

Exact Analysis of Entanglement Entropy in Gapped Quantum Spin Chains

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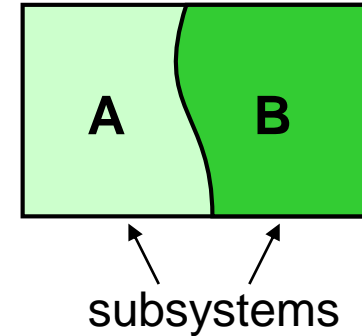
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Entanglement Entropy

Definition of Entanglement Entropy(EE)

- Many body ground state (assumed to be unique) : $|G\rangle$
- Density matrix : $\rho_{AB} = |G\rangle\langle G|$
- Reduced density matrix : $\rho_A = \text{Tr}_B \rho_{AB}$
- Entanglement Entropy : $S_A = -\text{Tr}_A \rho_A \log_2 \rho_A$



Physical Meaning of the EE

- Direct product state

$$|\Psi_{AB}\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle \quad \longrightarrow \quad S_A = 0$$

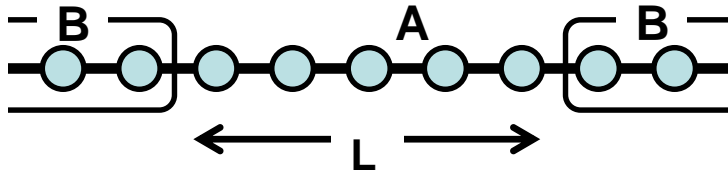
- Maximally entangled state

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{D}} \sum_{j=1}^D |\Psi_A^j\rangle \otimes |\Psi_B^j\rangle \quad \longrightarrow \quad S_A = \log_2 D$$

Entanglement Entropy in Spin Chains

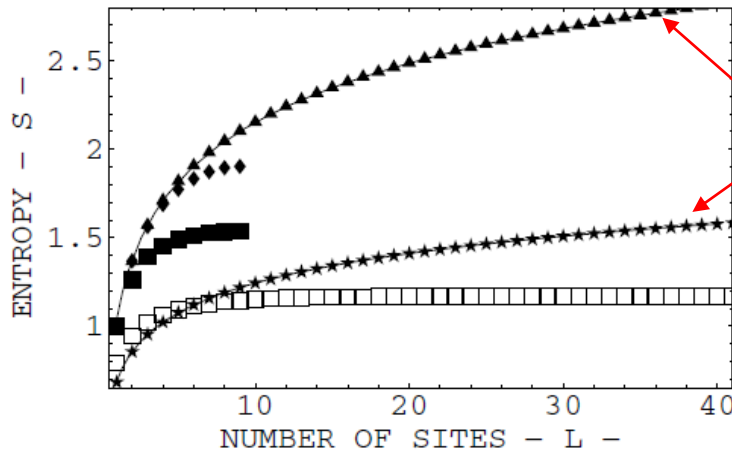
EE in the XXZ and the XY model with magnetic field

- Vidal *et al.*, *PRL* **90** (2003)



$$H_{XXZ} = \sum_{l=0}^{N-1} (\sigma_l^x \sigma_{l+1}^x + \sigma_l^y \sigma_{l+1}^y + \Delta \sigma_l^z \sigma_{l+1}^z - \lambda \sigma_l^z),$$

$$H_{XY} = - \sum_{l=0}^{N-1} \left(\frac{a}{2} [(1 + \gamma) \sigma_l^x \sigma_{l+1}^x + (1 - \gamma) \sigma_l^y \sigma_{l+1}^y] + \sigma_l^z \right).$$



□ : XY(a=1.1, γ=1)

■ : XXZ(Δ=2.5, λ=0)

★ : XY(a=1, γ=1)

▲ : XY(a=∞, γ=0)

◆ : XXZ(Δ=1, λ=0)

Gapless

Gapped

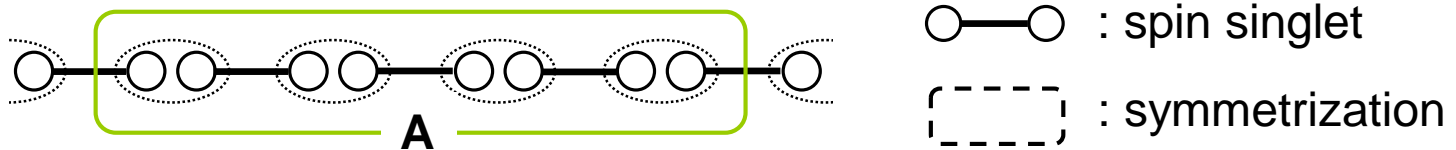
critical

Gapless point : $S_L \sim \frac{c + \bar{c}}{6} \log_2 L + k$ (Conformal field theory prediction)

Conjecture: gapped → saturation, gapless → logarithmic divergence

EE in the $S=1$ valence-bond-solid state (Haldane gapped systems)

- $S=1$ valence-bond-solid state

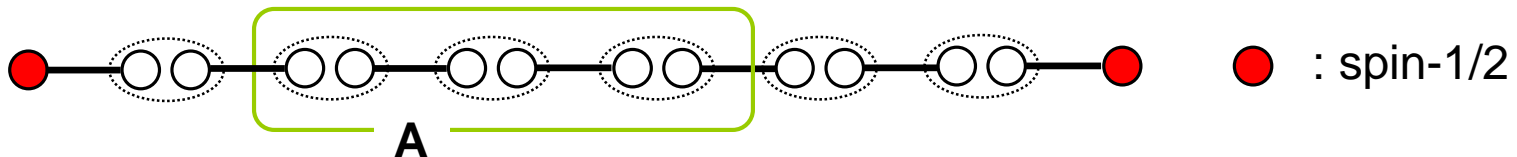


This state is a GS of the following Hamiltonian :

$$H = J \sum_j \vec{S}_j \cdot \vec{S}_{j+1} + \frac{1}{3} (\vec{S}_j \cdot \vec{S}_{j+1})^2$$

Affleck-Kennedy-Lieb-Tasaki(AKLT) model (1987)

- Fan, Korepin and Roychowdhury, *PRL* **94** (2004)



1. exact expression for the EE.
 2. $S_L \rightarrow \log_2 4 = 2$ in the thermodynamic limit.
- They 'partially' confirmed the conjecture proposed by Vidal et al.

Outline



1. Generic Valence-Bond-Solid with arbitrary integer spin- S
2. Exact expression for the entanglement entropy of VBS
 - a) Confirmation of the conjecture proposed by Vidal et al.
 - b) Relationship between the EE and correlation functions
3. Edge state interpretation and its application
4. Numerical results
5. Summary

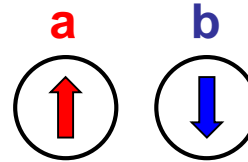


VBS with arbitrary integer-spin S

Preliminary Notions

Schwinger boson reps. of spin-operators

$$\begin{cases} S_j^+ = a_j^\dagger b_j, & S_j^- = b_j^\dagger a_j, \\ S_j^z = (a_j^\dagger a_j - b_j^\dagger b_j)/2, \end{cases}$$



$$\text{Constraint : } a_j^\dagger a_j + b_j^\dagger b_j = 2S.$$

Boson a/b creates up/down spin.

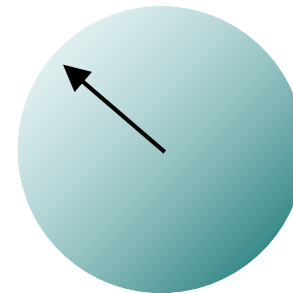
Coherent state representation of Schwinger bosons

$$|\hat{\Omega}\rangle = \frac{(ua^\dagger + vb^\dagger)^{2S}}{\sqrt{(2S)!}} |0\rangle,$$

$$\hat{\Omega} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

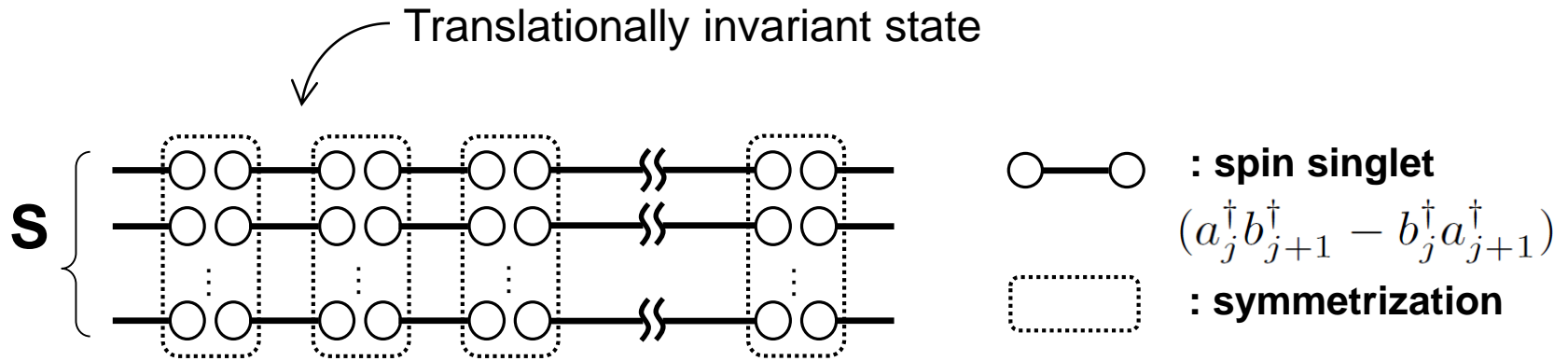
Spinor coordinate :

$$(u, v) = (\cos(\theta/2)e^{i\phi/2}, \sin(\theta/2)e^{-i\phi/2})$$



Advantage : The constraint $a_j^\dagger a_j + b_j^\dagger b_j = 2S$ is satisfied automatically.

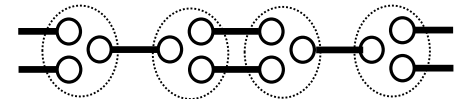
Construction of S=integer valence-bond-solid state



↓ Schwinger boson reps.

$$|\text{VBS}\rangle = \prod_{j=0}^L (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S |\text{vac}\rangle$$

We cannot construct a translationally invariant S=half-odd-integer VBS.



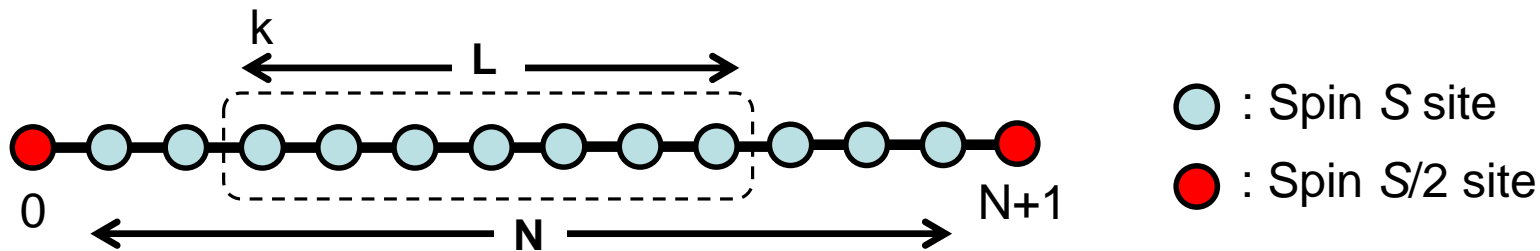
Corresponding Hamiltonian (Arovas-Auerbach-Haldane)

$$H = \sum_{j=1}^{N-1} \sum_{J=S+1}^{2S} A_J P_{j,j+1}^J + \pi_{0,1} + \pi_{N,N+1},$$

$P_{j,j+1}^J$ projects the bond spin onto the total spin J subspace.

$|\text{VBS}\rangle$ is a zero energy GS of the above Hamiltonian.

Our setting



- Density matrix : $\rho = |\text{VBS}\rangle\langle\text{VBS}| / \langle\text{VBS}|\text{VBS}\rangle$,
- Reduced density matrix : $\rho_L = \text{Tr}_{\overline{\mathcal{B}}_L} \rho$
- Entanglement Entropy : $\mathcal{S}_L = -\text{Tr}_{\mathcal{B}_L} \rho_L \log_2 \rho_L$

Resolution of identity

$$\text{Tr} \mathcal{O} = \frac{2S+1}{4\pi} \int d\hat{\Omega} \langle \hat{\Omega} | \mathcal{O} | \hat{\Omega} \rangle$$

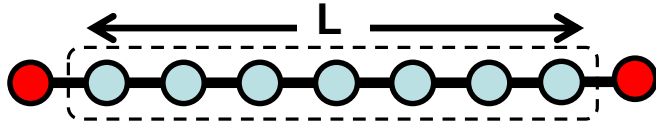
Integrating over $\hat{\Omega}_{k-l-1}$ ($l = 1, 2, \dots, k-1$) and $\hat{\Omega}_{k+L+m}$ ($m = 1, 2, \dots, N-L-k+1$) one can show the following

Theorem :

The reduced density matrix ρ_L does not depend on both the starting site k and the total length N .



We can set $N=L$ without loss of generality.



- : Spin S site
- : Spin S/2 site

Important Properties :

- Entanglement Entropy : $\mathcal{S}_L = \mathcal{S}_{\hat{L}}$ (∵ Schmidt decomposition)

(Reduced density matrix of two end spin-S/2's : $\rho_{\hat{L}}$) $|\text{vac}\rangle = |0,0\rangle_{0,L+1}$

⇒ We can focus on the RDM of two end spin-S/2's.

$$\rho_{\hat{L}} = \frac{\int \prod_{j=1}^L \frac{d\hat{\Omega}_j}{4\pi} \prod_{k=1}^{L-1} \left(\frac{1 - \hat{\Omega}_k \cdot \hat{\Omega}_{k+1}}{2} \right)^S P_0^\dagger Q_{L+1}^\dagger |\text{vac}\rangle \langle \text{vac}| P_0 Q_{L+1}}{(S!)^2 \int \left(\prod_{j=1}^L \frac{d\hat{\Omega}_j}{4\pi} \right) \prod_{k=1}^{L-1} \left(\frac{1 - \hat{\Omega}_k \cdot \hat{\Omega}_{k+1}}{2} \right)^S}$$

- Transformation property of spinor coordinates

$$\begin{array}{ccc}
 |\hat{\Omega}\rangle & \longrightarrow & |-\hat{\Omega}\rangle \\
 (\theta, \phi) & & (\pi - \theta, \phi + \pi) \\
 \begin{array}{c} \text{---} \\ \diagup \\ \text{---} \end{array} & & \begin{array}{c} \text{---} \\ \diagdown \\ \text{---} \end{array} \\
 (u, v) & \longrightarrow & (iv^*, -iu^*)
 \end{array}$$

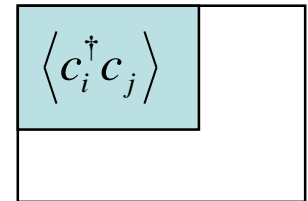
$$\begin{aligned}
 P_0^\dagger |0\rangle &= (a_0^\dagger v_1^* - b_0^\dagger u_1^*)^S |0\rangle \\
 &= (-i)^S \sqrt{S!} |-\hat{\Omega}_1\rangle \\
 (\langle 0| a^{S-l} b^{S+l} |\hat{\Omega}\rangle &= \sqrt{(2S)!} u^{S-l} v^{S+l})
 \end{aligned}$$

Then we can rewrite $\rho_{\hat{L}}$ as

$$\rho_{\hat{L}} = \frac{\int \prod_{j=1}^L \frac{d\hat{\Omega}_j}{4\pi} \prod_{k=1}^{L-1} \left(\frac{1 - \hat{\Omega}_k \cdot \hat{\Omega}_{k+1}}{2} \right)^S |\hat{\Omega}_1\rangle_0 \langle \hat{\Omega}_1| \otimes |\hat{\Omega}_L\rangle_{L+1} \langle \hat{\Omega}_L|}{\int \left(\prod_{j=1}^L \frac{d\hat{\Omega}_j}{4\pi} \right) \prod_{k=1}^{L-1} \left(\frac{1 - \hat{\Omega}_k \cdot \hat{\Omega}_{k+1}}{2} \right)^S}.$$

- This can be thought of as a correlation function between the density matrices $|\hat{\Omega}_1\rangle_0 \langle \hat{\Omega}_1|$ and $|\hat{\Omega}_L\rangle_{L+1} \langle \hat{\Omega}_L|$.
- Matrix elements of $\rho_{\hat{L}}$ are completely determined by the two point correlation functions such as $\langle \vec{S}_1 \cdot \vec{S}_L \rangle$.
- cf) Free fermionic models : correlation matrix $\langle c_i^\dagger c_j \rangle$

subsystem



Relation between EE and correlation functions

Eigenvalues of correlation matrix ($(S+1)^2 \times (S+1)^2$ matrix)

→ **Entanglement entropy**

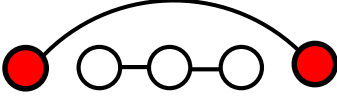
Eigenvalues of $\rho_{\hat{L}}$

The eigenvalues of $\rho_{\hat{L}}$ can be obtained using **transfer matrix**.

$$T_{k,k+1} = \left(\frac{1 - \hat{\Omega}_k \cdot \hat{\Omega}_{k+1}}{2} \right)^S = \frac{4\pi}{S+1} \sum_{l=0}^S \lambda(l) \sum_{m=-l}^l Y_l^m(\hat{\Omega}_k) \overline{Y_l^m(\hat{\Omega}_{k+1})}$$

$$\rho_{\hat{L}}(J) = \frac{4\pi}{(S+1)^2} \sum_{l=0}^S \frac{\lambda(l)^{L-1}}{I_l} \left(\frac{1}{2} J(J+1) - \frac{S}{2} \left(\frac{S}{2} + 1 \right) \right) \xrightarrow{L \rightarrow \infty} \frac{1}{(S+1)^2} \begin{pmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{pmatrix}$$

$$\lambda(l) \equiv (-1)^l S!(S+1)! / [(S-l)!(S+l+1)!]$$

Total spin of the edge spins $J (= 0, 1, 2, \dots, S)$ 

j -th order polynomial $I_j(X)$ $I_0(X) = \frac{1}{4\pi}$, $I_1(X) = \frac{3}{4\pi} \frac{X}{(S/2+1)^2}$, ...

Higher order polynomials are determined by the recursion relation :

$$I_{j+1}(X) = \frac{2j+3}{(S+j+2)^2} \left(\frac{4X}{j+1} + j \right) I_j(X) - \frac{j}{j+1} \cdot \frac{2j+3}{2j-1} \left(\frac{S-j+1}{S+j+2} \right)^2 I_{j-1}(X),$$

Entanglement Entropy

$$\mathcal{S}_L = - \sum_{J=0}^S (2J+1) \rho_{\hat{L}}(J) \log_2 \rho_{\hat{L}}(J) \longrightarrow$$

Saturation value

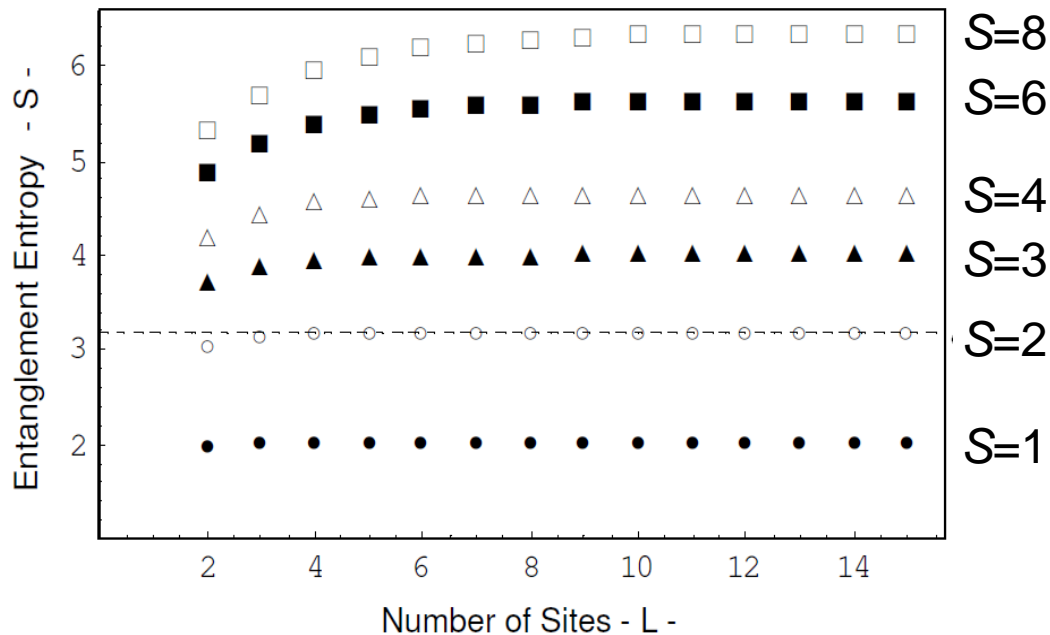
$$2 \log_2 (S+1)$$



Degrees of freedom

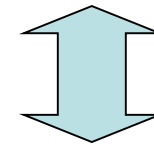
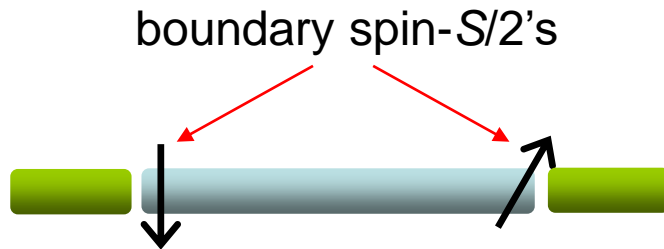
$$(2 \cdot S / 2 + 1)^2 = (S+1)^2$$

One can **exactly** calculate the finite size entanglement entropy by the recursion relation.



Edge State Interpretation and its application

	EE	Boundary spins	Degrees of freedom
1	$2\log_2 2$	Two spin-1/2's	$(2 \cdot 1/2 + 1)^2 = 4$
2	$2\log_2 3$	Two spin-1's	$(2 \cdot 1 + 1)^2 = 9$
S	$2\log_2 (S + 1)$	Two spin- $S/2$'s	$(2 \cdot S/2 + 1)^2 = (S + 1)^2$



Degeneracy (open boundary)
cf) Kennedy triplet + GS

Application of the Edge states

Each edge state behaves as a free spin- $S/2$.

→ This $(S+1)$ -level system can be used as a qubit (qudit)!



Open boundary condition

Numerical Results

- **S=1 Spin Hamiltonian** (J.Phys.Soc.Jpn, **76** (2007) (Hirano and Hatsugai))
- **S=2 Spin Hamiltonian**

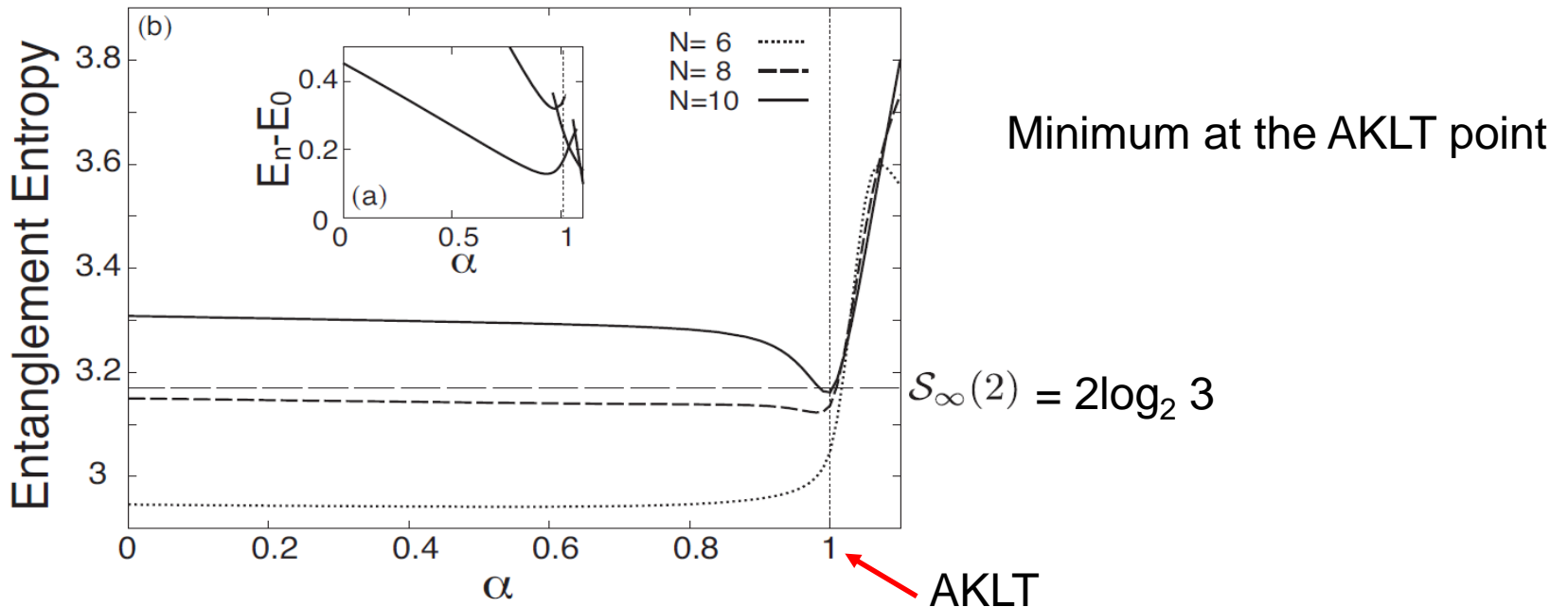
$$H = \sum_{i=1}^N \vec{S}_i \cdot \vec{S}_{i+1} + \alpha \left\{ \frac{2}{9} (\vec{S}_i \cdot \vec{S}_{i+1})^2 + \frac{1}{63} (\vec{S}_i \cdot \vec{S}_{i+1})^3 + \frac{10}{7} \right\},$$

$\alpha = 0$: Heisenberg,

$\alpha = 1$: AKLT

(VBS g.s. is the exact g.s.)

EE from Exact Diagonalization



Summary

- Obtained the exact expression for the EE in VBS states with generic integer-Spin S .
- Confirmed the saturation of the EE in the generic VBS.
- Clarified the relation between the EE and the correlation function
- Proposed a novel application of the edge state as a qubit/qudit for quantum computation.

