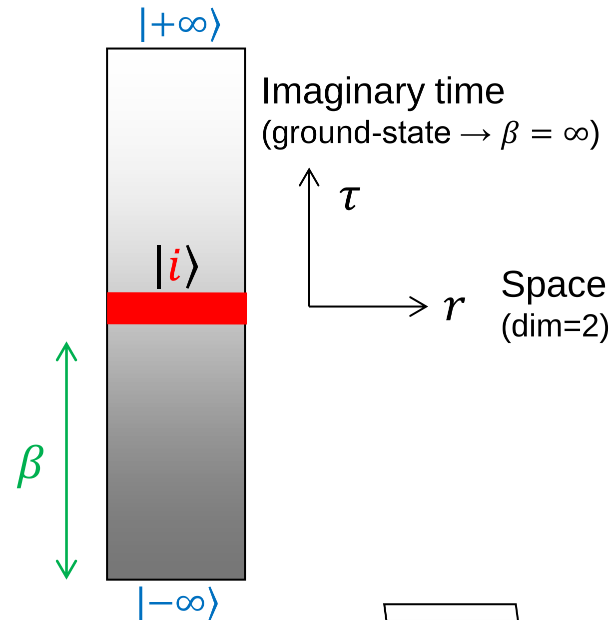
❑ Field-theory derivation ?

From now: we consider the Shannon entropy computed in the x –basis, for an XY ferromagnet (1 Nambu-Goldstone mode)

Replica formulation of the Rényi entropy

- Euclidian path integral

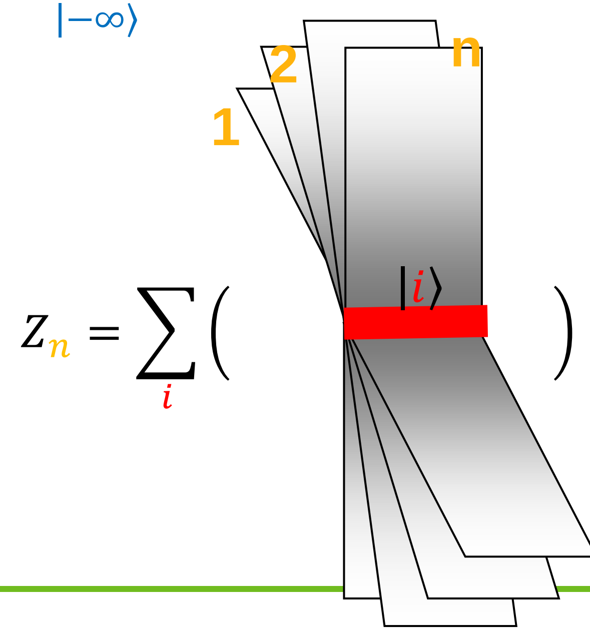
$$p_{i} = \langle\psi|i\rangle\langle i|\psi\rangle \sim \langle -\infty|e^{-\beta H}|i\rangle\langle i|e^{-\beta H}|+\infty\rangle$$
$$\beta \to \infty$$



- Replica formulation for $Z_n = \sum_i (p_i)^n$

The replica are glued together at $\tau = 0$. $n > 1$ integer.

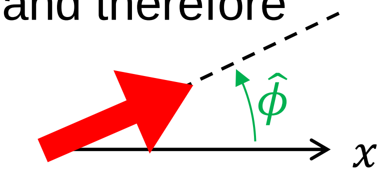
- How to compute (the universal terms in) such a partition function ?



GM, Pasquier & Oshikawa, arXiv:1607.02465

Replica formulation of the Rényi entropy

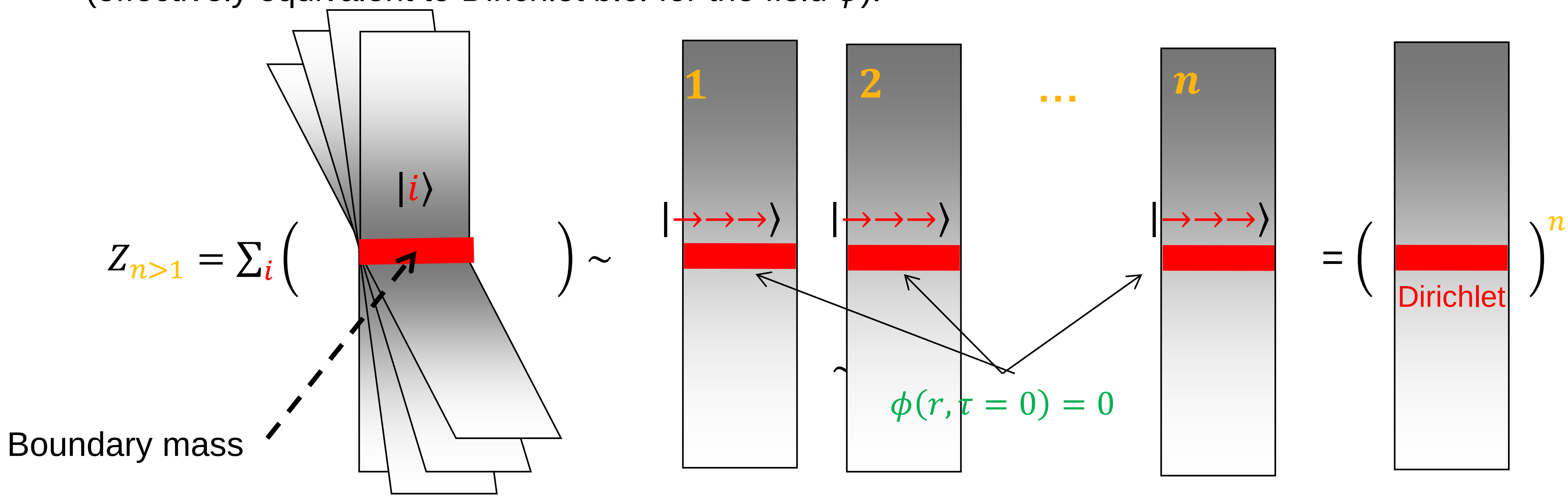
- $n > 1$: the basis choice selects a particular direction (x direction), and therefore explicitly breaks the $U(1)$ symmetry (spin rotations about the z axis)



→ Expect boundary mass term (since not forbidden by symmetry)

$$\sim \mathrm{m}^2 \int dr\, \phi(r, \tau = 0)^2$$

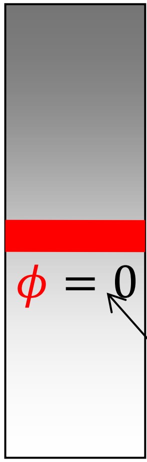
→ mass terms are relevant in $d = 2 + 1$ → « pin » the order parameter direction (effectively equivalent to Dirichlet b.c. for the field ϕ).



GM, Pasquier & Oshikawa, arXiv:1607.02465

p_{max} & free field

- Result of the previous slide:



$$Z_{n>1} \sim \left(\phi = 0 \right)^n \sim (p_{max})^n = |\langle \psi | \phi(r) = 0 \rangle|^{2n} \qquad S_{n>1} = \frac{1}{1-n} \log Z_n \sim \frac{n}{1-n} \log p_{max}$$

Dirichlet b.c.: $\phi(r, \tau = 0) = 0$

- Free-field approximation to compute $\langle \psi | \phi = 0 \rangle$:

  This approx. should not affect the universal part of p_{max}

  - Massless free-field: $H = \frac{1}{2} \int d^2 r [\chi_\perp \Pi_r^2 + \rho_s (\nabla \phi_r)^2] = \frac{1}{2} \sum_k \left[\frac{c^2}{\rho_s} \Pi_k^2 + \rho_s k^2 |\phi_k|^2 \right]$
  - Each mode = harmonic oscillator with mass $m_k = \rho_S / c^2$ and frequency $\omega_k = c|k|$. ρ_S: stiffness
  - Gaussian ground-state wave function

$$\langle \psi | \{\phi_k\} \rangle = \prod_{k \neq 0} \left(\frac{\rho_S |k|}{\pi c} \right)^{\frac{1}{4}} \exp\left(- \frac{\rho_S |k| {\phi_k}^2}{2\pi c} \right)$$

$p_{max}^{osc} = |\langle \psi | \{\phi_k = 0\} \rangle|^2 = \prod_{k \neq 0} \left(\frac{\rho_S |k|}{\pi c} \right)^{\frac{1}{2}}$ … needs some **regularization** to get the universal part.

GM, Pasquier & Oshikawa, arXiv:1607.02465

p_{max} & determinant of Laplacian

$$p_{max}^{osc} = |\langle\psi|\{\phi_k = 0\}\rangle|^2 = \prod_{k\neq 0}\left(\frac{\rho_S|k|}{\pi c}\right)^{\frac{1}{2}}$$

$$S_\infty = -\log p_{max}^{osc} = \underbrace{-\frac{1}{2}\sum_{k\neq 0}\log\frac{\rho_S}{\pi c}}_{=\mathcal{O}(N)\text{ volume term}} - \frac{1}{4}\sum_{k\neq 0}\log|k|^2$$

- We recognize the determinant' of the Laplacian $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = -|k|^2$:

  well known in Maths, CFT, …

in $D = 2$: $\log\det{}'\Delta = \sum_{k\neq 0}\log|k|^2 \simeq \mathcal{O}(N = \text{Area}) + \left(1 - \frac{\chi}{6}\right)\log N + \cdots$ [Kac 1966]

Topological term (Euler-Poincaré char.)

Torus case ($\chi = 0$) : $-\log p_{max}^{osc} = \mathcal{O}(N) - \frac{1}{4}\log N + \cdots$

Note: can also derive this $\log$ term using a lattice regularization + Euler-Maclaurin expansion.

- Compare with numerics

  Luitz, Alet & Laflorencie PRL 2014.

  XY model, $S = \frac{1}{2}$, square lattice: $S_\infty \simeq \mathcal{O}(N) + 0.269(1)\log N$

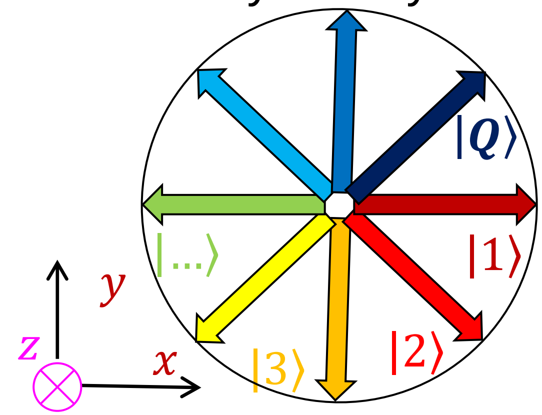
→ wrong sign ☹ ! Something is missing ?

GM, Pasquier & Oshikawa, arXiv:1607.02465

Tower of state – degeneracy factor

- Finite-size quantum antiferromagnet (or XY ferromagnet) :
  The ground-state $|\psi\rangle$ is rotationally invariant: $S^z_{\text{tot}} = 0$
  $\neq$ broken symmetry state

Broken-symmetry states



- The ground-state $|\psi\rangle$ is a linear combination
  of $\sim \boldsymbol{Q}$ symmetry-breaking states :

$$|\psi\rangle = \frac{1}{\sqrt{\boldsymbol{Q}}}\left(|1\rangle + |2\rangle + |3\rangle + \cdots + |\boldsymbol{Q}\rangle\right)$$

$\boldsymbol{Q} \sim \mathcal{O}(\sqrt{N})$
for broken $U(1)$

- Consequence for the $n = \infty$ -Rényi entropy ?

$$p_{max} = |\langle\rightarrow\rightarrow\rightarrow|\psi\rangle|^2 = \frac{1}{\boldsymbol{Q}}|\langle\rightarrow\rightarrow\rightarrow|1\rangle + \langle\rightarrow\rightarrow\rightarrow|2\rangle + \langle\rightarrow\rightarrow\rightarrow|3\rangle + \cdots|^2$$

neglect the contributions of $|2\rangle, |3\rangle, \cdots$ (the directions do not match $\rightarrow\rightarrow\rightarrow$)

$$\Rightarrow\ p_{max} \simeq \frac{1}{\boldsymbol{Q}}|\langle\rightarrow\rightarrow\rightarrow|1\rangle|^2 = \frac{1}{\boldsymbol{Q}}\, p^{\text{osc}}_{max} = N^{-\frac{1}{2}}\, p^{\text{osc}}_{max}$$

$$-\log p_{max} = \mathcal{O}(N) \quad + \left(\frac{1}{2} - \frac{1}{4}\right)\log N + \cdots$$

agreement with the QMC results
Luitz, Alet, & Laflorencie PRL 2014 :

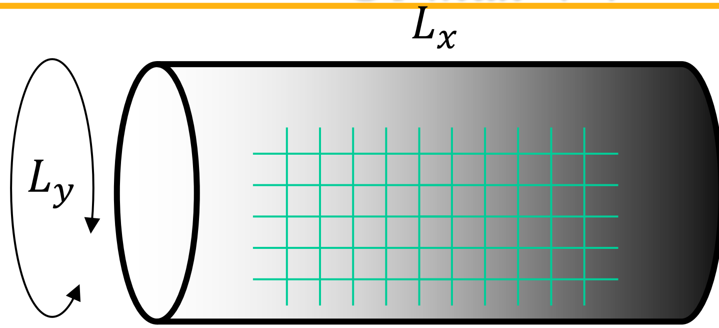
- Finite n: $S_{n>1} \sim \frac{n}{1-n}\log p_{max} \sim \mathcal{O}(N) + \frac{1}{4}\frac{n}{n-1}\log N$

GM, Pasquier & Oshikawa, arXiv:1607.02465

DMRG numerics for $-\log p_{max}$ (1)

Spin-$\frac{1}{2}$ « XY » model

$$H = -\sum_{<ij>} \left(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y\right)$$



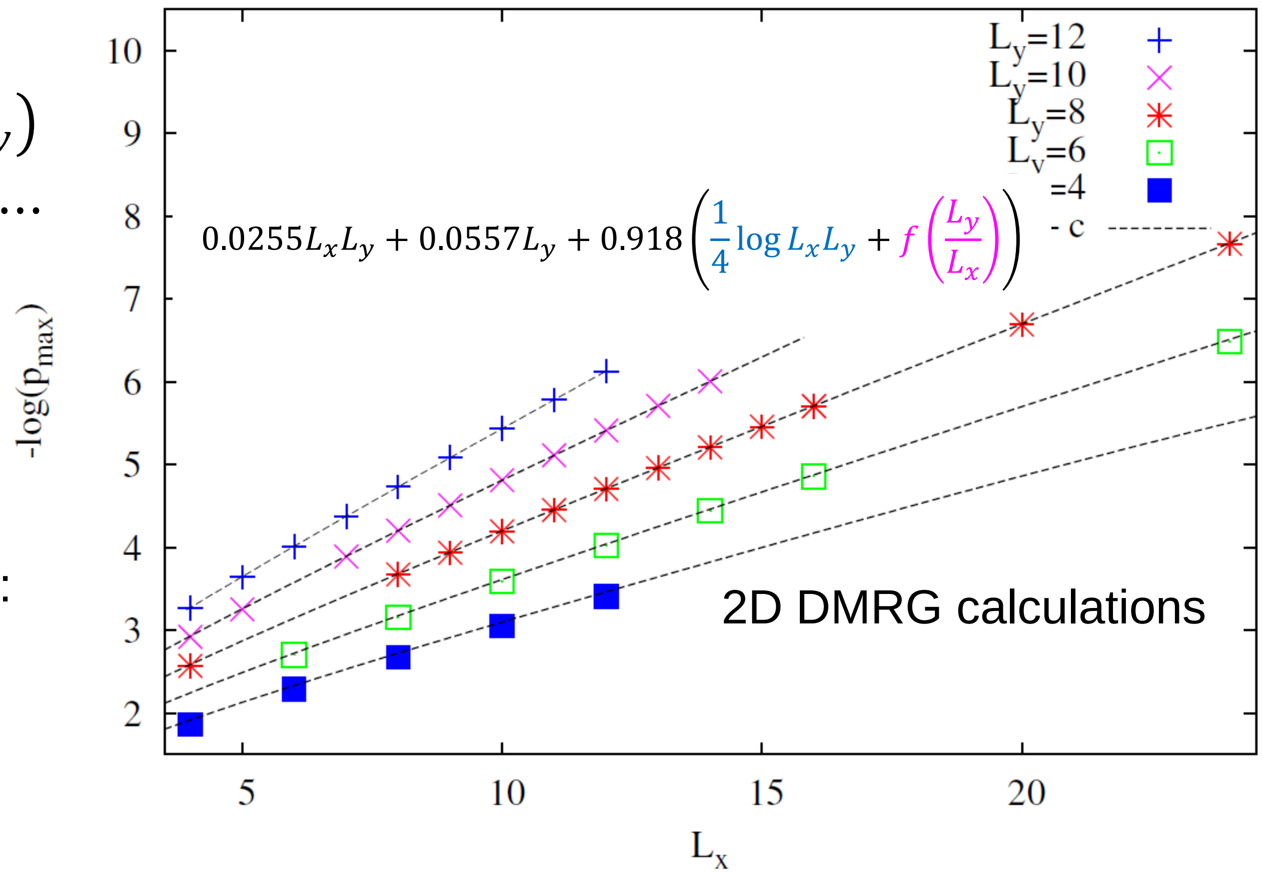
Cylinder aspect ratio $r = \frac{L_y}{L_x}$

$$-\log p_{max} = \mathcal{O}(L_x L_y) + \mathcal{O}(L_y) + \frac{1}{4}\log L_x L_y + f\left(\frac{L_y}{L_x}\right) + \cdots$$

Aspect-ratio dependent term in $-\log p_{max}$ (oscillator contribution):

$$f(r) = -\frac{1}{2}\log\left(\sqrt{r}\,\eta\left(i\frac{L_y}{2L_x}\right)\right)$$

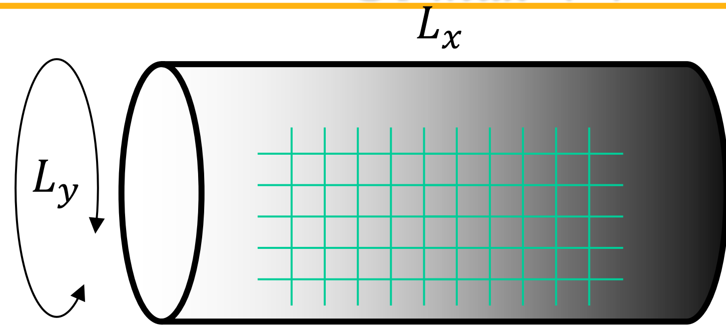
η: Dedekind η-function



GM, Pasquier & Oshikawa, arXiv:1607.02465

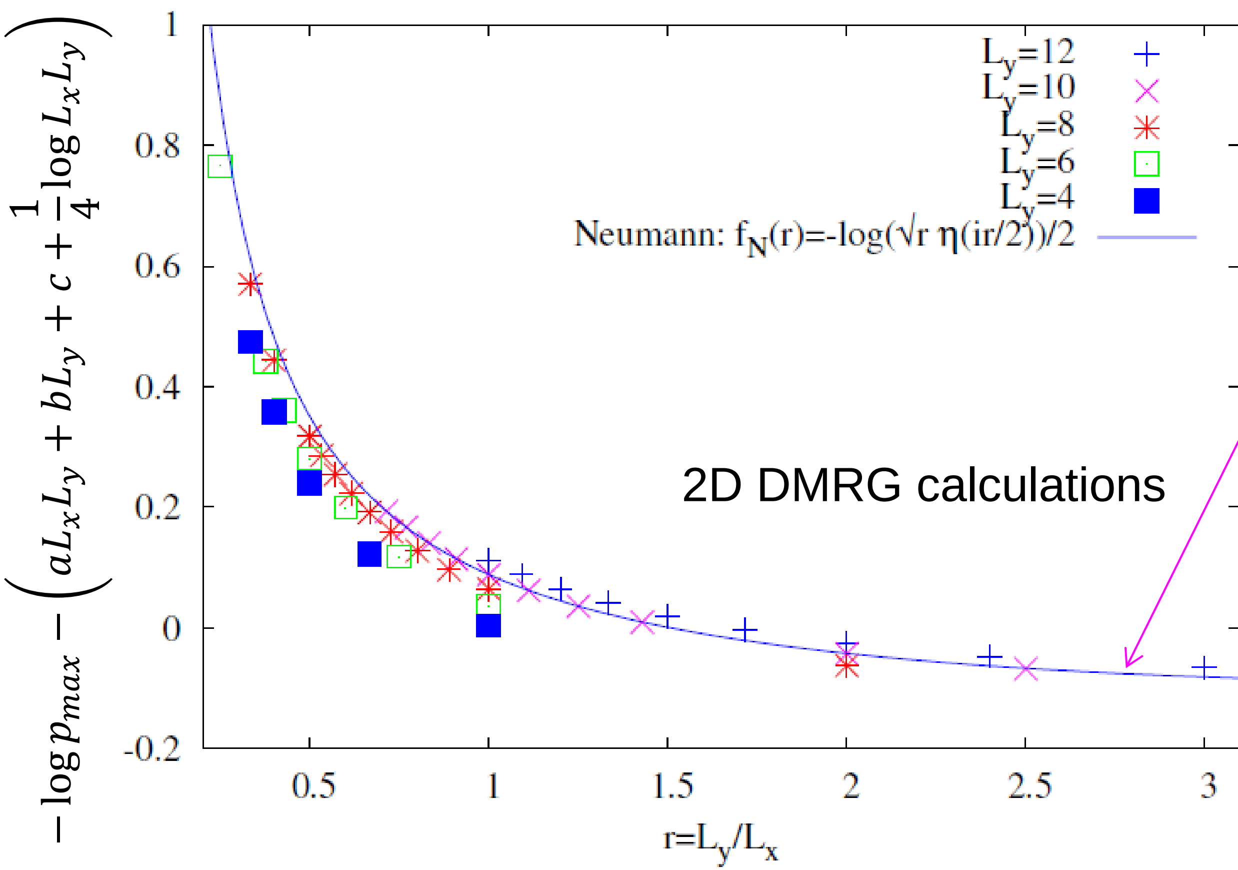
DMRG numerics for $-\log p_{max}$ (2)

$$H = -\sum_j \left(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y\right)$$



Cylinder aspect ratio $r = \frac{L_y}{L_x}$

GM, Pasquier & Oshikawa, arXiv:1607.02465



Aspect-ratio dependent term in $-\log p_{max}$ (oscillator contribution):

$$f(r) = -\frac{1}{2}\log\left(\sqrt{r}\,\eta\left(i\frac{L_y}{2L_x}\right)\right)$$

… obtained from $\log\det{}'\Delta$ with Neumann b.c.

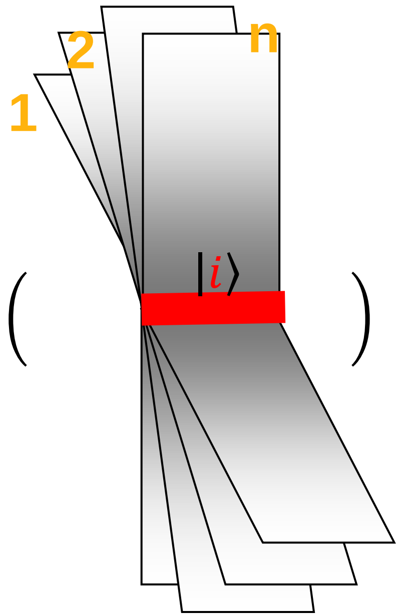
Dedekind η-function:

$$\eta(\tau) = q^{\frac{1}{24}}\prod_{n=1}^{\infty}(1-q^n)$$

$$q = \exp(2i\pi\tau) = \exp -\frac{L_y}{L_x}$$

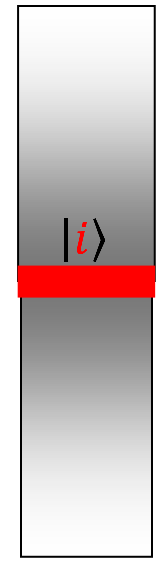
What about $n \to 1$?

$$Z_n = \sum_i \Big($$



$$\Big)$$

$$Z_1 = \sum_i \Big($$



$$\Big) = \langle \psi | \psi \rangle = 1$$

$$S_1 = \left.\frac{\partial \log Z_n}{\partial n}\right|_{n=1}$$

- $n \to 1$: no boundary (τ=0 is not a special line)
- U(1) symmetry is preserved, the mass term vanish when $n \to 1$

$\Rightarrow$ Use the Gaussian approx. to the wave-function to compute S_1^{osc}

$$S_1^{osc} = \mathcal{O}(N) - \frac{1}{4} \log N$$

$\Rightarrow$ U(1) symmetry $\to$ no deg. factor. $\to S_1 = S_1^{osc} \sim \mathcal{O}(N) - \frac{1}{4} \log N$

Numerical check ? Not easy…

GM, Pasquier & Oshikawa, arXiv:1607.02465

Concluding remarks

- A single weight ($p_{\max}$) in the wave-function "knows" about the long distance physics:
  - Compactification radius in TLL
  - Goldstone modes in D=2, …
- Goldstone in D=2
  - $\log N$ (& aspect-ratio dependent): strong similarity with von Neumann entropy
  - $n = n_c = 1$: new phase transition in Rényi entropies
  - Numerical checks at $n = 1$? Not easy for QMC or DMRG…
  - Higher dimension ?