The Asymmetric Valence-Bond-Solid States in Quantum Spin Chains

The Difference between Odd and Even Spins

Daisuke Maekawa and Hal Tasaki

webinar @ YouTube / May 2022

illustrations by Kfactory

motivation

Haldane's discovery

Haldane 1981, 1983, 1983

the spin S quantum antiferromagnetic Heisenberg chain

$$\hat{H}_{\mathrm{Heis}} = \sum_{j=1}^{L} \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1}$$

$$(\hat{\boldsymbol{S}}_j)^2 = S(S+1) \qquad S = \tfrac{1}{2}, 1, \tfrac{3}{2}, 2, \ldots$$

the ground state is

critical (unique, gapless) if $S = \frac{1}{2}, \frac{3}{2}, \ldots$

disordered (unique, gapped) if $S = 1, 2, \ldots$

how can we understand this qualitative difference between models with integer and half-odd-integer spins?

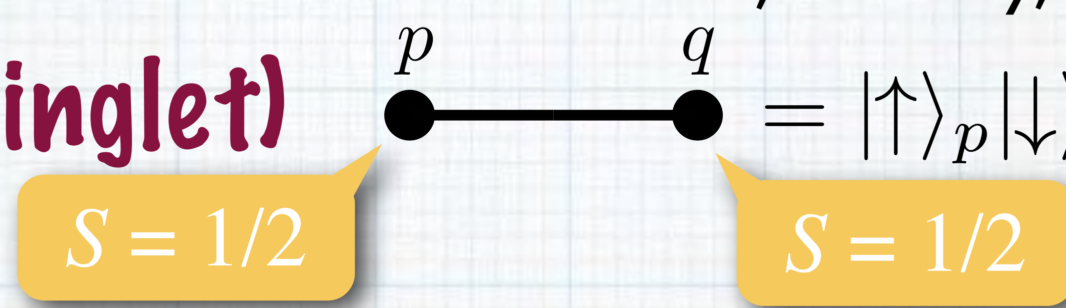
intuitive diagrammatic explanation

valence-bond picture

valence-bond picture

Affleck, Kennedy, Lieb, Tasaki 1987, 1988

valence-bond (spin singlet)

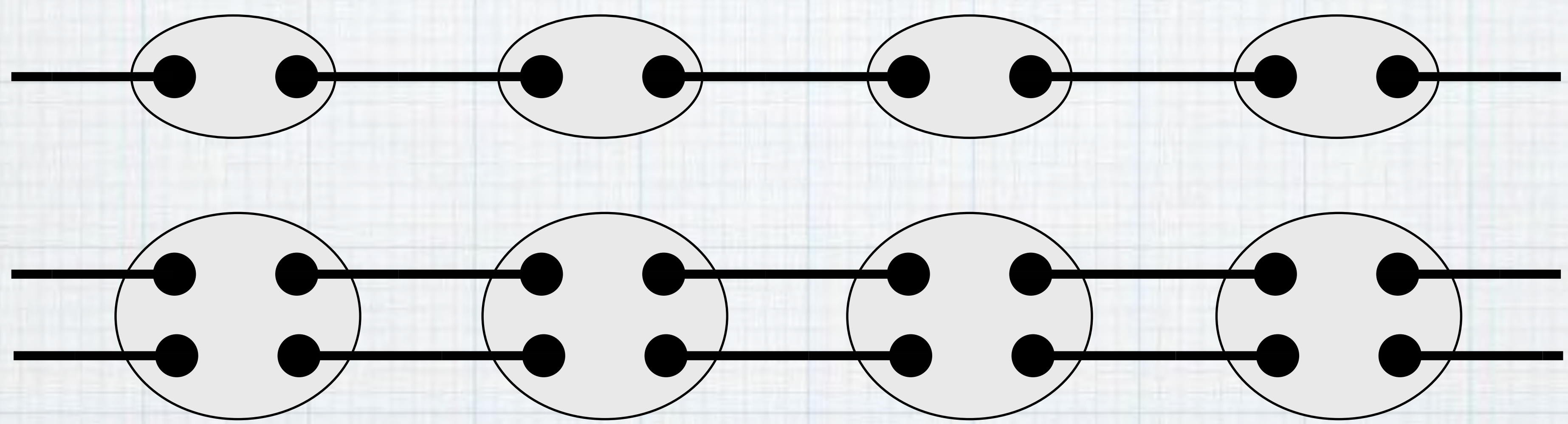


$= |\uparrow\rangle_p |\downarrow\rangle_q - |\downarrow\rangle_p |\uparrow\rangle_q$

can one form a translation-invariant state of a spin S chain from short-ranged valence-bonds?

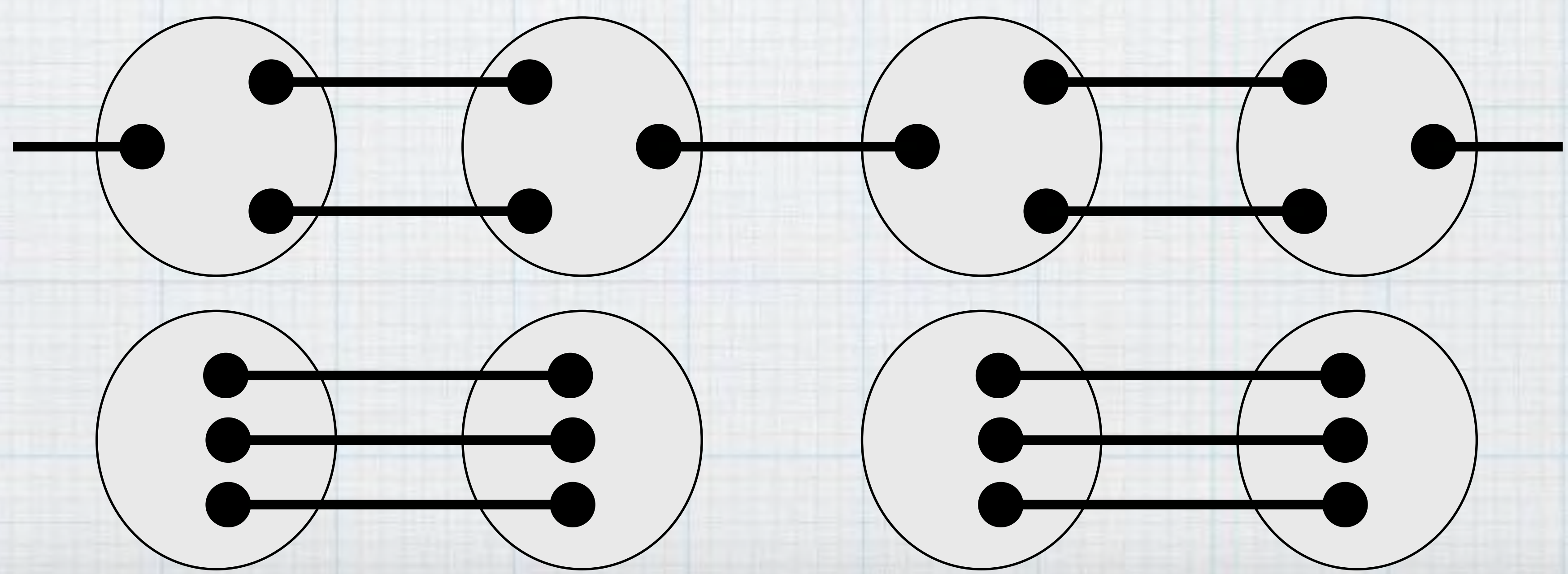
$S = 1$

$S = 2$



yes!

$S = \frac{3}{2}$



no!

the AKLT model and the AKLT state

Affleck, Kennedy, Lieb, Tasaki 1987, 1988

qualitatively similar to the AF Heisenberg chain

an artificial antiferromagnetic model with integer S

$$\hat{H}_{\mathrm{AKLT}} = \sum_{j=1}^{L} \hat{P}_{j,j+1}^{S_{\mathrm{tot}}>S}$$

rigorously known to have a unique gapped ground state

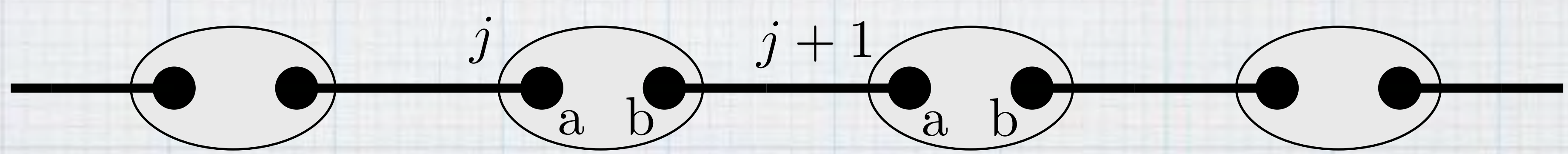
Affleck et al. 1988, Fannes, Nachtergaele, Werner 1992

exact ground state is known

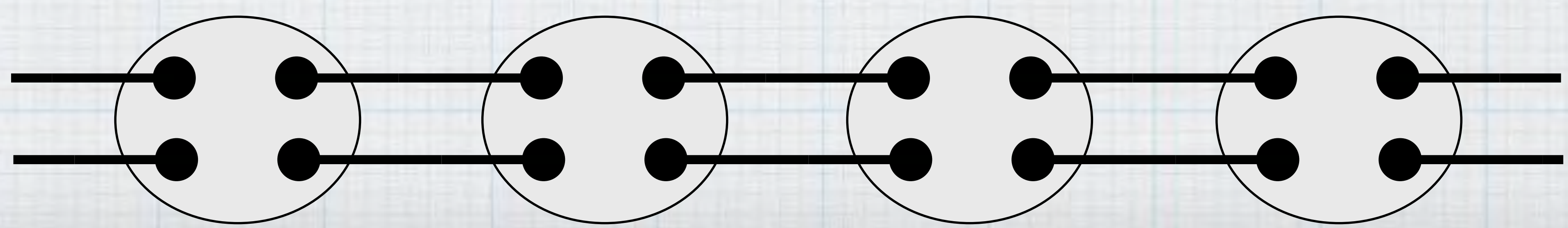
the VBS (valence-bond solid) state or the AKLT state

$S=1$

$$|\Phi_{\mathrm{AKLT}}\rangle = \Bigl(\bigotimes_{j=1}^{L} \hat{\mathcal{S}}_j\Bigr)\Bigl(\bigotimes_{j=1}^{L} \{|{\uparrow}\rangle_{(j,\mathrm{b})}|{\downarrow}\rangle_{(j+1,\mathrm{a})} - |{\downarrow}\rangle_{(j,\mathrm{b})}|{\uparrow}\rangle_{(j+1,\mathrm{a})}\}\Bigr)$$

$=$ 

$S=2$

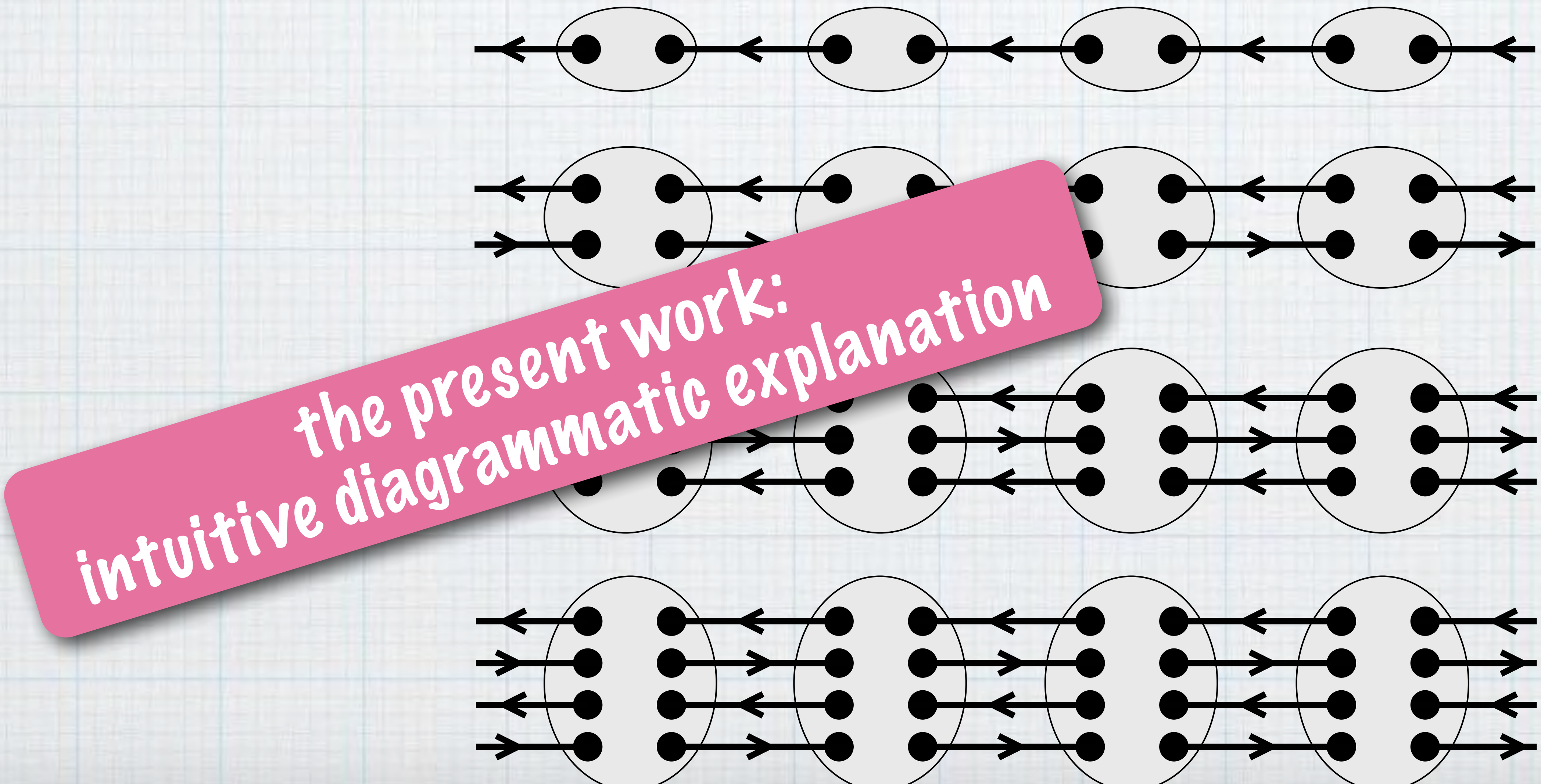
$|\Phi_{\mathrm{AKLT}}\rangle =$ 

further qualitative difference

there is a qualitative difference between the AKLT states with even S and odd S (hidden antiferromagnetic order)

Oshikawa 1992

the difference was finally understood in 2009 when the theory of symmetry protected topological (SPT) phases was developed Gu,Wen 2009, Pollmann, Turner, Berg, Oshikawa 2009



symmetry protected topological (SPT) phases

symmetry protected topological (SPT) phases

Gu, Wen 2009, Pollmann, Turner, Berg, Oshikawa 2010, 2012

chain with spin S

$\mathcal{M}$ space of all Hamiltonians with a disordered ground state

$\hat{H}_0, \hat{H}_1 \in \mathcal{M}$ are connected if there exists a continuous path $\hat{H}_s \in \mathcal{M}$ with $s \in [0,1]$

conjecture: all Hamiltonians in $\mathcal{M}$ are connected

Chen, Gu, Wen 2011

there is only one phase in $\mathcal{M}$

$\mathcal{M}_\Sigma$ space of Hamiltonians in $\mathcal{M}$ with symmetry Σ

$\hat{H}_0, \hat{H}_1 \in \mathcal{M}_\Sigma$ are connected in $\mathcal{M}_\Sigma$ if there exists a continuous path $\hat{H}_s \in \mathcal{M}_\Sigma$ with $s \in [0,1]$

$\mathcal{M}_\Sigma$ may consist of distinct connected components

symmetry protected topological (SPT) phases

symmetry protected topological (SPT) phases

Gu, Wen 2009, Pollmann, Turner, Berg, Oshikawa 2010, 2012

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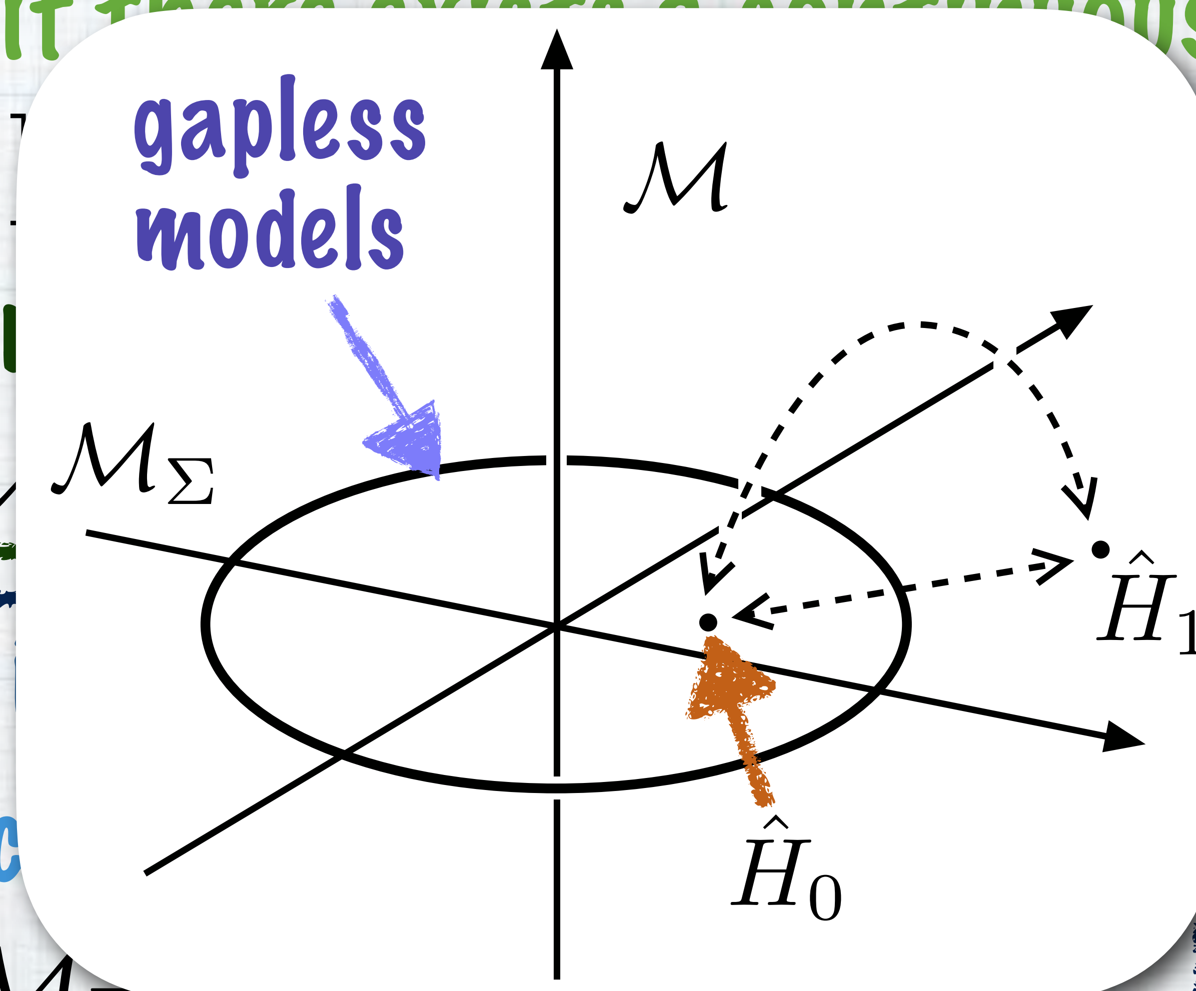


$\mathcal{M}_\Sigma$ space of Hamiltonians

$\hat{H}_0, \hat{H}_1 \in \mathcal{M}_\Sigma$ are connec

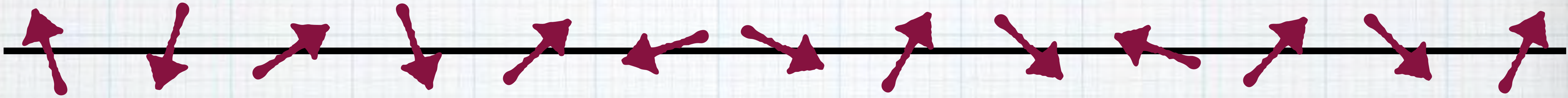
a continuous path $\hat{H}_s \in \mathcal{M}_\Sigma$ with $s \in [0, 1]$

$\mathcal{M}_\Sigma$ may consist of distinct connected components

symmetry protected topological (SPT) phases

SPT phases in spin chains with integer S

Gu, Wen 2009, Pollmann, Turner, Berg, Oshikawa 2010, 2012, Ogata 2020, 2022



theorem

when Σ is $\begin{cases} \text{the bond-centered inversion symmetry} \\ \text{the time-reversal symmetry} \\ \text{the } \mathbb{Z}_2 \times \mathbb{Z}_2 \text{ symmetry} \end{cases}$

$\mathcal{M}_\Sigma$ consists of at least two SPT phases

$\hat{H}_{\mathrm{trivial}} = \sum_{j=1}^{L} (\hat{S}_j^{(\mathrm{z})})^2$ belongs to the trivial phase

disordered ground state $|\Phi_{\mathrm{zero}}\rangle = \bigotimes_{j=1}^{L} |0\rangle_j$

$\hat{H}_{\mathrm{AKLT}}$ belongs to $\begin{cases} \text{a nontrivial phase if } S \text{ is odd} \\ \text{the trivial phase if } S \text{ is even} \end{cases}$

the essence of the difference between odd and even S

intuitive diagrammatic explanation

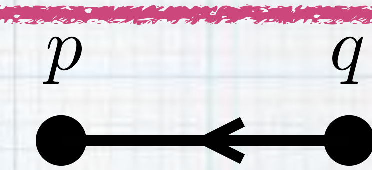
asymmetric VBS states

asymmetric valence-bond

the building block of the asymmetric VBS state

a state of two $S = 1/2$'s parametrized by $\mu \in [0, 1]$

$$|\psi_{p,q}^{(\mu)}\rangle = |\uparrow\rangle_p|\downarrow\rangle_q - \mu\,|\downarrow\rangle_p|\uparrow\rangle_q =$$



not invariant under $\left\{ \begin{array}{l} \text{inversion} \\ \text{time-reversal} \\ \mathbb{Z}_2 \times \mathbb{Z}_2 \text{ transformation} \end{array} \right\}$ if $\mu \neq 1$

inversion transformation

$$\hat{\mathcal{I}}\,|\psi_{p,q}^{(\mu)}\rangle = |\psi_{q,p}^{(\mu)}\rangle =$$

time-reversal transformation

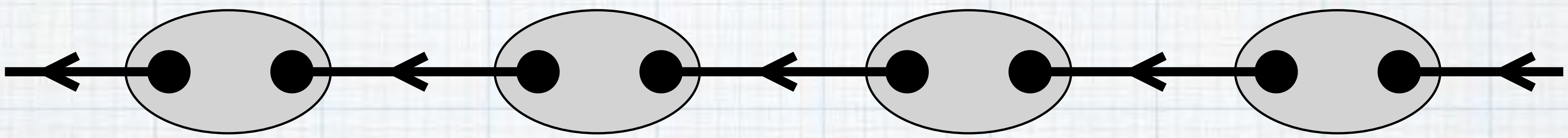
$$\hat{\Theta}|\psi_{p,q}^{(\mu)}\rangle = -|\psi_{q,p}^{(\mu)}\rangle$$

$\mathbb{Z}_2 \times \mathbb{Z}_2$ transformation

$$\hat{U}^{(\mathrm{y})}|\psi_{p,q}^{(\mu)}\rangle = -|\psi_{q,p}^{(\mu)}\rangle, \quad \hat{U}^{(\mathrm{z})}|\psi_{p,q}^{(\mu)}\rangle = |\psi_{p,q}^{(\mu)}\rangle$$

$S = 1$ asymmetric VBS state

$$|\Psi_\mu\rangle = \left(\bigotimes_{j=1}^{L} \hat{\mathcal{S}}_j\right)\left(\bigotimes_{j=1}^{L} |\psi^{(\mu)}_{(j,\mathrm{b}),(j+1,\mathrm{a})}\rangle\right)$$

$=$ 

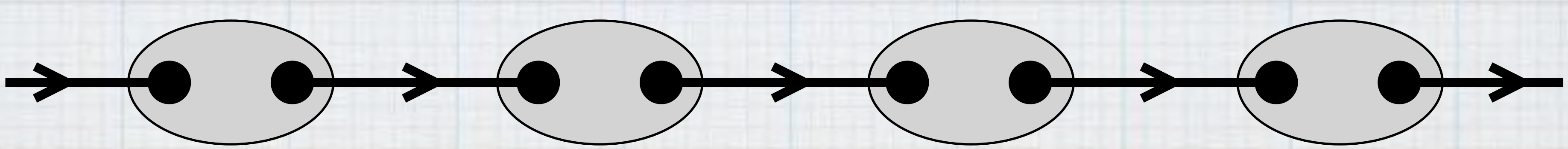
disordered states that continuously interpolate between the AKLT and the zero states

Bachmann, Nachtergaele 2012, 2014

$$|\Psi_1\rangle = |\Phi_{\mathrm{AKLT}}\rangle \qquad |\Psi_0\rangle = |\Phi_{\mathrm{zero}}\rangle$$

there is Hamiltonian $\hat{H}_\mu$ whose unique gaped g.s. is $|\Psi_\mu\rangle$

not invariant under the three transformations

$\hat{\mathcal{I}}\,|\Psi_\mu\rangle =$ 

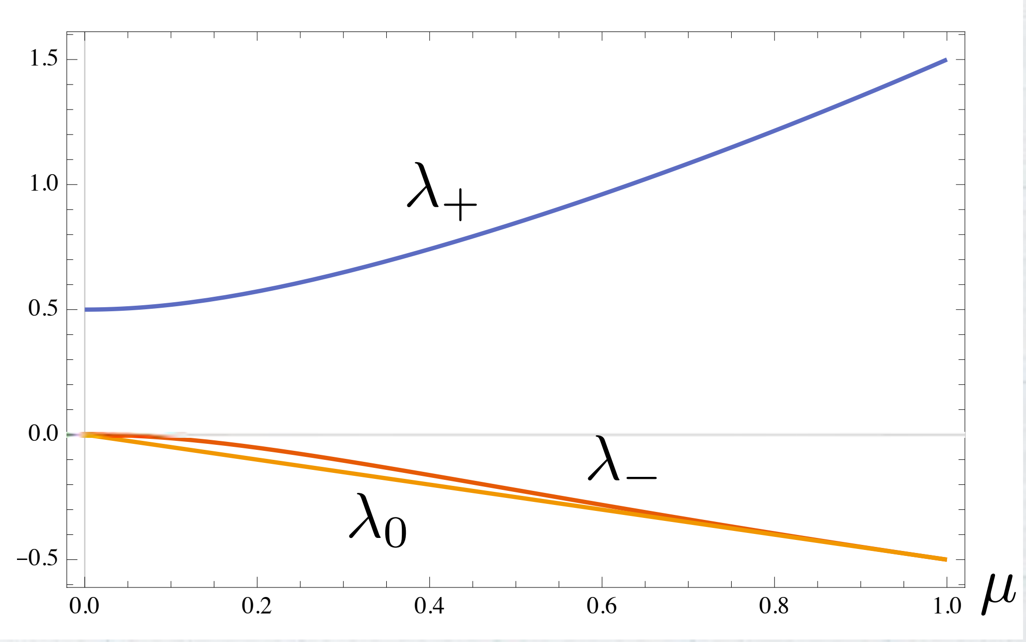
matrix product representation

$$|\Psi_\mu\rangle = \sum_{m_1,\ldots,m_L=-S}^{S} \mathrm{Tr}[\mathsf{A}^{(m_1)}\cdots\mathsf{A}^{(m_L)}]\,|m_1\rangle_1\otimes\cdots\otimes|m_L\rangle_L$$

$$\mathsf{A}^{(1)} = \begin{pmatrix} 0 & 0 \\ -\sqrt{\mu} & 0 \end{pmatrix},\quad \mathsf{A}^{(0)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & -\mu \end{pmatrix},\quad \mathsf{A}^{(-1)} = \begin{pmatrix} 0 & \sqrt{\mu} \\ 0 & 0 \end{pmatrix}$$

$$\mathsf{T} = \begin{pmatrix} \frac{1}{2} & \mu & 0 & 0 \\ \mu & \frac{\mu^2}{2} & 0 & 0 \\ 0 & 0 & -\frac{\mu}{2} & 0 \\ 0 & 0 & 0 & -\frac{\mu}{2} \end{pmatrix}$$

$$\lambda_0 = -\frac{\mu}{2},\qquad \lambda_\pm = \frac{\mu^2+1\pm\sqrt{\mu^4+14\mu^2+1}}{4}$$



$$\langle\,\cdot\,\rangle_\mu = \lim_{L\uparrow\infty}\frac{\langle\Psi_\mu|\cdot|\Psi_\mu\rangle}{\langle\Psi_\mu|\Psi_\mu\rangle}$$

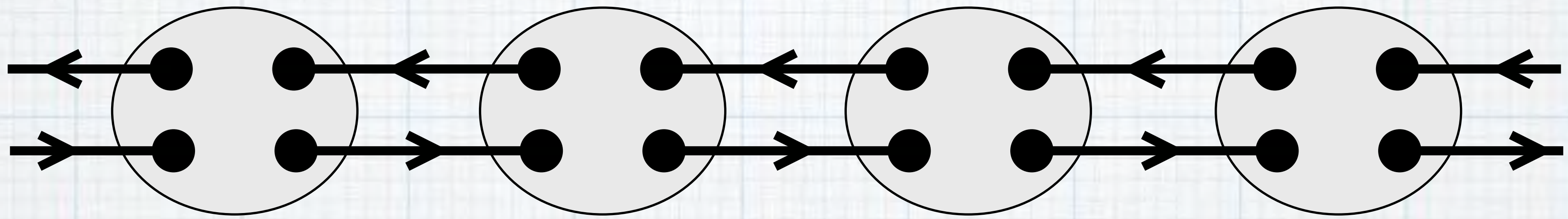
$$\langle\hat{S}_j^{(\mathrm{z})}\,\hat{S}_k^{(\mathrm{z})}\rangle_\mu = \frac{4}{3}\Bigl(\frac{\lambda_-}{\lambda_+}\Bigr)^{|j-k|}$$

$$\langle\hat{S}_j^{(\mathrm{x})}\,\hat{S}_k^{(\mathrm{x})}\rangle_\mu = \langle\hat{S}_j^{(\mathrm{y})}\,\hat{S}_k^{(\mathrm{y})}\rangle_\mu = \frac{(\lambda_+ + \frac{1}{2})(\lambda_+ + \frac{\mu^2}{2})}{2(\lambda_+ - \frac{\mu^2+1}{4})\lambda_+}\Bigl(\frac{\lambda_0}{\lambda_+}\Bigr)^{|j-k|}$$

$S=2$ asymmetric VBS state

$$|\Psi_\mu\rangle = \left(\bigotimes_{j=1}^{L}\hat{S}_j\right)\left(\bigotimes_{j=1}^{L}|\psi^{(\mu)}_{(j,\mathrm{b}),(j+1,\mathrm{a})}\rangle\otimes|\psi^{(\mu)}_{(j+1,\mathrm{c}),(j,\mathrm{d})}\rangle\right)$$

$=$



disordered states that continuously interpolate between the AKLT and the zero states

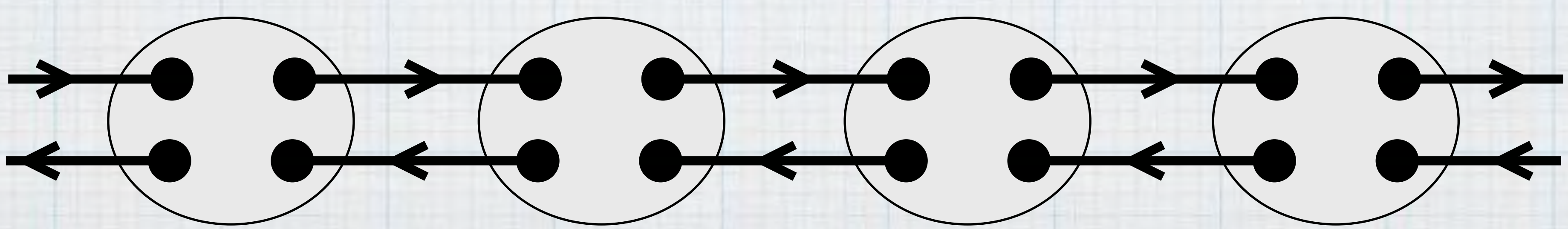
Pollmann, Turner, Berg, Oshikawa 2012

$$|\Psi_1\rangle = |\Phi_{\mathrm{AKLT}}\rangle \qquad |\Psi_0\rangle = |\Phi_{\mathrm{zero}}\rangle$$

there is Hamiltonian $\hat{H}_\mu$ whose unique gaped g.s. is $|\Psi_\mu\rangle$

invariant under the three transformations

$\hat{\mathcal{I}}\,|\Psi_\mu\rangle =$



$= |\Psi_\mu\rangle$

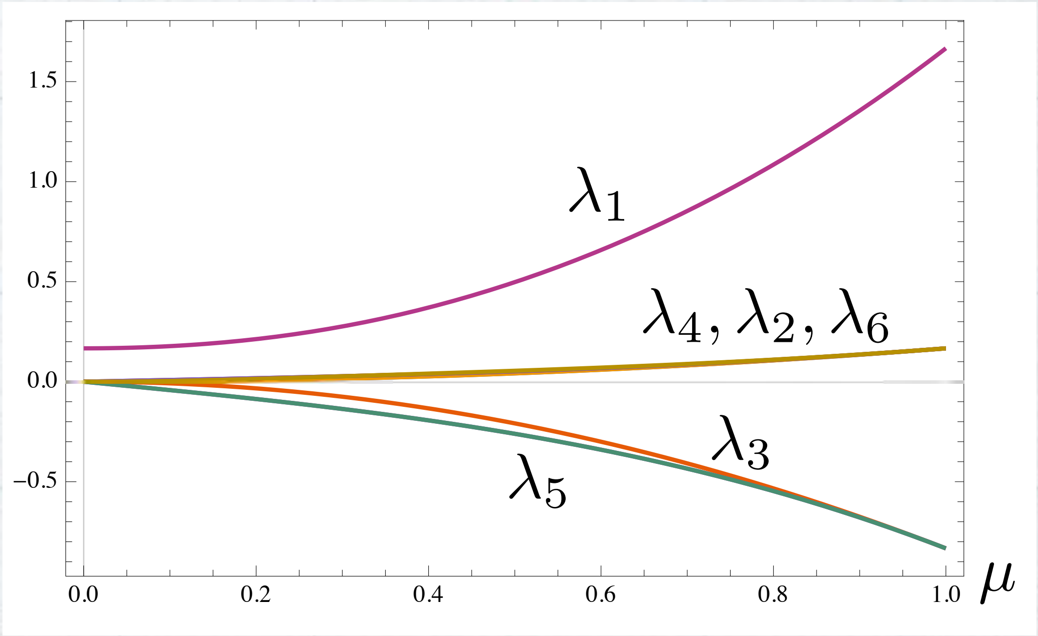
matrix product representation

$$|\Psi_\mu\rangle = \sum_{m_1,\dots,m_L=-S}^{S} \mathrm{Tr}[\mathsf{A}^{(m_1)}\cdots\mathsf{A}^{(m_L)}]\,|m_1\rangle_1\otimes\cdots\otimes|m_L\rangle_L$$

$$\mathsf{A}^{(2)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\mu & 0 & 0 \end{pmatrix}, \quad \mathsf{A}^{(1)} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 \\ \sqrt{\mu(1+\mu^2)} & 0 & 0 \\ 0 & -\sqrt{\mu(1+\mu^2)} & 0 \end{pmatrix}, \quad \mathsf{A}^{(0)} = \frac{1}{\sqrt{6}}\begin{pmatrix} -\mu & 0 & 0 \\ 0 & 1+\mu^2 & 0 \\ 0 & 0 & -\mu \end{pmatrix},$$

$$\mathsf{A}^{(-1)} = \frac{1}{2}\begin{pmatrix} 0 & -\sqrt{\mu(1+\mu^2)} & 0 \\ 0 & 0 & \sqrt{\mu(1+\mu^2)} \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathsf{A}^{(-2)} = \begin{pmatrix} 0 & 0 & -\mu \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\mathsf{T} = \begin{pmatrix}
\frac{\mu^2}{6} & \frac{\mu(1+\mu^2)}{4} & \mu^2 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{\mu(1+\mu^2)}{4} & \frac{(1+\mu^2)^2}{6} & \frac{\mu(1+\mu^2)}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\
\mu^2 & \frac{\mu(1+\mu^2)}{4} & \frac{\mu^2}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -\frac{\mu(1+\mu^2)}{6} & -\frac{\mu(1+\mu^2)}{4} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -\frac{\mu(1+\mu^2)}{4} & -\frac{\mu(1+\mu^2)}{6} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\frac{\mu(1+\mu^2)}{6} & -\frac{\mu(1+\mu^2)}{4} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\frac{\mu(1+\mu^2)}{4} & -\frac{\mu(1+\mu^2)}{6} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\mu^2}{6} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\mu^2}{6}
\end{pmatrix}$$



$$\lambda_1 = \tfrac{1}{12}\{1+9\mu^2+\mu^4+\sqrt{1+8\mu^2+63\mu^4+8\mu^6+\mu^8}\},$$

$$\lambda_2 = \tfrac{1}{12}\{1+9\mu^2+\mu^4-\sqrt{1+8\mu^2+63\mu^4+8\mu^6+\mu^8}\}, \quad \lambda_3 = -5\mu^2/6,$$

$$\lambda_4 = \tfrac{1}{12}\mu(1+\mu^2), \quad \lambda_5 = -\tfrac{5}{12}\mu(1+\mu^2), \quad \lambda_6 = \mu^2/6,$$

asymmetric VBS state and SPT phases

disordered states that continuously interpolate between the AKLT state and the trivial zero state

there is Hamiltonian $\hat{H}_\mu$ whose unique gaped g.s. is $|\Psi_\mu\rangle$

$|\Psi_\mu\rangle$ and $\hat{H}_\mu$ are invariant under the three transformations for $S=2$, but not for $S=1$

$S=1$

$\hat{H}_{\mathrm{AKLT}}$ belongs to a nontrivial SPT phase

$\hat{H}_{\mathrm{AKLT}}$ and $\hat{H}_{\mathrm{trival}}$ are $\begin{cases}\text{connected within } \mathcal{M} \\ \text{not connected within } \mathcal{M}_\Sigma\end{cases}$

$S=2$

$\hat{H}_{\mathrm{AKLT}}$ belongs to the trivial SPT phase

$\hat{H}_{\mathrm{AKLT}}$ and $\hat{H}_{\mathrm{trival}}$ are connected within $\mathcal{M}_\Sigma$

the difference between odd and even S

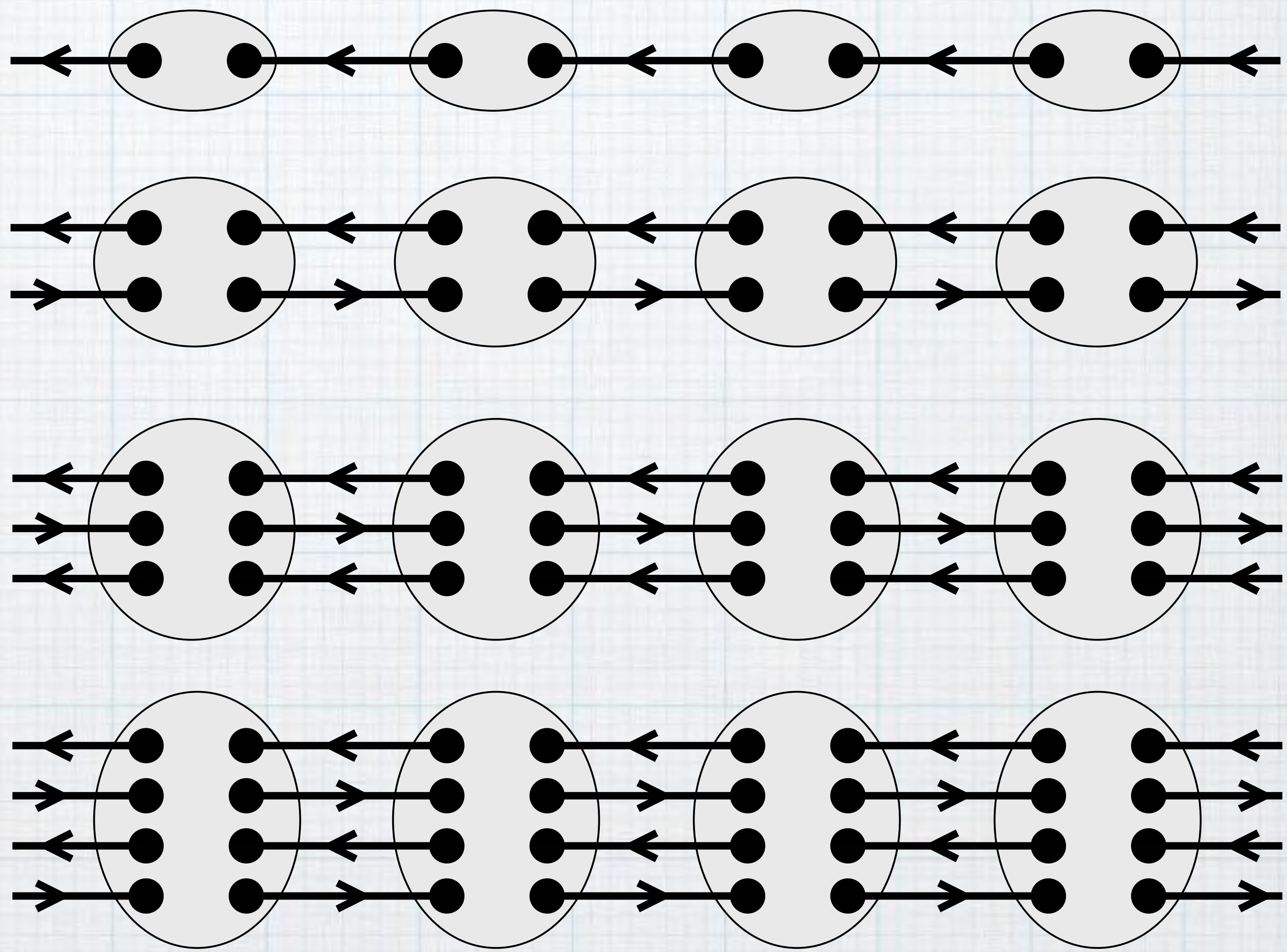
the asymmetric VBS state is invariant under the three transformations if the arrows on every pair of neighboring sites cancel

$S = 1$

$S = 2$

$S = 3$

$S = 4$



invariant state is possible only for even S

summary

- we defined the asymmetric VBS state, which interpolates between the AKLT and the zero states
- the asymmetric VBS state has all the three symmetries relevant to the SPT phases for $S = 2$, but has none of the symmetries for $S = 1$
- these observations are consistent with the theory of SPT phases in quantum spin chains, and provide us with an intuitive explanation of the difference between odd and even S
- if we had come up with this idea in 1992 ....

illustrations by Kfactory and Naruse Chisato