Part 2

"Quantum spin liquid" in the ground states of low dimensional quantum spin systems

Haldane gap / for S=1 AF chains

and the VBS state

⟨Haldane conjecture and related results⟩

$d=1$ (almost throughout the present part)

§ Haldane conjecture

Heisenberg AF chain $\hat{H}=\sum_{x=1}^{L}\hat{\mathbf{S}}_x\cdot\hat{\mathbf{S}}_{x+1}$ $(\hat{\mathbf{S}}_{L+1}=\hat{\mathbf{S}}_1)$

$(S=\frac{1}{2},1,\frac{3}{2},\cdots)$ (L even)

(Marshll-Lreb-Mattis theorem
→ the g.s. is unique for finite L.)

$\boxed{S=\frac{1}{2}}$ Common beliefs based on the Bethe ansatz solution (1931)

i) the g.s. is unique (also for $L\uparrow\infty$) → NO LRO or SSB

ii) no energy gap above the g.s. energy $\equiv$ $E_{1st}-E_{GS}\doteqdot O(\frac{1}{L})$

iii) the g.s. correlation funct. decays by a power law as

$$\langle\Phi_{GS},\hat{\mathbf{S}}_x\cdot\hat{\mathbf{S}}_y\,\Phi_{GS}\rangle\approx(-1)^{x-y}|x-y|^{-1}$$

Haldan 1983

- non-linear σ-model with a topological term
- sem-classical quantization of solitons

large S limit

$S=\frac{1}{2}, \frac{3}{2}, \cdots$ half-odd-integer spins

i)
ii)
iii)

as in $S=\frac{1}{2}$

$S=1,2,3,\cdots$ integer spins

i)' the g.s. is unique (also for $L\uparrow\infty$) → No LRO or SSB

ii)' ∃ a nonvanishing energy gap above the g.s energy

Haldane gap ($\Delta E \simeq 2Se^{-\pi S}$) $\updownarrow O(1)$

iii)' the g.s. correlation function decays exponentially

$$\langle \Phi_{GS}, \hat{S}_x \cdot \hat{S}_y \Phi_{GS} \rangle \simeq (-1)^{x-y} \exp\left[-\frac{|x-y|}{3}\right]$$

disordered (massive) behavior at $T=0$

strong "quantum fluctuation"

at least in mid 80's

Surprising points of the conjecture

- a drastic difference between the systems with half-odd-integer S and integer S

- it is natural that a one-dim. system with a continuous symmetry has low-energy excitations.

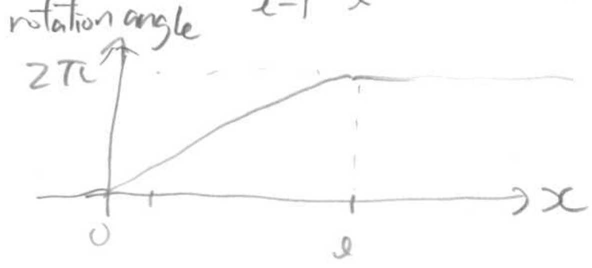
see the next section

Rem

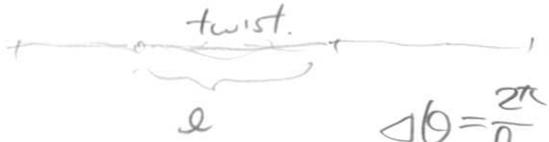
(i') + ii') $\Rightarrow$ iii') was finally proved by Hastings and Koma 2006

§ Theorem which rules out "unique g.s. + gap"

twist operator $\hat{U}_\ell = \exp\left[i \sum_{x=1}^{\ell} \frac{2\pi x}{\ell} \hat{S}_x^{(3)} \right]$ $\qquad \ell < L$



$\Psi = \hat{U}_\ell \Phi_{GS}$



$\Delta\theta = \frac{2\pi}{\ell}$

$$\langle \Psi, \hat{H} \Psi \rangle - E_{GS} = \ell \cdot O((\Delta\theta)^2) = O\left(\frac{1}{\ell}\right)$$

always gapless ?!

One can prove $\langle \Phi_{GS}, \Psi \rangle = 0$ only for $S = \frac{1}{2}, \frac{3}{2}, \cdots$

Theorem (Lieb-Schultz-Mattis 1961, Affleck-Lieb 1986)

For $S = \frac{1}{2}, \frac{3}{2}, \cdots$ "unique g.s. + gap" is impossible.

No information for $S = 1, 2, \cdots$

generalization

(Yamanaka-Oshikawa-Affleck 1997)

DATE

§ Semi-classical approach

$$\hat{H} = \underbrace{\overset{\text{classical (Ising)}}{\sum_{x=1}^{L} \hat{S}^{(3)}_x \hat{S}^{(3)}_{x+1}}}_{\hat{H}_c} + \underbrace{\overset{\text{"quantum"}}{\frac{1}{2}\sum_{x=1}^{L}\left\{ \hat{S}^{+}_x \hat{S}^{-}_{x+1} + \hat{S}^{-}_x \hat{S}^{+}_{x+1} \right\}}}_{\hat{H}_Q}$$

treat as "perturbation"

<u>$S=\frac{1}{2}$</u> G.S. of $\hat{H}_c$

↑ ↓ ↑ ↓ ↑ ↓ ↑ ↓

$\hat{S}^+\hat{S}^-$

↑ ↓ ↑ ↑ ↓ ↓ ↑ ↓

$\hat{S}^+\hat{S}^-$

↑ ↓ ↑ ↑ ↓ ↑ ↓ ↓

- <u>pair creation</u> of kinks
- kinks <u>hop</u> by twice the lattice spacing

also <u>pair annihilation</u>.

Note that there are <u>two kinds of kinks</u> → even, odd

different kinds of kinks never pair-annihilate

↑ ↓ ↑ ↑ ↓ ↑ ↑ ↓ ↑

↑ ↓ ↑ ↑ ↑ ↓ ↑ ↓ ↑

noway!!

$\underline{S=1}$ GS of $\hat{H}_c$

$+ - + - + - + -$

$\hat{S}^- \hat{S}^+$

$+ - 0\ 0 + - + -$ <u>pair creation</u> of kinks (0's)

$S^+ S^-$

$+ - 0 + 0 - + -$ kinks <u>hop</u> by a single lattice spacing

$S^- S^+$

$+ - 0 + - 0 + -$

- <u>only one kind of kinks</u>, pairly created and annihilated.

⇑

$\boxed{\text{essential difference from the } S=\tfrac{1}{2} \text{ case}}$

- This construction generates only special states like

$+ 0 - + - 0 0 + 0 - + 0 - 0 + \cdots$

+ and − alternate with arbitrary number of 0's in between them. → (hidden AF order)

$\tilde{\mathcal{H}}$: restricted Hilbert space generated by these basis states

<u>Theorem</u> (Tasaki '86 unpublished)

The Heisenberg AF on $\tilde{\mathcal{H}}$ has a unique g.s. with a gap and exponentially decaying correlation function

<AKLT model and the VBS picture>

§ AKLT model for $S=1$

$S=1$ (AF) chain with

$$\hat{H}_{AKLT} = \sum_{x=1}^{L} \left\{ \hat{\mathbf{S}}_x \cdot \hat{\mathbf{S}}_{x+1} + \frac{1}{3}\left(\hat{\mathbf{S}}_x \cdot \hat{\mathbf{S}}_{x+1}\right)^2 \right\}$$

still AF, and $SU(2)$ invariant

<u>Theorem</u> (Affleck-Kennedy-Lieb-Tasaki 1987)

- The g.s. is unique (for finite and infinite L)
- $\exists$ a nonvanishing energy gap (uniform in L)
- $\langle \Phi_{GS}, \hat{\mathbf{S}}_x \cdot \hat{\mathbf{S}}_y \Phi_{GS} \rangle = (-1)^{|x-y|} \, 4 \cdot 3^{-|x-y|}$ $\quad (|x-y| \geq 2)$

strong support to the Haldane conjecture

$\rightarrow$ <u>BUT NOT A PROOF !!</u>

a stability theorem (very difficult but important)

<u>Theorem</u> (Yarotsky 2006)

$\hat{V}$: any short ranged translation invariant interaction

$\hat{H} = \hat{H}_{AKLT} + \varepsilon \hat{V}$ For suff. small ε,

the g.s. is unique, $\exists$ a gap, exp. decay.

§VBS (valence-bond-solid) state

exact g.s. of the AKLT model

$$\hat{\mathbb{S}}_x \cdot \hat{\mathbb{S}}_{x+1} + \frac{1}{3}(\hat{\mathbb{S}}_x \cdot \hat{\mathbb{S}}_{x+1})^2 = 2\hat{P}_2(\hat{\mathbb{S}}_x + \hat{\mathbb{S}}_{x+1}) - \frac{2}{3}$$

the e.v. of $(\hat{\mathbb{S}}_x + \hat{\mathbb{S}}_{x+1})^2 \to S'(S'+1)$ with $S'=0, 1, 2$.

$\hat{P}_2$: the proj. onto the space with $S'=2$

$\hat{H}_{AKLT}$ is essentially the same as

$$\hat{H}'_{AKLT} = \sum_{x=1}^{L-1} \hat{P}_2(\hat{\mathbb{S}}_x + \hat{\mathbb{S}}_{x+1})$$

We shall construct Φ_{VBS} s.t. $\hat{P}_2(\hat{\mathbb{S}}_x + \hat{\mathbb{S}}_{+1})\,\Phi_{VBS} = 0$ for $\forall x$.

Then it is a g.s. of $\hat{H}'_{AKLT}$ (and $\hat{H}_{AKLT}$)

Construction of the VBS state

- two $S=\frac{1}{2}$'s. $\quad$ L $\uparrow$ $\quad$ R $\downarrow$ $\qquad \psi_L^{\sigma} \otimes \psi_R^{\sigma'} \qquad \sigma, \sigma' = \uparrow, \downarrow$

$$\hat{\mathcal{S}}\left(\psi_L^{\sigma} \otimes \psi_R^{\sigma'}\right) = \underbrace{\frac{1}{2}\left\{\psi_L^{\sigma} \otimes \psi_R^{\sigma'} + \psi_L^{\sigma'} \otimes \psi_R^{\sigma}\right\}}_{\text{total spin } 1.}$$

$\hat{\mathcal{S}}$ → symmetrization

→ projection op. onto the supspace with $S_{tot}=1$.

- duplicated chain. with sites $(x,L), (x,R)$ $\quad x=1,\cdots,L$

put $S=\frac{1}{2}$'s on each site

$$\Phi_{\text{pre-VBS}} := \bigotimes_{x=1}^{L} \underbrace{\frac{1}{\sqrt{2}}\left\{\psi_{x,R}^{\uparrow} \otimes \psi_{x+1,L}^{\downarrow} - \psi_{x,R}^{\downarrow} \otimes \psi_{x+1,L}^{\uparrow}\right\}}$$

→ singlet pair = valence-bond

a state for $2L$ spin $\frac{1}{2}$'s.

$\Phi_{\mathrm{VBS}} := \left(\bigotimes_x \hat{\mathcal{S}}_x\right) \Phi_{\text{pre-VBS}}$

valence-bond solid state

a state for the $S=1$ chain.

$S=1$

BUT note that

$$\hat{P}_2(\hat{\mathbf{S}}_x+\hat{\mathbf{S}}_{x+1})\,\Phi_{\mathrm{VBS}} = \hat{P}_2(\hat{\mathbf{S}}_x+\hat{\mathbf{S}}_{x+1})\left(\bigotimes_x \hat{\mathcal{S}}_x\right)\Phi_{\text{pre-VBS}}$$

$$= \left(\bigotimes_x \mathcal{S}_x\right) \underbrace{\hat{P}_2(\hat{\mathbf{S}}_{x,L}+\hat{\mathbf{S}}_{x,R}+\hat{\mathbf{S}}_{x+1,L}+\hat{\mathbf{S}}_{x+1,R})\,\Phi_{\text{pre-VBS}}}_{=\,0}$$

singlet!

Φ_{VBS} is an exact g.s. of $\hat{H}_{\mathrm{AKLT}}$

the theorem is proved based on the exact g.s. and the special properties of the model

gap : a simpler proof Knabe 88

$\downarrow$

(general theory Fannes, Nachtergaele, Werner 92)

SKIP

§ Proof of the eristence of a gap (Knabe, 1988)

When $E_{GS}=0$, gap $\geq \varepsilon \iff \hat{H}^2 \geq \varepsilon \hat{H}$

show this

Write $\hat{P}_x = \hat{P}_2(\hat{S}_x + \hat{S}_{x+1})$

note $\hat{P}_x \hat{P}_y \geq 0$ unless $|x-y|=1$

$$\hat{H} = \sum_{x=1}^{L} \hat{P}_x \quad (\text{pbc})$$

fix $n \geq 2$, and let $\hat{h}_x = \sum_{y=x}^{x+n-1} \hat{P}_x$

then

$$\sum_{x=1}^{L} (\hat{h}_x)^2 = n \sum_{x=1}^{L} \hat{P}_x + (n-1) \sum_{|x-y|=1} \hat{P}_x \hat{P}_y + (n-2) \sum_{|x-y|=2} \hat{P}_x \hat{P}_y + \cdots + \sum_{|x-y|=n-1} \hat{P}_x \hat{P}_y$$

$$\leq n \sum_{x=1}^{L} \hat{P}_x + (n-1) \sum_{x \neq y} \hat{P}_x \hat{P}_y$$

$$= \underbrace{\sum_{x=1}^{L} \hat{P}_x}_{= \hat{H}} + (n-1) \hat{H}^2.$$

$$\therefore \hat{H}^2 \geq -\frac{1}{n-1} \hat{H} + \frac{1}{n-1} \sum_{x=1}^{L} (\hat{h}_x)^2$$

use $(\hat{h}_n)^2 \geq \varepsilon_n \hat{h}_n$ ($\overset{>0}{\varepsilon_n}$: the gap of $\hat{h}_x$)

SKIP

$$\hat{H}^2 \geq -\frac{1}{n-1}\hat{H} + \frac{1}{n-1}\varepsilon_n \underbrace{\sum_{x=1}^{L}\hat{h}_x}_{=n\hat{H}}$$

$$= \frac{n}{n-1}\left(\varepsilon_n - \frac{1}{n}\right)\hat{H}$$

So $\hat{H}$ has a nonvanishing gap (indep. of L)

if $\varepsilon_n - \frac{1}{n} > 0$ for some n

check numerically.

VBS-1 **

Extend the method of Knabe J. Stat. Phys. 52, 627-638 (1988) to prove the existence of a nonvanishing gap of the Majumdar-Ghosh model

$S=1/2$ periodic chain with L even

$$H_{MG} = \sum_{x=1}^{L}\left\{\hat{\mathbf{S}}_x\cdot\hat{\mathbf{S}}_{x+1} + \frac{1}{2}\hat{\mathbf{S}}_x\cdot\hat{\mathbf{S}}_{x+2}\right\}$$

See also Section 5 of AKLT 88.

§VBS state in the standard basis — hidden AF order

o——o = (↑—↓) − (↓—↑)

Φ_{VBS} is a sum of many basis states

—↓↑—↓↓—↑↓—↑↑—↓↑—↓↑—↓↓—↑↑—

0 − 0 + 0 0 − + ...

+ and − alternate with arbitrary numbers of 0's in between them!

$$\Phi_{VBS} = \sum_{\sigma}{}' (-1)^{z(\sigma)} \, 2^{n(\sigma)/2} \, \Psi^{\sigma}$$

satisfies the constraint

$z(\sigma)$ the number of 0's on odd sites
$n(\sigma)$ the number of $\pm$'s.

· "quantum spin liquid" with hidden AF order

· one gets exactly the same expansion whatever "quantization axis" is taken.

standard AF order → appears in a specific direction

hidden AF order → appears in any directions!

(rem. $\mathcal{S}(\uparrow\uparrow) = \psi^{+}$ $\quad \mathcal{S}(\downarrow\downarrow) = \psi^{-}$

$\mathcal{S}(\uparrow\downarrow) = \frac{1}{2}(\uparrow\downarrow + \downarrow\uparrow) = \frac{1}{\sqrt{2}}\psi^{0}$)

the complicated coefficient with ~~a~~ the long range constraint can be expressed using matrix products.

Fannes, Nachtergaele, Werner 89. 92

Klümper, Schadschneider, Zittarz 91

$$\Phi_{VBS} = \sum_{\sigma} \mathrm{Tr}[A_{\sigma_1} A_{\sigma_2} \cdots A_{\sigma_n}]\, \Psi^{\sigma} \quad \text{—} \circledast$$

no constranits $A_+ = \begin{pmatrix} 0 & 0 \\ -\sqrt{2} & 0 \end{pmatrix}, A_- = \begin{pmatrix} 0 & \sqrt{2} \\ 0 & 0 \end{pmatrix}, A_0 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

Finitely correlate states
Matrix product states (MPS)

very general but still very special!

VBS-2

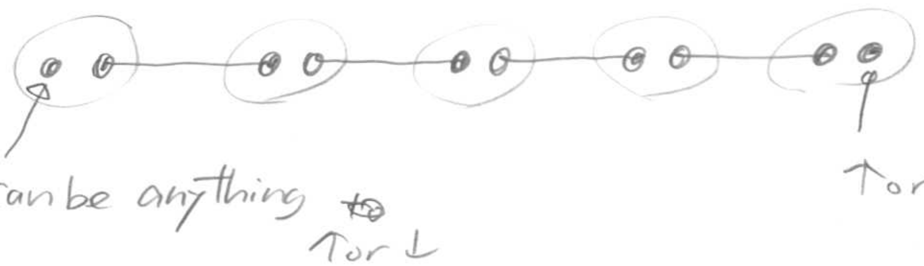
Confirm $\circledast$ (starting from the def. of VBS)

Find a similar expression for the $S=\frac{3}{2}$ state

§ VBS states open chains — edge states

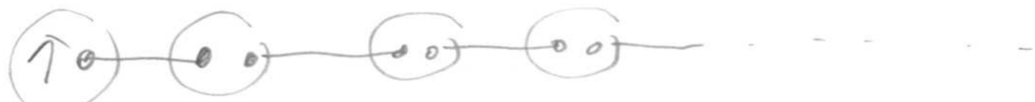
AKLT model on periodic chain, infinite chain
→ the <u>g.s. is unique</u>.

on open chain



There are four ground states

~~Semi-infinite~~ long chain with extra ↑

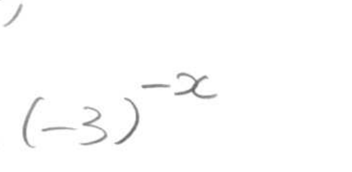
$\Phi'_{VBS} =$ 

the edge spin is not completely localized

$$\langle \Phi'_{VBS}, \hat{S}^{(1)}_x \Phi'_{VBS} \rangle = \langle \Phi'_{VBS}, \hat{S}^{(2)}_x \Phi'_{VBS} \rangle = 0$$

$$\langle \Phi'_{VBS}, \hat{S}^{(3)}_x \Phi'_{VBS} \rangle = -2(-3)^{-x}$$

$$\sum_{x=1}^{\infty} \langle \quad \downarrow \quad \rangle = \frac{1}{2}.$$



$$\Lambda_L = \{-\tfrac{L}{2}+1, -\tfrac{L}{2}+2, \cdots, \tfrac{L}{2}\}$$

$\downarrow$

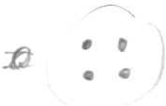
the four g.s. converges to a single inf. vol gr. st. as $L \uparrow \infty$

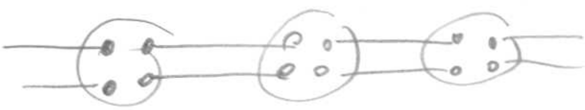
recall that

	finite. L	$L \uparrow \infty$
Heisenberg AF $d \geq 2$	unique g.s.	infinitely many g.s.
AKLT open chain	four g.s.	unique g.s

§ VBS picture

Can we form VBS states for other S ?

$S=2$  four $S=\frac{1}{2}$'s



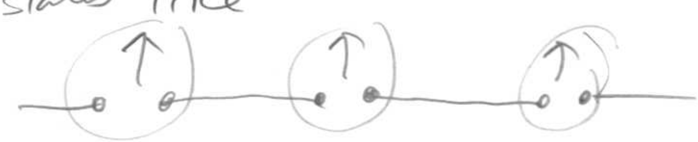
$S=\frac{3}{2}$  three $S=\frac{1}{2}$'s

translation inv. is broken.

We can construct translation invariant VBS only for integer S.

Skip

BUT under magnetic field one may have a g.s. states like



for $S=\frac{3}{2}$ chain VBS like state

here $S^{(3)}_{Tot} = \frac{L}{2}$

YOA filling factor is $\nu = \frac{1}{2} + \frac{3}{2} = \underset{\text{integer!}}{2}$

<Haldane phase>

§ Haldane conj. for the $S=1$ Heisenberg AF chain

$$\hat{H} = \sum_{x=1}^{L} \hat{\mathbf{S}}_x \cdot \hat{\mathbf{S}}_{x+1}$$

numerical results → gap is also observed experimentally!

- $\exists$ a gap $\simeq 0.41$ above the unique g.s.
- correlation in g.s. decays exponentially

BUT STILL NO PROOF → AKLT is at the "center" of the "Haldane phase", and the Heisenberg AF happens to belong to that phase ? ? ?

§. The model with anisotropy

$S=1$ chain (pbc)

$$\hat{H}_{aniso} = \sum_{x=1}^{L} \{ \hat{\mathbf{S}}_x \cdot \hat{\mathbf{S}}_{x+1} + \underbrace{D(\hat{S}_x^{(3)})^2}_{\text{anisotropy}} \} \qquad D \geq 0$$

note that

$$\hat{H}_0 = \sum_{x=1}^{L} D(\hat{S}_x^{(3)})^2 \quad \text{is trivial}$$

G.S. $\Phi_0 = \bigotimes_{x=1}^{L} \psi_x^0$ $\qquad$ 0 0 0 0 0 0 0

$E_0 = 0$

1st excited $\qquad$ 0 0 0 + 0 0 0 $\quad$ or $\quad$ 0 0 0 − 0 0 0

$E_{1st} = E_0 + D$ ← energy gap

if $D \gg 1$

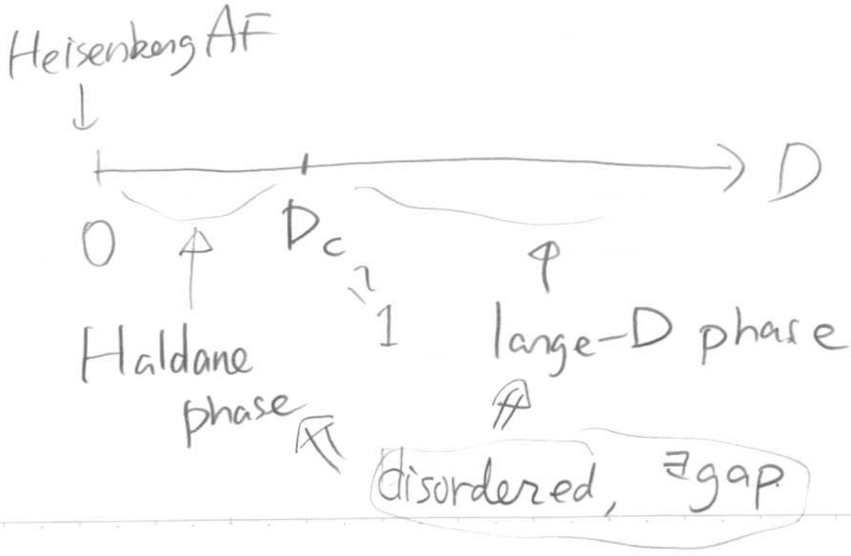
- The g.s. is unique and is close to Φ_0
- $\exists$ a gap $\simeq D$
- The g.s. correlation decays exponentially

all rigorous and trivial
(cluster expansion)

Is the Haldane gap smoothly connected to this trivial gap?

numerical results

gapless point?



§ Peculiar features of the Haldane phase

Hidden AF order

The g.s. of $\hat{H}_{\mathrm{aniso}}$ $\quad \Phi_{GS} = \sum_{\sigma} C_\sigma \tilde{\Psi}^\sigma$

$C_\sigma > 0$ for $\forall \sigma$ (Marshall-Lieb-Mattis)

(different from the VBS state)

BUT in the Haldane phase most states (with considerable weight) look like

$$+\ 0\ -\ +\ -\ 0\ 0\ \underbrace{-\ 0\ +}_{\text{defect}}\ 0\ +\ 0\ -\ +\ -$$

the long-range hidden AF order still presents

$$\underset{\substack{\uparrow\\ \text{even}}}{+}\ -\ +\ -\ \underbrace{-\ +}\ +\ -\ \underset{\substack{\uparrow\\ \text{even}}}{+}\ -\ +$$

den Nijs - Rommelse string order parameter 1989

$$O^{(\alpha)}_{\mathrm{string}} := -\lim_{|x-y|\uparrow\infty} \lim_{L\uparrow\infty} \langle \Phi_{GS}, \hat{S}^{(\alpha)}_x \underbrace{\exp\Big[i\pi \sum_{z=x+1}^{y-1} \hat{S}^{(\alpha)}_z\Big]}_{\parallel \ (-1)^{\sum \hat{S}^{(\alpha)}_z}} \hat{S}^{(\alpha)}_y \Phi_{GS} \rangle$$

$\alpha = 1, 2, 3$

for the VBS state $O^{(\alpha)}_{string} = \frac{4}{9}$ $\alpha = 1, 2, 3.$

heuristic arguments
+ numerical res. for $\hat{H}_{aniso}$

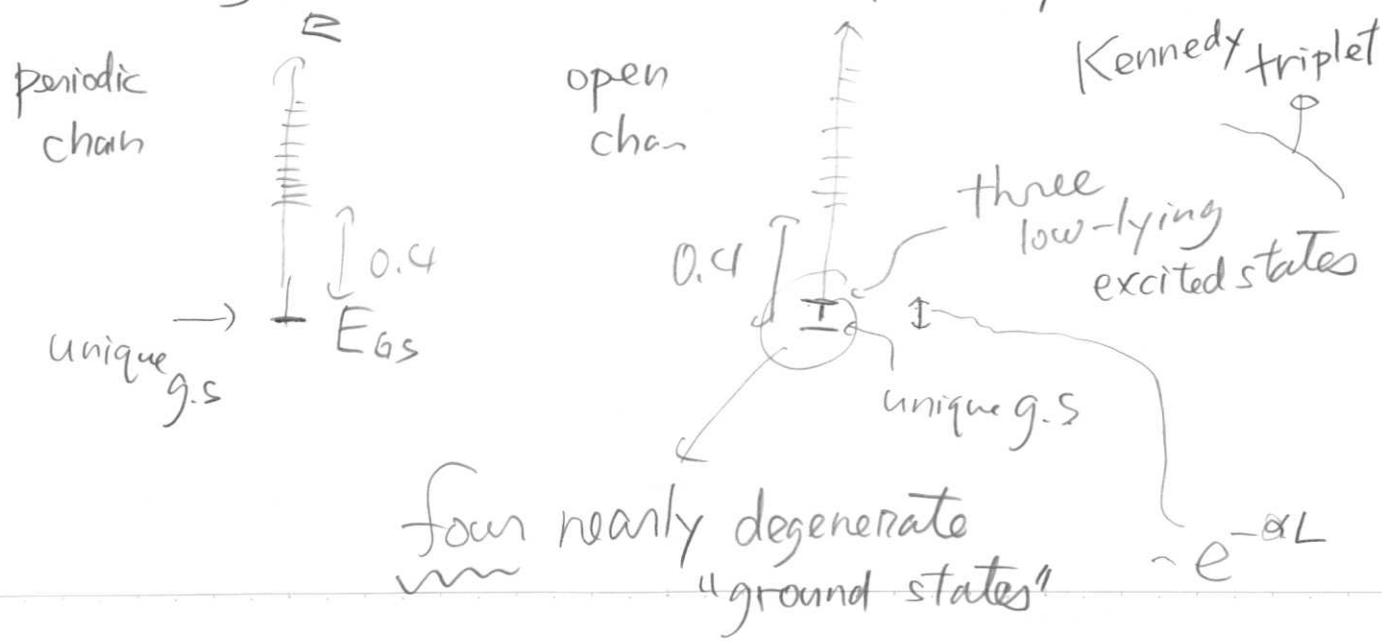
$\begin{cases} \text{Haldne phase} & O^{(1)}_{string} = O^{(2)}_{string} > 0, \; O^{(3)}_{string} > 0 \\ \text{large-D phase} & O^{(1)}_{string} = O^{(2)}_{string} = O^{(3)}_{string} = 0 \end{cases}$

$\boxed{\text{The hidden AF order (measured by the string order par.) characterizes the Haldane phase.}}$

Near four-fold degeneracy and the edge state

- AKLT model on $\begin{cases} \text{a periodic chain} \rightarrow \text{unique g.s. + a gap} \\ \text{an open chain} \rightarrow \text{four g.s. + a gap} \end{cases}$

- Heisenberg AF (numeical)   Kennedy 1990



hidden AF order $\Longrightarrow$ near four-fold degeneracy

1) Harsch-von der Liden Theorem

$$\hat{O}^{(\alpha)}_{string} := \sum_{x=1}^{L} \hat{S}^{(\alpha)}_x \exp\left[i\pi \sum_{y=1}^{x-1} \hat{S}^{(\alpha)}_y\right]$$

if $O^{(\alpha)}_{string} \neq 0$

Then $\langle \Phi_{GS}, (\hat{O}^{(\alpha)}_{string})^2 \Phi_{GS} \rangle \geq \alpha . L^2$ $\quad \alpha > 0$

Thus $\dfrac{O^{(\alpha)}_{string} \Phi_{GS}}{\| O^{(\alpha)}_{string} \Phi_{GS} \|}$ is a low-lying state

$\alpha = 1, 2, 3$

they are orthogonal

2) 0, +, − configuration

config. with complete hidden AF order

$|0 + 0 - + \cdots - + 0 0 -|$

$|0 0 - + \cdots +|$

$|- \cdots -|$

$|+ \cdots +|$

four kinds

edges states

Thus. "Haldane phase" is a distinct phase

0 Haldane $D_c \simeq 1$ large-D → D

hidden AF order | no order

near-four-fold degeneracy in open chain (edge states) | unique GS with a gap in open chain.

quite exotic!

observed experimentally!