Entanglement in Valence-Bond-Solid States on Symmetric Graphs

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History of VBS and MPS

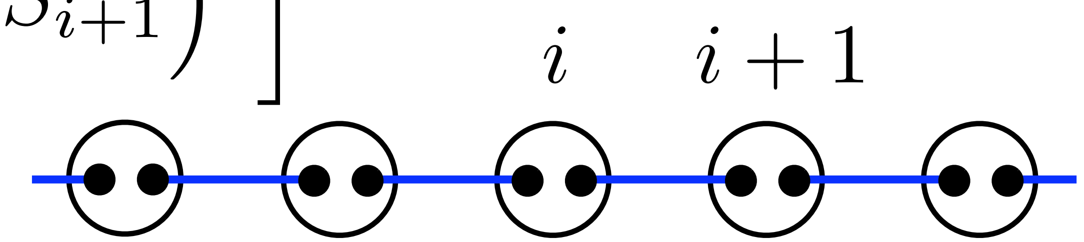
✓ **Haldane's conjecture** PRL **50** (1983)

Integer-S antiferromagnetic Heisenberg chains are gapped.

✓ **Affleck-Lieb-Kennedy-Tasaki(AKLT) model** PRL **59** (1987) CMP **115** (1987)

$$\mathcal{H}_{\mathrm{AKLT}} = J \sum_i \left[\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} \left(\vec{S}_i \cdot \vec{S}_{i+1} \right)^2 \right]$$

Valence-Bond-Solid (VBS) state



✓ **Schwinger boson representation**

Arovas, Auerbach, Haldane, PRL **60** (1989)

$$|\mathrm{VBS}\rangle = \prod_{i=1}^{L} \left(a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger \right) |\mathrm{vac}\rangle$$

✓ **Matrix Product State(MPS)**

Fannes, Nactergaele, Werner, EPL **24** (1989),
Kluemper, Schadschneider, Zittarz, JPA **24** (1991).

$$|\mathrm{VBS}\rangle = \mathrm{Tr}\left(A^{[1]} A^{[2]} \cdots A^{[L]} \right), \qquad A^{[i]} = \begin{pmatrix} |0\rangle_i & +\sqrt{2}|+\rangle_i \\ -\sqrt{2}|-\rangle_i & -|0\rangle_i \end{pmatrix}$$

Quantum Information Science

- ✓ **Projected Pair Entangled State (PEPS)**
  Tensor Network States (TNS)
  Verstraete, Cirac, PRA **70** (2004).
  Gross, Eisert, PRL **98** (2007).

- ✓ **Measurement based Quantum Computation (MQC)**
  MQC using AKLT chains
  Verstraete, Cirac, PRA **70** (2004).
  Brennen, Miyake, PRL **101** (2008).

- ✓ **Universal quantum computation using 2d VBS states**
  Wei, Affleck, Raussendorf, arXiv:1009.2840.
  Miyake, arXiv:1009.3491.

- ✓ **Optical lattice**
  Optical lattice can be realize AKLT model
  S.K. Yip, PRL **90** 250402 (2003)
  J.J. Garcia-Ripoll et al. PRL. **93** 250405 (2004)
  G.K.Brennen et al. NJP **9** 138 (2007)

Our aim is to obtain the entanglement entropy of VBS state!

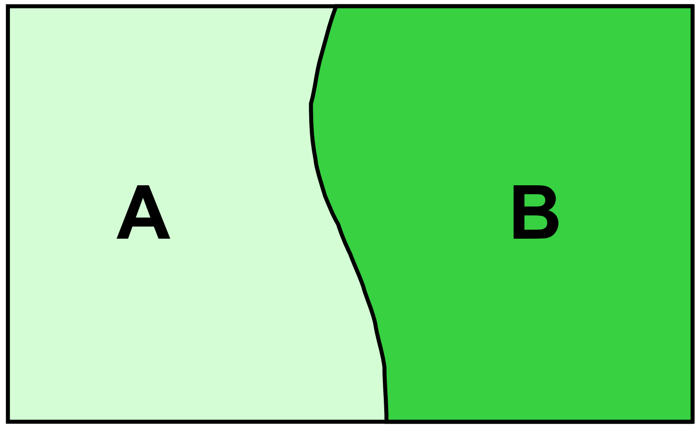
Entanglement Entropy

Schmidt decomposition

$$|\Psi\rangle = \sum_\alpha \lambda_\alpha |\phi_\alpha^{[A]}\rangle \otimes |\phi_\alpha^{[B]}\rangle$$

$\{|\phi_\alpha^{[A]}\rangle\}, \{|\phi_\alpha^{[B]}\rangle\}$ orthonormal basis

$|\Psi\rangle$ is normalized. $(\langle\Psi|\Psi\rangle = 1)$



Reduced density matrix

$$\rho_A = \mathrm{Tr}_B |\Psi\rangle\langle\Psi| = \sum_\alpha \lambda_\alpha^2 |\phi_\alpha^{[A]}\rangle\langle\phi_\alpha^{[A]}|$$

Entanglement Entropy (von Neumann entropy)

$$\mathcal{S} = -\sum_\alpha \lambda_\alpha^2 \log \lambda_\alpha^2$$

e.g.) maximally entangled state

$$|\Psi\rangle = \frac{1}{\sqrt{D}} \sum_{\alpha=1}^{D} |\phi_\alpha^{[A]}\rangle \otimes |\phi_\alpha^{[B]}\rangle$$

$$\Downarrow$$

$$\mathcal{S} = \log D$$

Reflection Symmetry

Pre-Schmidt decomposition

$$|\Psi\rangle = \sum_{\alpha=1}^{D} |\phi_\alpha^{[A]}\rangle \otimes |\phi_\alpha^{[B]}\rangle$$

$|\Psi\rangle$ is not necessarily normalized.

$\{|\phi_\alpha^{[A]}\rangle\}, \{|\phi_\alpha^{[B]}\rangle\}$ may not be orthonormal.

Overlap matrices

$$(\mathcal{M}^{[A]})_{\alpha\beta} = \langle\phi_\alpha^{[A]}|\phi_\beta^{[A]}\rangle \qquad (\mathcal{M}^{[B]})_{\alpha\beta} = \langle\phi_\alpha^{[B]}|\phi_\beta^{[B]}\rangle$$

Useful fact

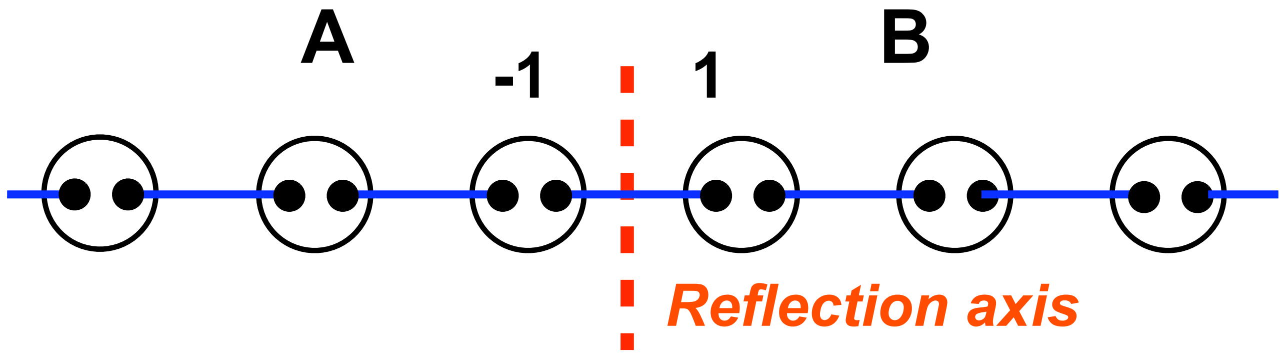
If $\mathcal{M}^{[A]} = \mathcal{M}^{[B]} = \mathcal{M}$ and $\mathcal{M}$ is real symmetric matrix, then

$$\mathcal{S} = -\sum_\alpha p_\alpha \log p_\alpha, \;\; p_\alpha = \frac{d_\alpha^2}{\sum_\alpha d_\alpha^2}$$

where d_α are the eigenvalues of $\mathcal{M}$.

This technique can be applied to VBS state on a reflection symmetric graph!

Application to 1d VBS states



$$|\mathrm{VBS}\rangle = a^\dagger_{-1}|\mathrm{VBS}^{[A]}\rangle \otimes b^\dagger_{+1}|\mathrm{VBS}^{[B]}\rangle - b^\dagger_{-1}|\mathrm{VBS}^{[A]}\rangle \otimes a^\dagger_{+1}|\mathrm{VBS}^{[B]}\rangle$$

$$|\phi^{[A]}_\uparrow\rangle = a^\dagger_{-1}|\mathrm{VBS}^{[A]}\rangle, |\phi^{[A]}_\downarrow\rangle = b^\dagger_{-1}|\mathrm{VBS}^{[A]}\rangle$$

$$(\mathcal{M}^{[A]})_{\alpha\beta} = (\mathcal{M}^{[B]})_{\alpha\beta} = d\delta_{\alpha\beta}$$

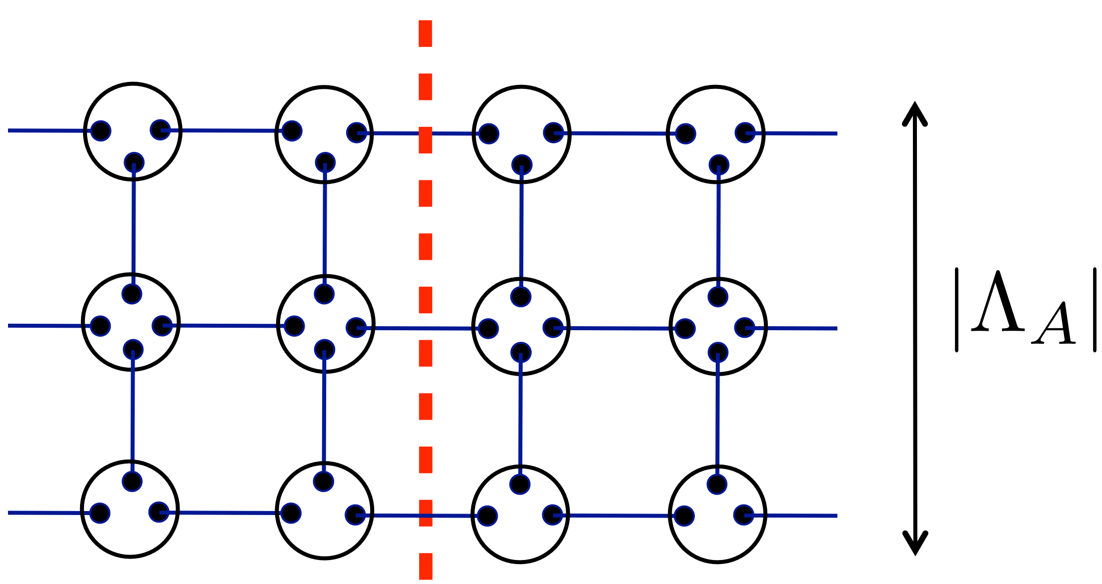
$$\mathcal{S} = \log 2$$

$$\mathcal{S} = \log(S+1)$$

1d results

Fan, Korepin, Roychowdhury, PRL **93** (2004),
Katsura, Hirano, Hatsugai, PRB **76** (2007), Xu, Katsura, Hirano, Korepin, JSP **133** (2008).

What about 2d VBS states?

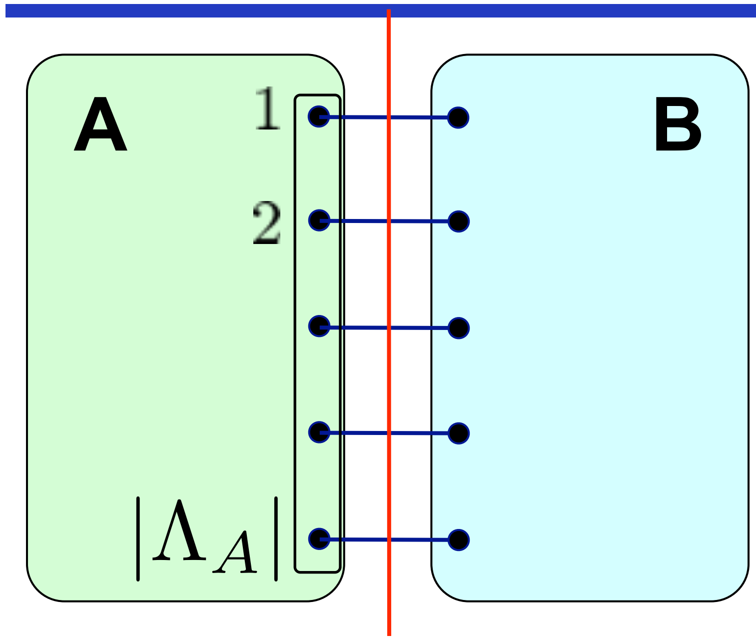


Symmetry is not large enough to determine the overlap matrix $\mathcal{M}^{[A]}$.
Numerics are required.

Naive guess (valence bond EE)

$$\mathcal{S} = |\Lambda_A| \log 2$$ (crossed out)

Overlap matrix



Schwinger boson rep. -> Coherent state rep.

1. Matrix elements can be calculated by Monte Carlo integrations.
2. Exact diagonalization of $2^{|\Lambda_A|}$ dimensional matrix.

$$\mathcal{M} = \int \left[\prod_{i \in A} \frac{(2S_i+1)!}{4\pi} d\hat{\Omega}_i \right] \prod_{k \in \Lambda_A} \left(\frac{1 + \hat{\Omega}_k \cdot \vec{\sigma}_k}{2} \right) \prod_{(i,j) \in \mathcal{B}_A} \left(\frac{1 - \hat{\Omega}_i \cdot \hat{\Omega}_j}{2} \right)$$

σ_k^α s act on the auxiliary spaces. (dim = $2^{|\Lambda_A|}$).

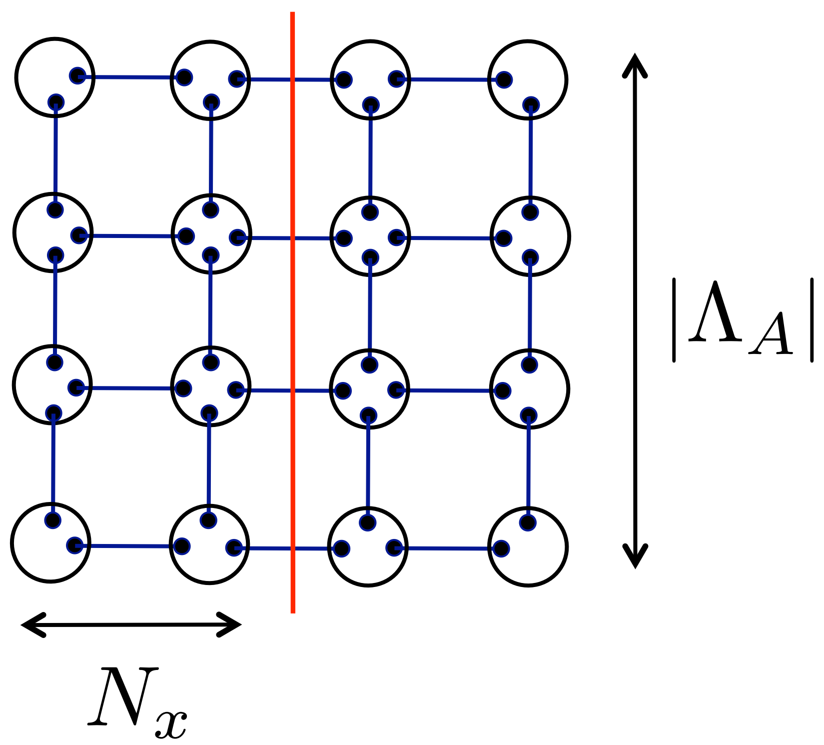
If and only if $\mathcal{M}$ is proportional to the identity matrix, $\mathcal{S} = |\Lambda_A| \log 2$

Conjecture

The von Neumann (entanglement) entropy is strictly less than $|\Lambda_A| \log 2$ even in the 2d infinite-size limit.

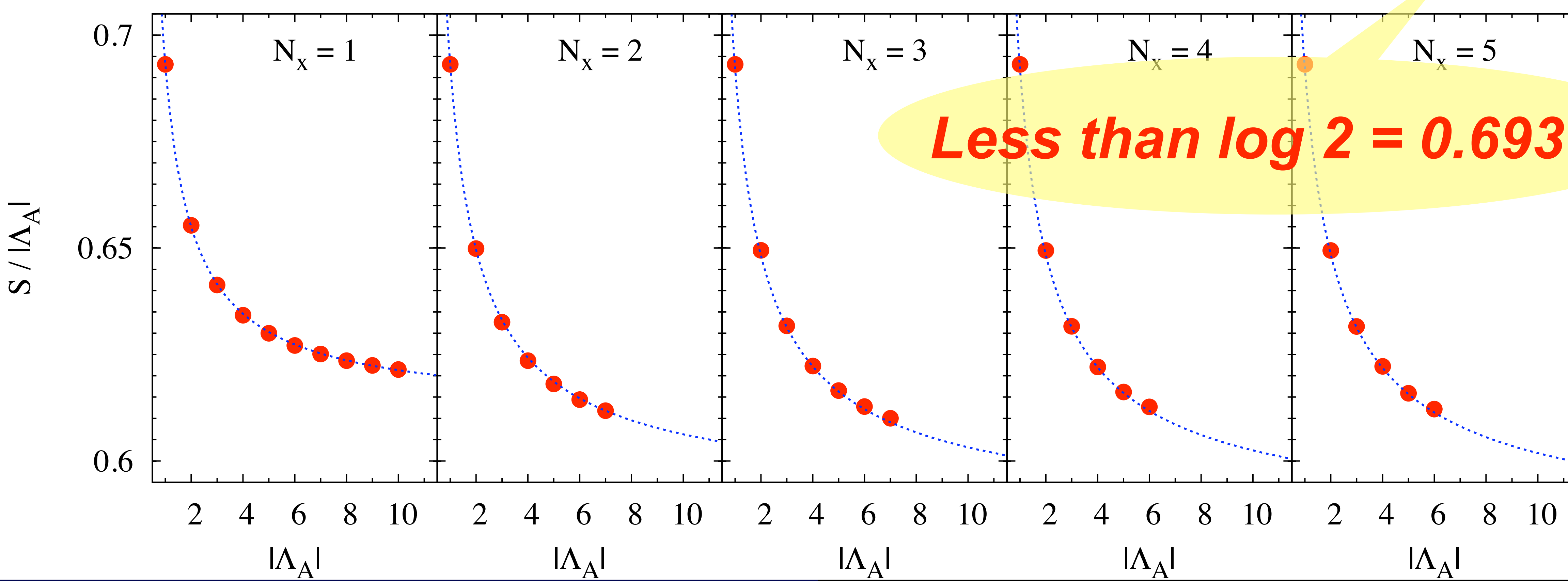
EE per valence bond = $\dfrac{\mathcal{S}}{|\Lambda_A|} < \log 2$ ***different from 1d !***

Numerical results (square lattice)



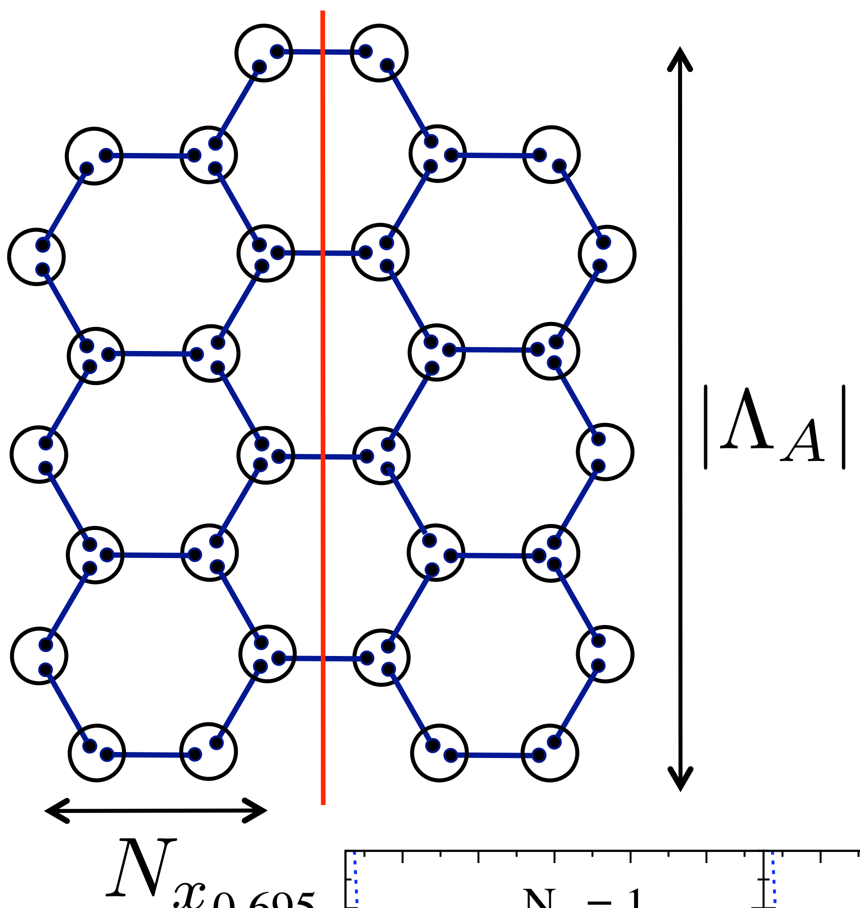
Fitting Function $$\frac{S}{|\Lambda_A|} = \frac{C}{|\Lambda_A|^{\Delta}} + \alpha$$

	C	Δ	α
Nx=1	0.0821(4)	0.90(1)	0.6110(4)
Nx=2	0.104(1)	0.78(2)	0.589(1)
Nx=3	0.108(1)	0.75(2)	0.584(1)
Nx=4	0.110(2)	0.73(3)	0.582(2)
Nx=5	0.112(1)	0.71(2)	0.580(1)



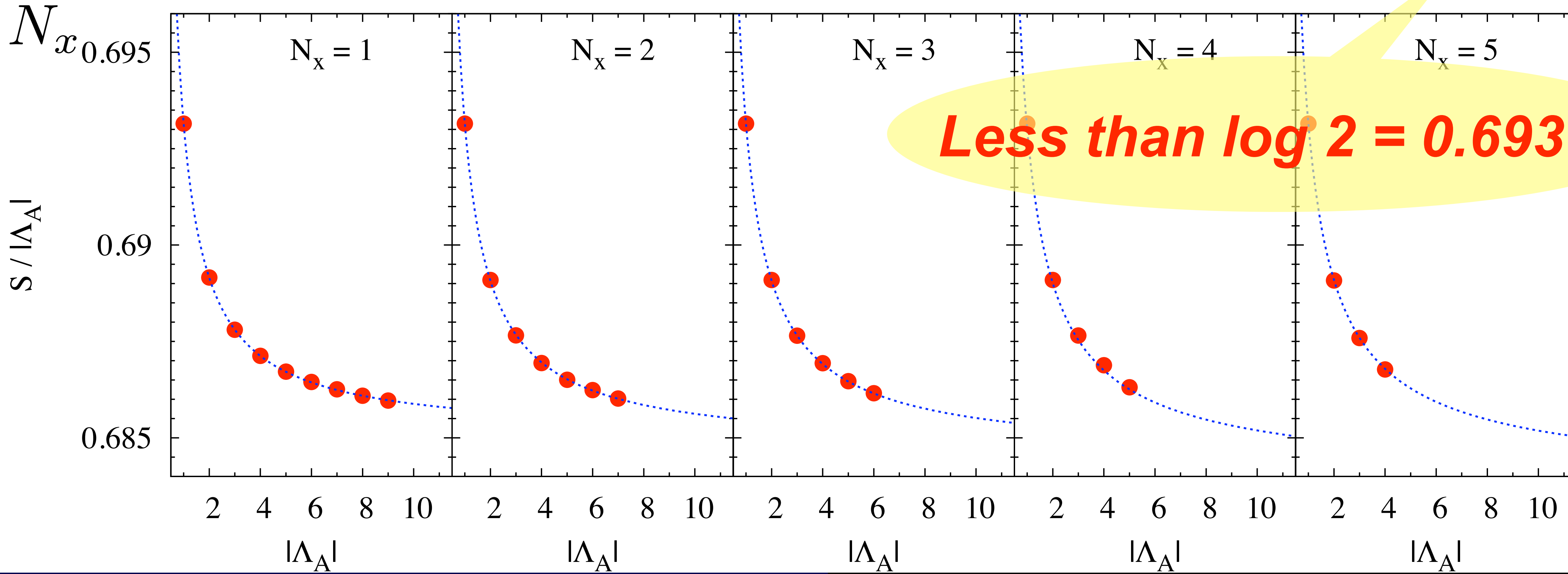
Less than log 2 = 0.6931...

Numerical results (hexagonal lattice)



Fitting Function $$\frac{\mathcal{S}}{|\Lambda_A|} = \frac{C}{|\Lambda_A|^{\Delta}} + \alpha$$

	C	Δ	α
Nx=1	0.00812(1)	0.974(4)	0.68502(1)
Nx=2	0.00849(4)	0.94(1)	0.68465(5)
Nx=3	0.00870(3)	0.904(7)	0.68443(3)
Nx=4	0.0092(2)	0.82(3)	0.6838(2)
Nx=5	0.00941(7)	0.81(1)	0.68373(7)



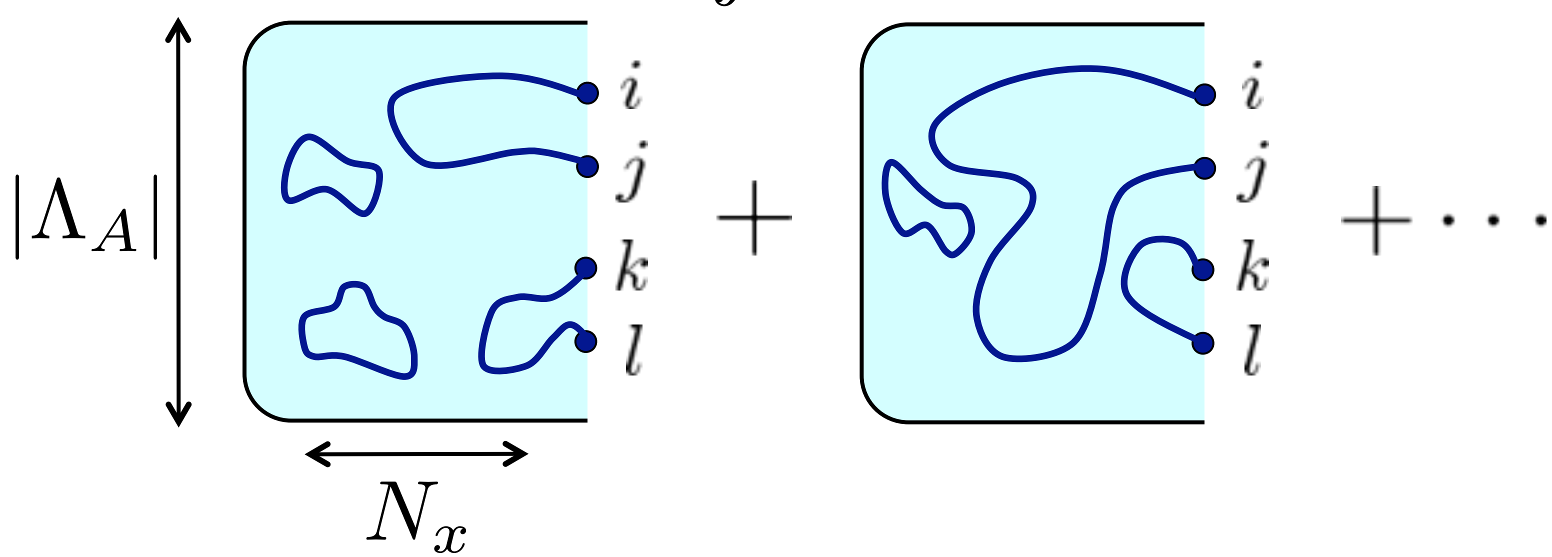
Less than log 2 = 0.6931...

Analytical results (loop model)

Overlap matrix = holographic spin chain (polynomial in $(\vec{\sigma}_i \cdot \vec{\sigma}_j)$)

$$\mathcal{M} = \int \left[\prod_{i \in A} \frac{(2S_i+1)!}{4\pi} d\hat{\Omega}_i \right] \prod_{k \in \Lambda_A} \left(\frac{1+\hat{\Omega}_k \cdot \vec{\sigma}_k}{2} \right) \prod_{(i,j) \in \mathcal{B}_A} \left(\frac{1-\hat{\Omega}_i \cdot \hat{\Omega}_j}{2} \right)$$

Useful formula: $\int \frac{d\hat{\Omega}}{4\pi} (\hat{\Omega}_1 \cdot \hat{\Omega})(\hat{\Omega} \cdot \hat{\Omega}_2) = \frac{1}{3} (\hat{\Omega}_1 \cdot \hat{\Omega}_2)$



Bond weight: 1/3
Loop weight: 3

Non-critical loop model

Transfer matrix approach for ladder systems

✓ Recursion relation between $N_x = n$ and $N_x = n+1$.

✓ Perron-Frobenius vector of the transfer matrix ->$\mathcal{M}$ in the limit of large N_x . We can obtain $\mathcal{M}(N_x \to \infty)$ without using MC.

Conjecture is true for quasi-1d (fixed $|\Lambda_A|$) systems.

Comparison of analytical and numerics

Square Lattice		Nx = 1	Nx = 2	Nx = 3	Nx = 4	Nx = 5
Ny = 2	Exact	0.6553433	0.6498531	0.6494635	0.6494368	0.6494349
	MC	0.6553431	0.6498533	0.6494621	0.6494342	0.6494373
Ny = 3	Exact	0.6413153	0.6325619	0.6316999	0.6316095	0.6315995
	MC	0.6413145	0.6325626	0.6316999	0.6316080	0.6315866

Honeycomb Lattice		Nx = 1	Nx = 2	Nx = 3	Nx = 4	Nx = 5
Ny = 4	Exact	0.6891577	0.6890932	0.6890927	0.6890927	0.6890927
	MC	0.6891575	0.6890924	0.6890929	0.6890925	0.6890840
Ny = 6	Exact	0.6878024	0.6876554	0.6876523	0.6876522	0.6876522
	MC	0.6878027	0.6876558	0.6876513	0.6876537	0.6875899
Ny = 8	Exact	0.6871254	0.6869344	0.6869295	0.6869293	0.6869293
	MC	0.6871243	0.6869385	0.6869363	0.6868834	0.6867750

Summary

We studied the entanglement entropy of VBS state on square lattice and hexagonal lattice.

✓ New method for calculating entanglement entropy.

✓ Numerical (and analytical) support for the conjecture.

The von Neumann (entanglement) entropy is strictly less than $|\Lambda_A| \log 2$ even in 2-dim inifinite size limit.

EE per valence bond = $\dfrac{\mathcal{S}}{|\Lambda_A|} < \log 2$

EE < log[#edge states]

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