S=1 ダイマー・トライマー模型の基底状態相図

桂 法称 (東大院理)

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➢ *Phys. Rev. B*, **96**, 165126 (2017). [arXiv:1709.01344]

What are dimers and trimers?

■ Spin-1 dimer

Dimer = SU(2) singlet state of two *S*=1

$$\mathbf{1} \otimes \mathbf{1} = \mathbf{2} \otimes \mathbf{1} \otimes \boxed{\mathbf{0}}$$

g.s. of 2-site AFM Heisenberg chain

$$\frac{1}{\sqrt{3}}(|+\rangle_i|-\rangle_j - |0\rangle_i|0\rangle_j + |-\rangle_i|+\rangle_j)$$

- Projection operator

$$\mathcal{P}_D(i,j) = \frac{1}{3}[(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^2 - 1]$$

■ Spin-1 trimer

Trimer = SU(2) singlet state of three *S*=1

$$\mathbf{1} \otimes \mathbf{1} \otimes \mathbf{1} = \mathbf{3} \oplus \mathbf{2} \oplus \mathbf{2} \oplus \mathbf{1} \oplus \mathbf{1} \oplus \mathbf{1} \oplus \boxed{\mathbf{0}}$$

g.s. of 3-site AFM Heisenberg chain

SU(3) singlet

$$\frac{1}{\sqrt{6}} \sum_{a,b,c=-1}^{1} \epsilon^{abc} |a\rangle_i |b\rangle_j |c\rangle_k$$

- Projection operator

$$\mathcal{P}_T(i,j,k) = -\frac{1}{144}(\boldsymbol{S}_{ijk}^2 - 2)(\boldsymbol{S}_{ijk}^2 - 6)(\boldsymbol{S}_{ijk}^2 - 12)$$

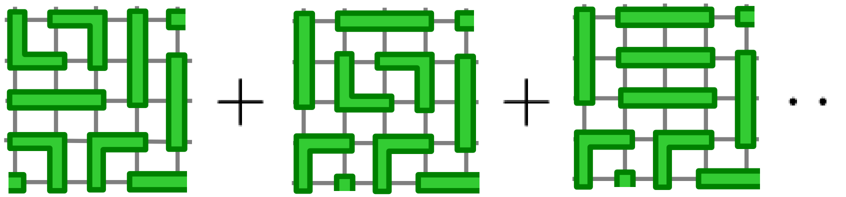
$$\boldsymbol{S}_{ijk} = \boldsymbol{S}_i + \mathbf{S}_j + \mathbf{S}_k$$

Motivation

- Trimer RVB state

  Lee, Oh, Han & H.K., *PRB* **95**, 060413(R) (2017).

  - Rokhsar-Kivelson type model
  - Exact g.s. = trimer RVB state
  - Z3 topological order



- Orthogonality issue

  Different configs. are not orthogonal

  → Hard to write down a microscopic spin Hamiltonian

  As a warm-up, consider the 1D case first

Results

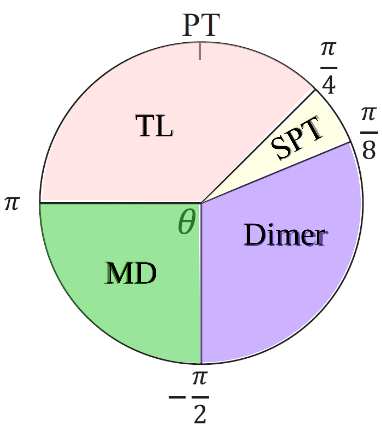
- Hamiltonian with competing dimer-, trimer int.

$$H_{\mathrm{DT}} = -\sum_i [\cos\theta D(i) + \sin\theta T(i)]$$

- Map out g.s. phase diagram

  4 phases: Dimer, SPT, Trimer Liquid and MD

- Model hosts trimer liquid ground state



S=1 bilinear-biquadratic (BLBQ) chain

■ Hamiltonian

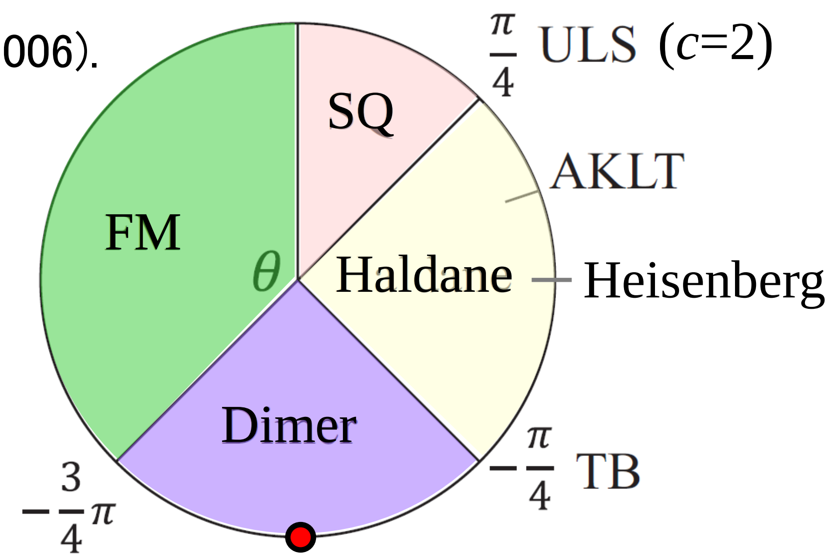
$$H_{\mathrm{BLBQ}} = \sum_{i=1}^{N} [\cos\theta (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + \sin\theta (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2]$$

■ Phase diagram

Lauchli, Schmid, Trebst, *PRB* **74**, 144426 (2006).

- Haldane:
  gapped, unique g.s., SPT!
- Spin-quadrupolar (SQ):
  gapless, dominant nematic correlation
- Ferromagnetic (FM)
- Dimer: gapped, 2-fold degenerate g.s.

Several solvable/integrable points.



Pure dimer $\theta = \frac{\pi}{2} \to \tilde{\theta} = 0$

Another way to write

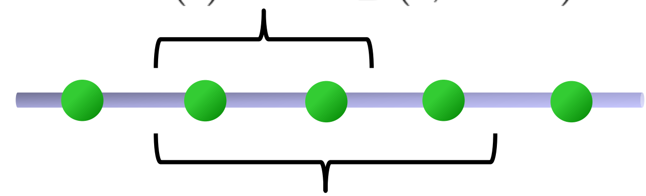
$$H_{\mathrm{BLBQ}} \propto -\sum_{i} [\cos\tilde{\theta}\, P^{(0)}_{i,i+1} + \sin\tilde{\theta}\, P^{(1)}_{i,i+1}]$$

S=1 dimer-trimer (DT) chain

■ Hamiltonian

$$H_{\rm DT} = -\sum_{i=1}^{N}[\cos\theta\, D(i) + \sin\theta\, T(i)]$$

$D(i) = 3\mathcal{P}_D(i, i+1)$

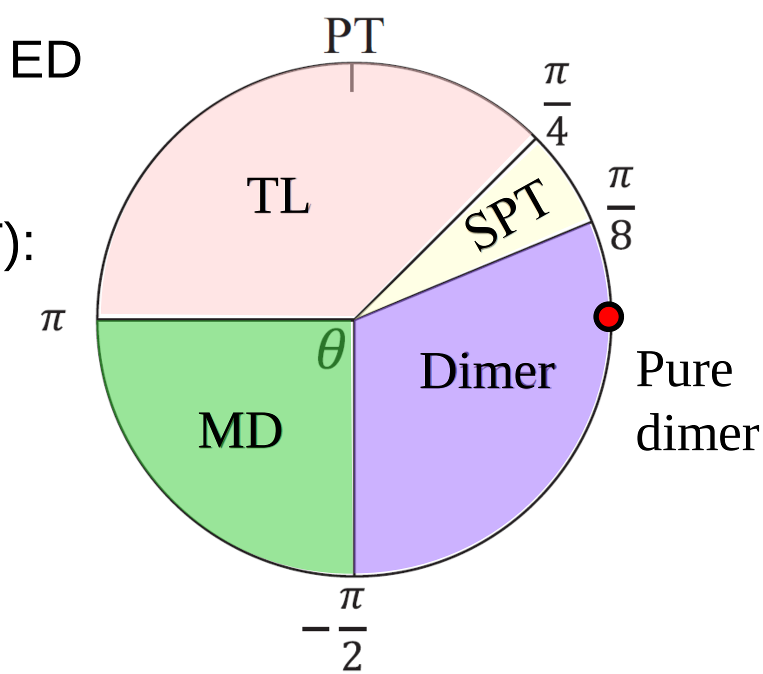


$T(i) = 6\mathcal{P}_T(i, i+1, i+2)$

■ Phase diagram

Methods: DMRG (ITensor library) and ED

- Dimer: same as dimer in BLBQ
- Symmetry-protected topological (SPT):
  gapped, unique g.s., ~ Haldane phase
- Trimer-liquid (TL):
  gapless, ~ SQ phase
- Macroscopically-degenerate (MD):
  similar to $\theta = \pi$ in BLBQ



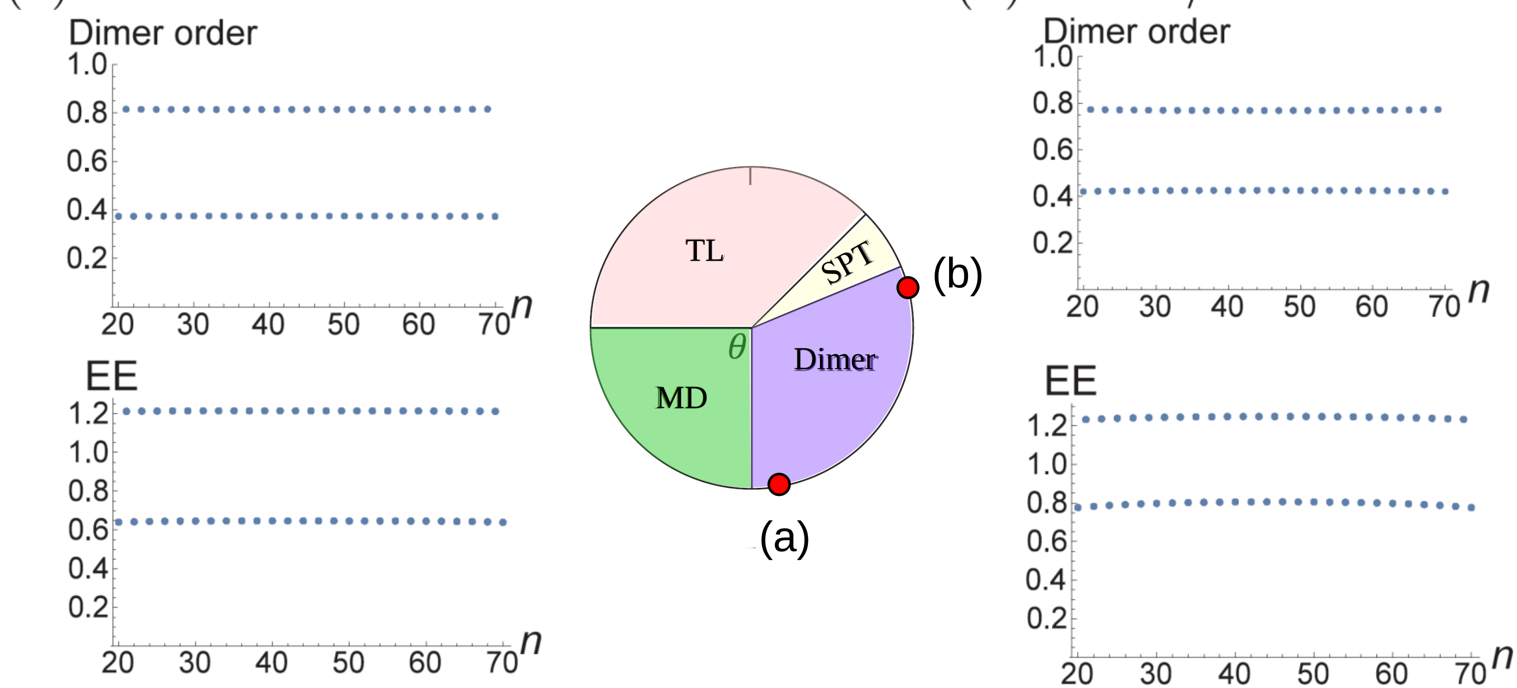
Gapless, translation-invariant, trimer liquid is realized in TL!

Phase boundaries: likely to be first order

Dimer phase

- Dimer order $\langle \mathcal{P}_D(n, n+1) \rangle \approx D_0 + (-1)^n D_1$
- Similar oscillations in entanglement entropy (EE)
- Zero Trimer order $\langle \mathcal{P}_T(n, n+1, n+2) \rangle \approx 0$
- Exponentially decaying correlations

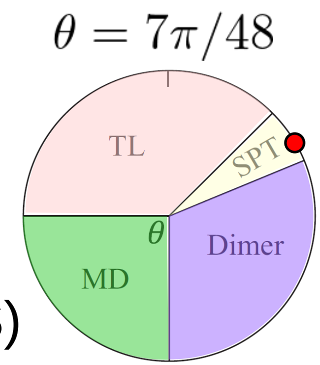
(a) $\theta = -0.45\pi$ (b) $\theta = \pi/12$

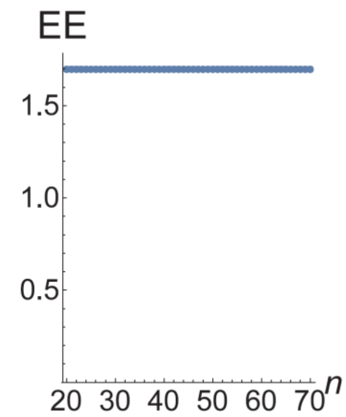


SPT phase

■ Characterization

- Nonzero dimer & trimer average
- Translation symmetry, Flat EE
- 4-fold deg. in entanglement spectrum (ES)
- Exponentially decaying correlations





■ Double degeneracy in ES

Pollmann, Turner, Berg, Oshikawa, *PRB* **81**, 064439 (2010).

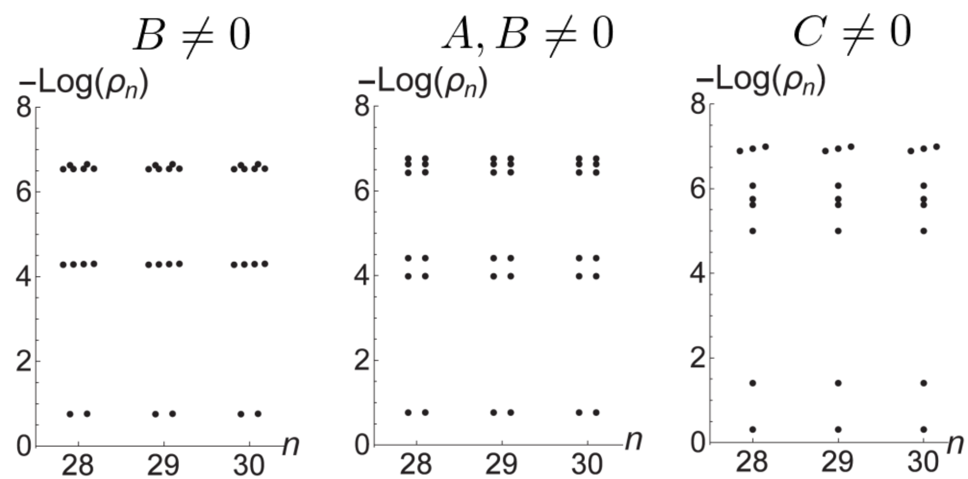
Perturbations:

$$A\sum_i (S_i^x S_i^y + S_i^y S_i^x) + B\sum_i S_i^z$$

$$+\,C\sum_i (S_i^z - S_{i+1}^z)(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)$$

$$+\,C\sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)(S_i^z - S_{i+1}^z)$$

C-term breaks inversion symmetry.



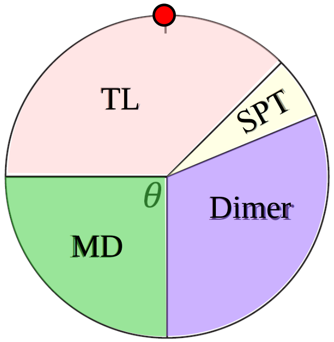
Robust double degeneracy!

TL phase

■ SU(3) symmetry at $\theta=\pi/2$

$$\mathcal{P}_T(i,j,k) = \frac{1}{6}(1 + P_{ijk} + P_{ijk}^{-1} - P_{ij} - P_{jk} - P_{ki})$$

ULS model: $H_{\mathrm{ULS}} = \sum_i P_{i,i+1}$



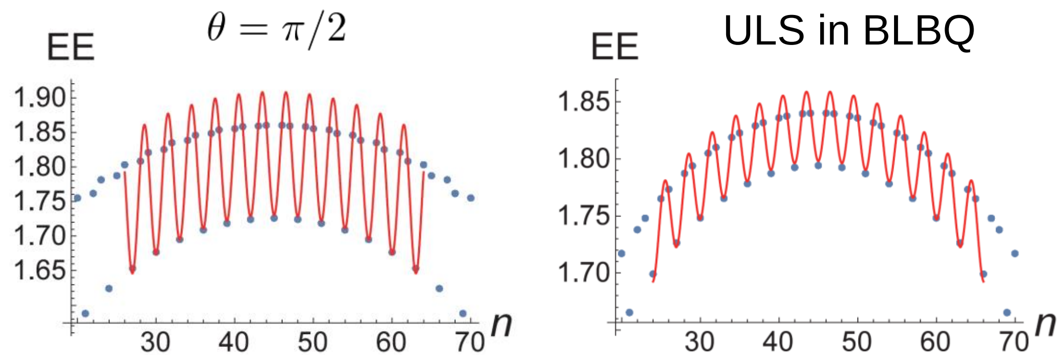
■ Characterization

- Entanglement properties

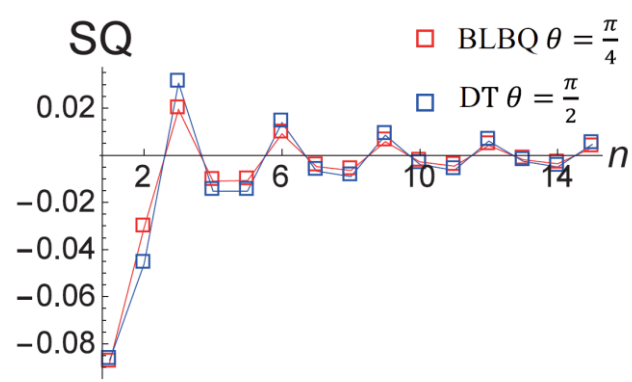
Calabrese-Cardy

$$S_n = S_n^{\mathrm{CFT}} + S_n^{\mathrm{osc}} + c',$$

$$S_n^{\mathrm{CFT}} = \frac{c_N}{6} \log\left[\frac{2L}{\pi}\sin\left(\frac{\pi n}{L}\right)\right]$$



- Consistent with $SU(3)_1$ WZW (c=2)
- Similar EE in the entire phase
- Same ES pattern as ULS



- Algebraically decaying correlations
- $\langle \Psi_0^{\mathrm{PT}} | \Psi_0^{\mathrm{ULS}} \rangle \sim 1$ for small N

MD phase

■ The number of g.s. (OBC) by ED

	N	3	4	5	6	7	8	9	10
(i)	$\theta = \pi$	21	55	144	377	987	2584	6765	17711
(ii)	$\pi < \theta < 3\pi/2$	20	49	119	288	696	1681	4059	9800
(iii)	$\theta = 3\pi/2$	26	75	216	622	1791	5157	14849	42756

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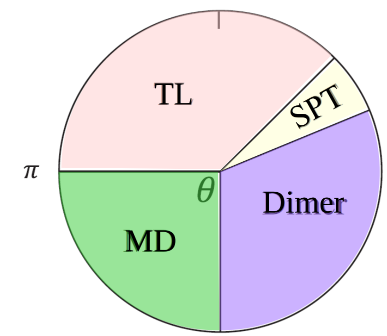
Surprisingly, they match (i) A001906, (ii) A048739, (iii) A076264

■ Residual entropy/site (conjecture)

$$s = \begin{cases} 2\ln\varphi & \sim 0.962 \quad \text{(i)} \\ \ln(1+\sqrt{2}) & \sim 0.881 \quad \text{(ii)} \\ \ln x^* & \sim 1.06 \quad \text{(iii)} \end{cases}$$

[φ: golden ratio]

$[(x^*)^3 + 3(x^*)^2 + 1 = 0]$



Consistent with lower bounds obtained by transfer matrix

For (i), see also Nomura & Takada, *JPSJ* **60**, 389 (1991).

Summary

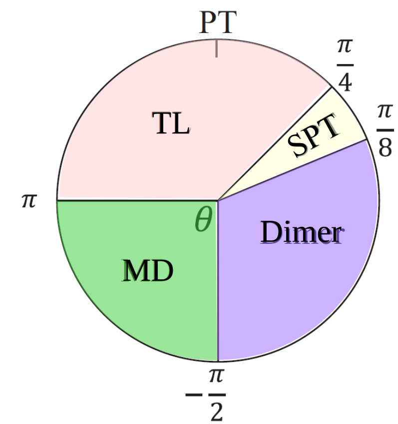
■ Dimer-Trimer chain

- Competition of dimer- & trimer formations

$$H_{\mathrm{DT}} = -\sum_i [\cos\theta D(i) + \sin\theta T(i)]$$

- 4 g.s. phases: Dimer, SPT, TL & MD
  Physical & entanglement properties

- Trimer liquid ground state is realized in TL



Future directions

■ Analytical approach

- Trimer plane waves are eigenstates @ $\theta=\pi/2$
  Bethe ansatz “approximation”: Kiwata & Akutsu, *JPSJ* **63**, 3598(1994).

■ 2D models?

- Microscopic spin Hamiltonians for RVB
  Fujimoto, *PRB* **72** (2005), Seidel, *PRB* **80** (2009), …

- What about trimer RVB?