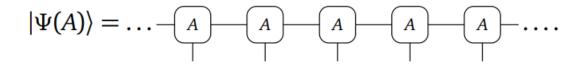
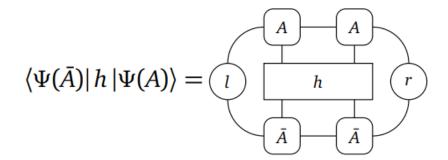
AD_excitation

Xingyu Zhang 2022.11.4

background

Ground state





• Quasiparticle ansatz(single-mode approximation)

$$|\Phi(B)_{k}\rangle = \sum_{n} e^{ikn} \dots - A \longrightarrow A \longrightarrow B \longrightarrow A \longrightarrow A \longrightarrow A \longrightarrow S_{n-1} \longrightarrow S_{n} \longrightarrow S_{n+1} \longrightarrow \cdots$$

2

Steps summary and difficulties

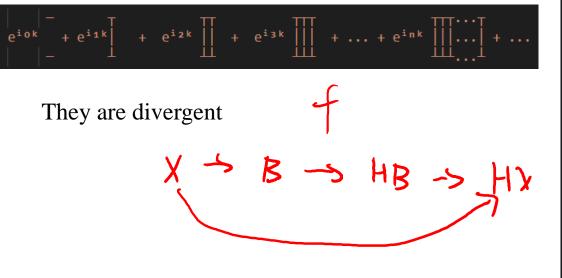
Correct graph summation

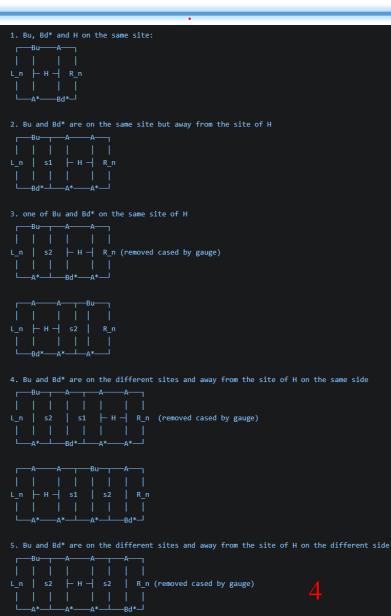
Correct series summation

s1 is series summation of



s2 is series summation of

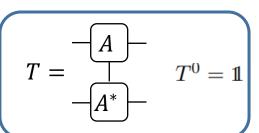




Geometric Sums of Transfer Matrices (1/3)

Geometric Sums

$$(y| = (x|\sum_{n=0}^{\infty} T^n)$$
 $|y| = \sum_{n=0}^{\infty} T^n|x)$ $T = A$ $T^0 = 1$



decomposition

$$T = \sum_{j=0}^{D^2 - 1} \lambda_j |j)(j| \qquad T^n = |0)(0| + \sum_{j=1}^{D^2 - 1} \lambda_j^n |j)(j| \qquad \begin{pmatrix} (j|k) = \delta_{jk} \\ \lambda_0 = 1 & |\lambda_{j>0}| < 1 \end{pmatrix}$$

$$(j|k) = \delta_{jk}$$
 $\lambda_0 = 1 \quad |\lambda_{j>0}| < 1$

$$\sum_{n=0}^{\infty} T^n = \sum_{n=0}^{\infty} |0)(0| + \sum_{j=1}^{D^2 - 1} \sum_{n=0}^{\infty} \lambda_j^n |j)(j|$$

$$= |\mathbb{N}||0)(0| + \sum_{j=1}^{D^2 - 1} (1 - \lambda_j)^{-1} |j)(j|$$

Geometric Sums of Transfer Matrices (2/3)

• projectors

$$P = |0)(0| Q = 1 - |0)(0|$$

$$\mathcal{T} = \sum_{j=1}^{D^2 - 1} \lambda_j |j| (j| = QT = TQ = T - P.$$

$$\sum_{n=0}^{\infty} T^n = |\mathbb{N}||0)(0| + Q(\mathbb{1} - \mathcal{T})^{-1}Q$$

$$(y| = |\mathbb{N}| (x|0) (0| + (x|Q(\mathbb{1} - \mathcal{T})^{-1}) |y| = |\mathbb{N}| (0) (0|x) + (\mathbb{1} - \mathcal{T})^{-1}Q|x).$$

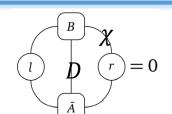
The diverging contributions can typically be safely discarded, as they correspond to a constant (albeit infinite) offset of some extensive observable (e.g. the Hamiltonian).

Geometric Sums of Transfer Matrices (3/3)

Linear solve

Orthogonal Parameterization of $\Phi(B)(1/2)$

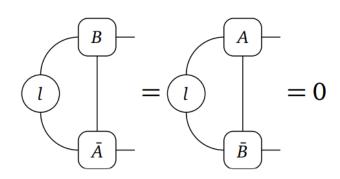
• $\Phi(B)$ is Orthogonal to $\psi(A)$



Gauge Invariant of Tangent vector

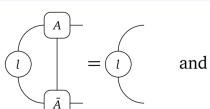
Parameters $D\chi^2 \to D\chi^2 - 1 \to D\chi^2 - \chi^2$

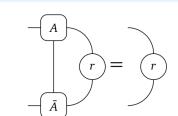
• Left gauge-fixing condition

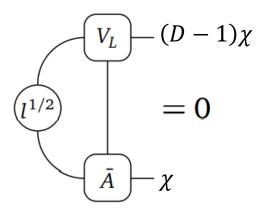


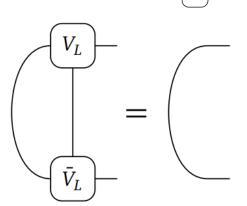
Orthogonal Parameterization of $\Phi(B)(2/2)$

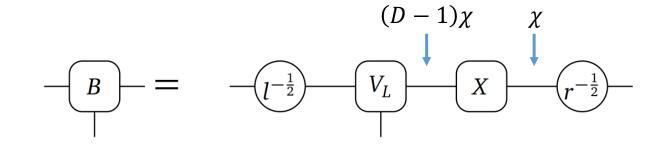
parameterization





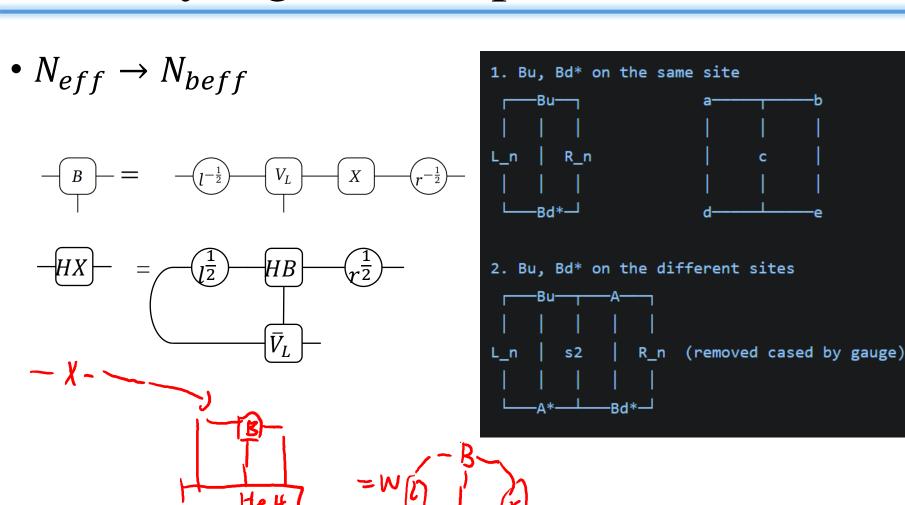






test

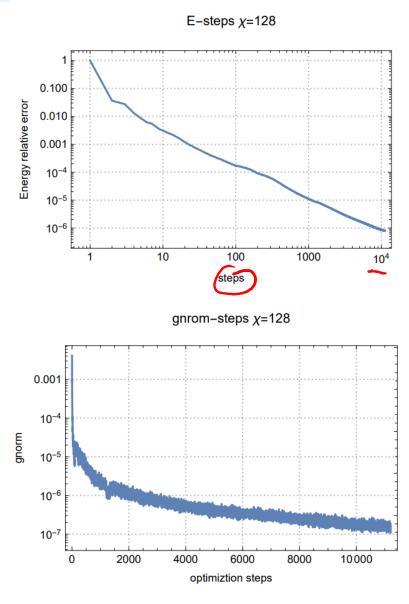
ordinary eigenvalue problem



Ground state by AD

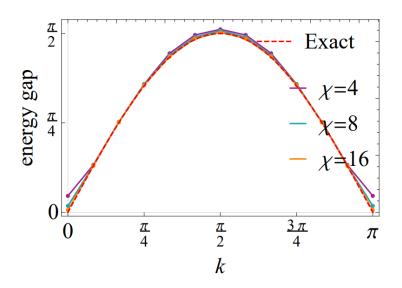
• Heisenberg S = 1/2

error exponentially-dependent on χ **ADMPS** 0.010 Energy relative error 10^{-5} 10^{-6} 10 50 5 100 X

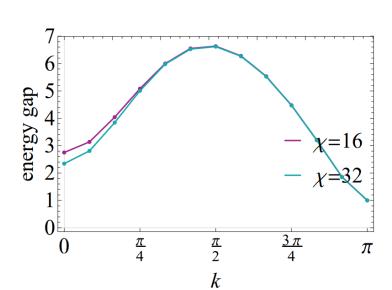


gap

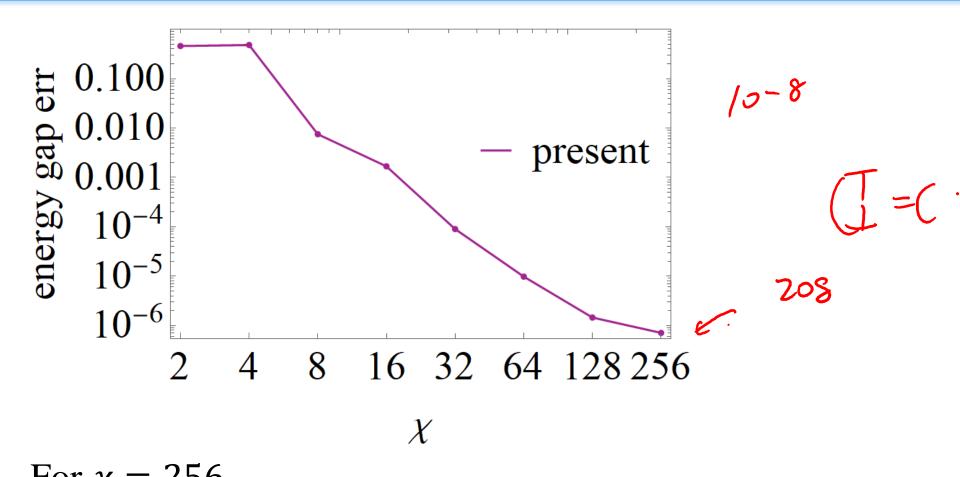
• Heisenberg S = 1/2



• Heisenberg S = 1

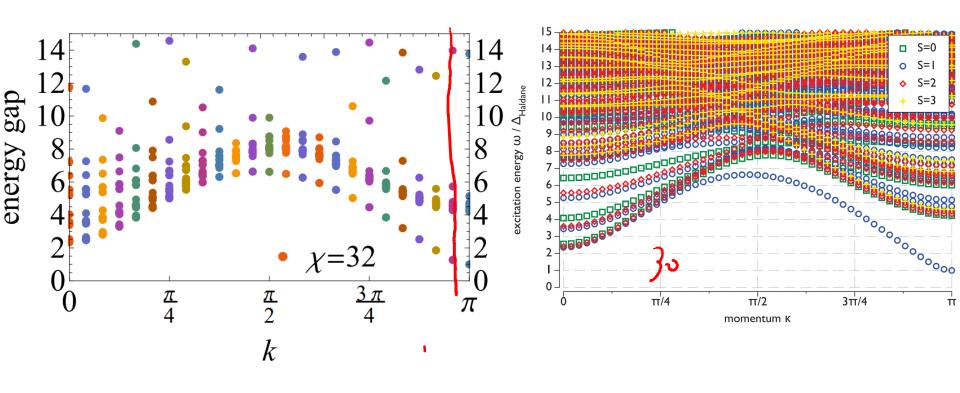


$k = \pi$ Haldane gap error

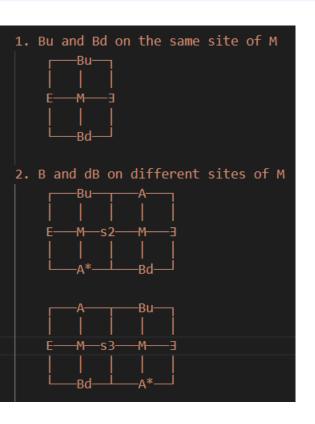


For $\chi = 256$ AD for ground state ~ 8h 10000 steps Eigsolve for excitation state ~ 500s

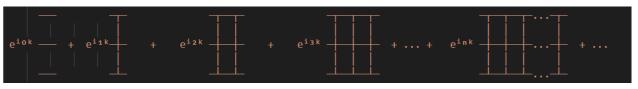
Heisenberg S = 1 excitation spectrum



MPO graph summation



s2



MPO

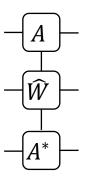
• TFIsing

$$H_{\text{TFI}} = -J \sum_{j} \sum_{n>0} \lambda^{n-1} X_j X_{j+n} - h \sum_{j} Z_j$$

$$\hat{W} = \begin{bmatrix} 1 & 0 & 0 \\ -JX & 1 & 0 \\ -hZ & X & 1 \end{bmatrix}$$

$$\hat{w}_L = \begin{bmatrix} -hZ & X & 1 \end{bmatrix}$$

$$\hat{w}_R = \begin{bmatrix} 1 & -JX & -hZ \end{bmatrix}^T$$



The \pm MPO transfer matrix contains Jordan blocks and that the dominant eigenvalue is one and of twofold algebraic degeneracy.

Overlap(E, \exists) = 0 E \exists \exists = 0

MPO transfer matrices technically do not have well defined fixed points. → quasi fixed points

Fixed point equations

• Left and right environment E3

$$C_a = C_a \perp^{aa} + C_a \qquad C_a = \sum_{b>a} C_b \perp^{ba}$$

$$D_a = \perp^{aa} D_a + D_a \qquad D_a = \sum_{b < a} \perp^{ab} D_b$$

• $\perp^{aa} = 0$

$$C_a = C_a$$

 $C_a = C_a$

•
$$\Box^{aa} = \lambda_a \Box$$

 $C_a = \lambda_a C_a \Box + C_a$
 $C_a = \lambda_a \Box C_a \Box + C_a$
 $C_a (1 - \lambda_a \Box) = C_a$
 $C_a (1 - \lambda_a \Box) = C_a$

•
$$\perp^{aa} = \perp$$

$$(1 - \bot) \Im_a = \Im_a$$

$$C_a (1 - \bot - \circ c) = C_a - C_a \circ c$$

$$(1 - \bot - \circ c) \Im_a = \Im_a - \circ c \Im_a$$

$$energy = c \Im_w = C_1 \circ$$

 $C_a(1-\perp)=C_a$

$$\Box^{ab} = \widehat{\widehat{W}}^{ab} \\
-\widehat{A}^*$$

$$\perp = A$$

$$-A^*$$

$$(y| = (x|\sum_{n=0}^{\infty} T^n)$$
 $|y| = \sum_{n=0}^{\infty} T^n|x)$

$$(y| = |\mathbb{N}| (x|0) (0| + (x|Q(\mathbb{1} - \mathcal{T})^{-1})$$

$$|y| = |\mathbb{N}| |0| (0|x) + (\mathbb{1} - \mathcal{T})^{-1} Q|x|.$$

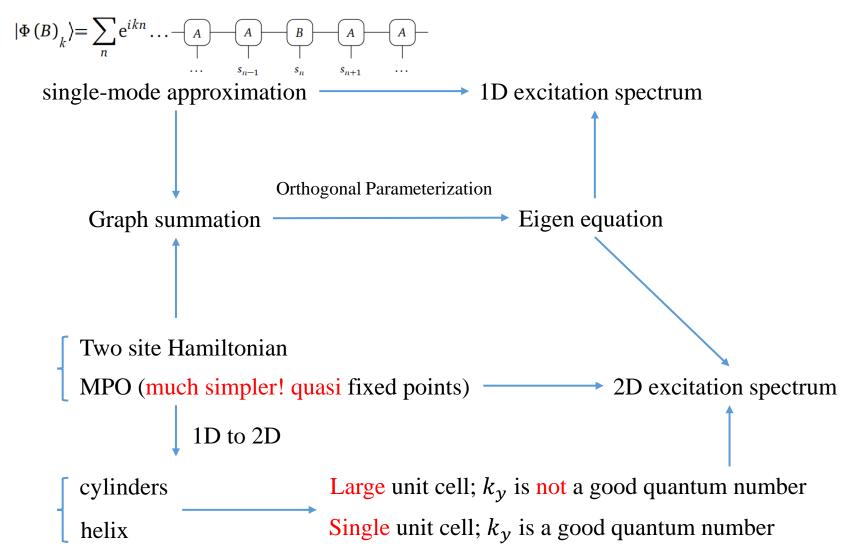
$$\begin{array}{ccc}
(\overline{\pm}) \\
(e-e') \\
(\overline{\pm}) \neq \\
(\overline{\pm})
\end{array}$$

$$\begin{array}{cccc}
(\overline{\pm}) \neq \\
k \\
(\overline{\pm})
\end{array}$$

2D excitation spectrum on Helix

Xingyu Zhang 2023.1.5

Review and contents



Direct 2D single-mode approximation

Spin excitation spectra of the spin-1/2 triangular Heisenberg antiferromagnets from tensor networks

Run-Ze Chi, ^{1,2,*} Yang Liu, ^{1,2,*} Yuan Wan, ^{1,3} Hai-Jun Liao, ^{1,3,†} and T. Xiang ^{1,2,4,‡}

¹Beijing National Laboratory for Condensed Matter Physics and Institute of Physics,

Chinese Academy of Sciences, Beijing 100190, China.

²School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China.

³Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China.

⁴Beijing Academy of Quantum Information Sciences, Beijing, China.

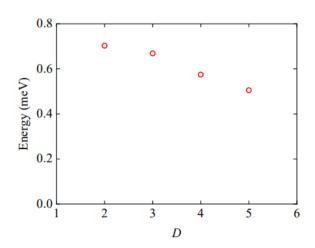
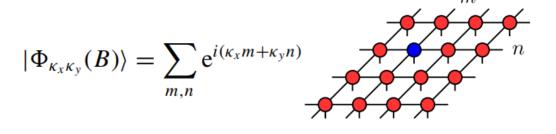


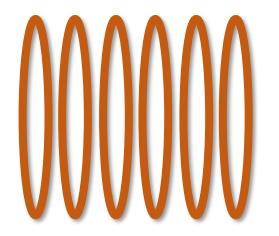
FIG. S2. Minimal spectral gap as a function of bond dimension D. The lowest spectral gap of the XXZ model occurs at the K point (see. Fig. S1) in the Brillouin zone. The gap values are obtained by contracting the effective Hamiltonian tensor network states of the excited states using the corner transfer matrix renormalization group method with a bond dimension $\chi=50$ for D=2,3,4 and $\chi=60$ for D=5.



- High computational cost
- No innovation point

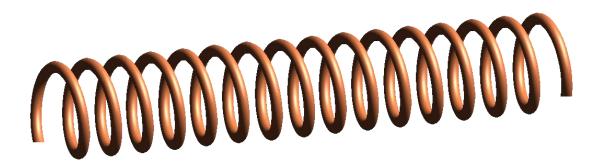
1D→2D map

Cylinder



W

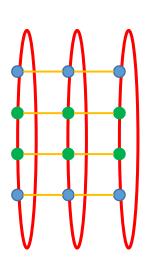
Helix

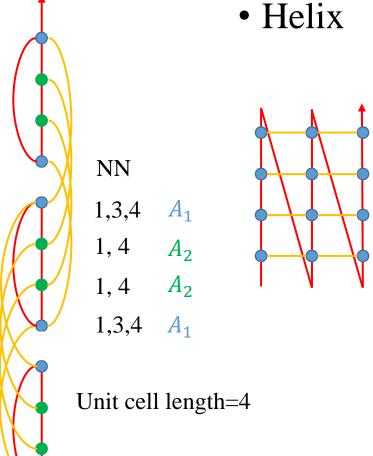


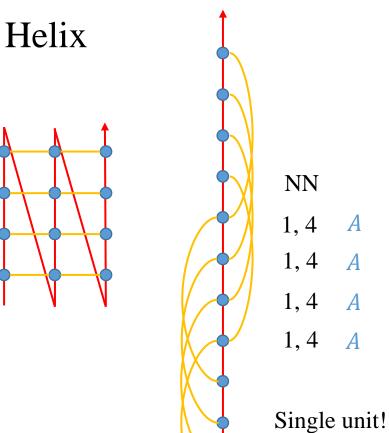
1D→2D map

W = 4 for example

• Cylinders







25

MPO from matrix product (MP) diagram

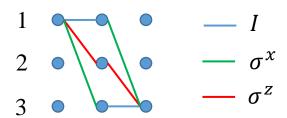
• 1D TFIsing

$$H = \sum_{i} -\sigma_{i}^{z} \sigma_{i+1}^{z} - \lambda \sigma_{i}^{x}$$

$$= -\sigma_{1}^{z} \sigma_{2}^{z} I_{3} I_{4} \dots -\sigma_{1}^{x} I_{2} I_{3} I_{4}$$

$$-I_{1} \sigma_{2}^{z} \sigma_{3}^{z} I_{4} \dots -I_{1} \sigma_{2}^{x} I_{3} I_{4}$$

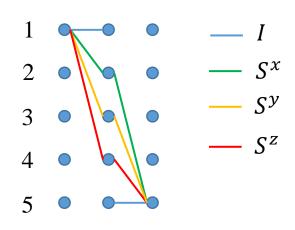
$$-I_{1} I_{2} \sigma_{3}^{z} \sigma_{4}^{z} \dots -I_{1} I_{2} \sigma_{3}^{x} I_{4}$$



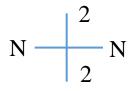
$$M = \begin{bmatrix} I & -\sigma^z & -\sigma^x \\ 0 & 0 & \sigma^z \\ 0 & 0 & I \end{bmatrix}$$
$$N = 3$$

• 1D Heisenberg

$$H = \sum_{i} -\sigma_{i}^{z} \sigma_{i+1}^{z} - \lambda \sigma_{i}^{x} \qquad H = \sum_{i} S_{i}^{x} S_{i+1}^{x} + S_{i}^{y} S_{i+1}^{y} + S_{i}^{z} S_{i+1}^{z}$$



$$M = \begin{bmatrix} I & S^x & S^y & S^z & 0\\ 0 & 0 & 0 & 0 & S^x\\ 0 & 0 & 0 & 0 & S^y\\ 0 & 0 & 0 & 0 & I \end{bmatrix}$$

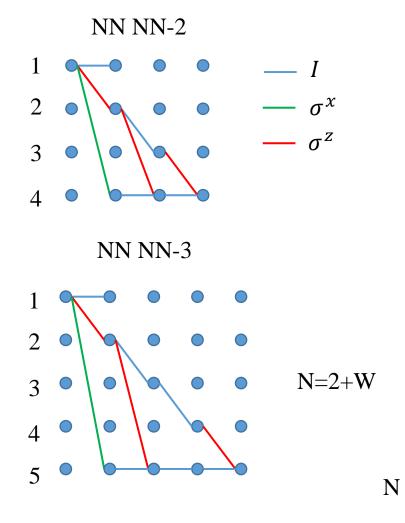


$$V = 5$$
 26

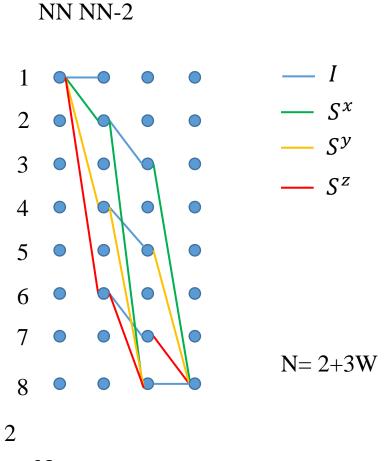
MPO from matrix product (MP) diagram

2

• TFIsing



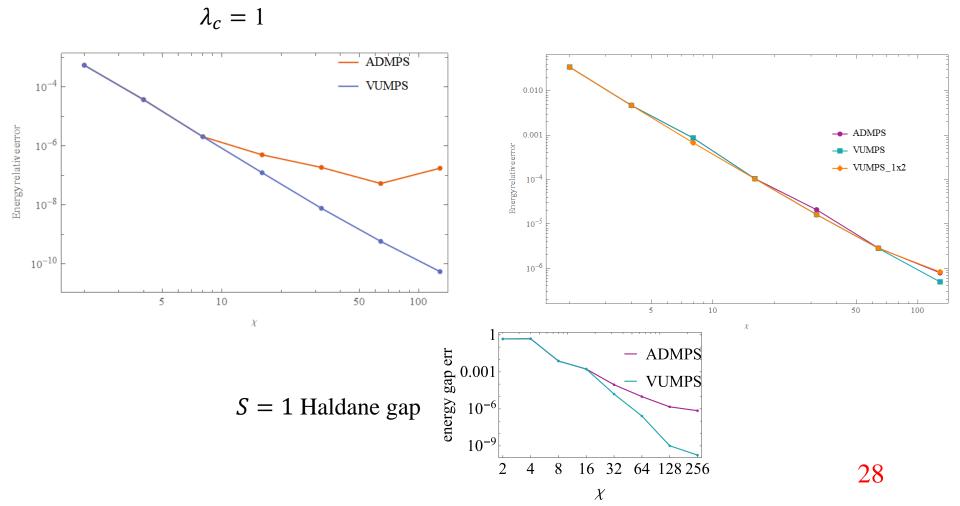
Heisenberg



Ground state vumps

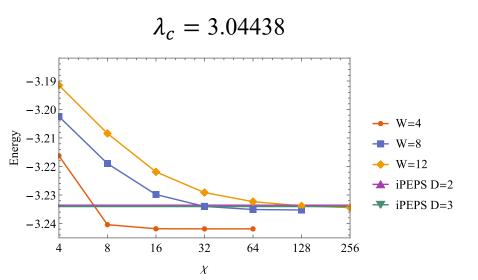
• 1D TFIsing NN

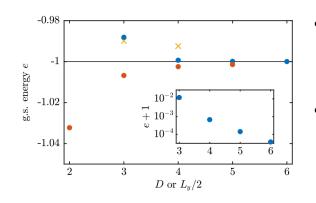
• 1D Heisenberg NN



Ground state vumps

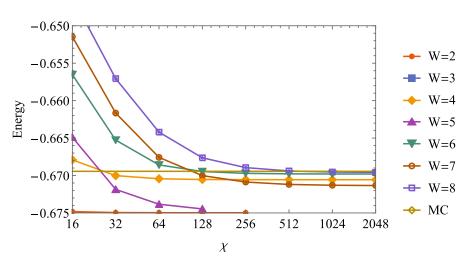
• 2D TFIsing

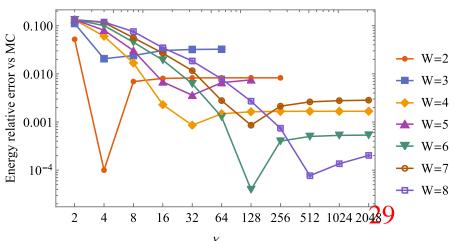




- Different approach with *D* v.s. *W*
- Nonmonotoni city with W and χ

• 2D Heisenberg NN





excitation spectrum

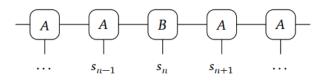
• Cylinder

$|\Phi_{p_x}(B)\rangle = \sum_{n} e^{ip_x n} T_x^n$ $A_1 \qquad A_2 \qquad B \qquad A_1 \qquad A_N$

with

Helix

$$\left|\Phi_{k_x,k_y}(B)\right\rangle = \sum_n e^{ik_x \lfloor n/W \rfloor + ik_y (n \bmod W)} T_x T_y$$



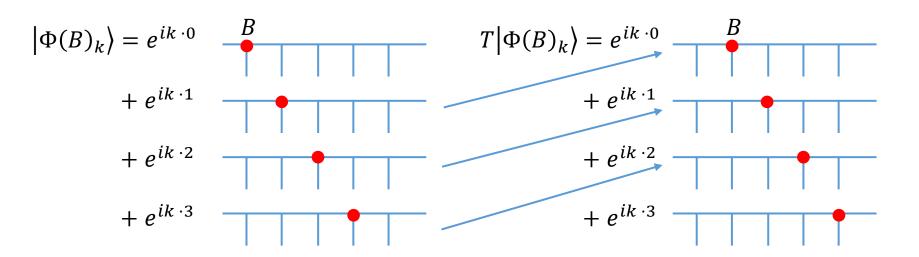
No k_y because k_y is not a good quantum number

 k_y is a good quantum number

Recover by directly calculating

$$\frac{1}{2\pi\delta(p_x - p_x')} \frac{\langle \Phi_{p_x'}(B) | T_y | \Phi_{p_x}(B) \rangle}{\langle \Psi(A) | T_y | \Psi(A) \rangle}$$

translation operator



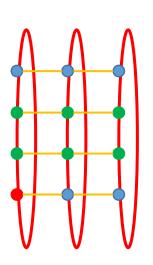
$$e^{-ik} |\Phi(B)_k\rangle = T |\Phi(B)_k\rangle$$

translation operator T_{ν}

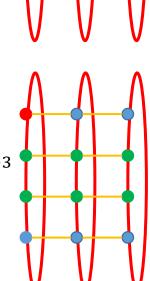
W = 4 for example

• Cylinder

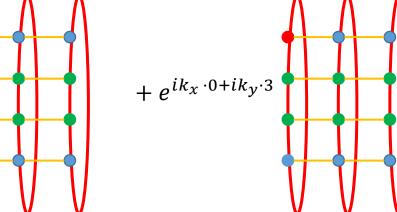
$$T_{\mathcal{Y}}\Big|\Phi(B)_{k_{\mathcal{X}},k_{\mathcal{Y}}}\Big\rangle = e^{ik_{\mathcal{X}}\cdot 0 + ik_{\mathcal{Y}}\cdot 0}$$



$$+e^{ik_x\cdot 0+ik_y\cdot 1}$$



$$+e^{ik_x\cdot 0+ik_y\cdot 2}$$

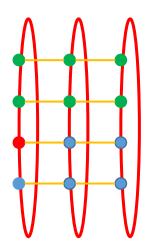


translation operator T_y

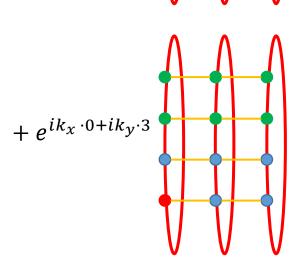
W = 4 for example

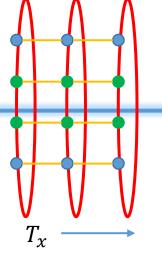
• Cylinder

$$T_{y} \left| \Phi(B)_{k_{x},k_{y}} \right\rangle = e^{ik_{x} \cdot 0 + ik_{y} \cdot 0}$$



$$+e^{ik_x\cdot 0+ik_y\cdot 1}$$





 k_{y} is not a good quantum number!

 $+e^{ik_x\cdot 0+ik_y\cdot 2}$

translation operator T_y

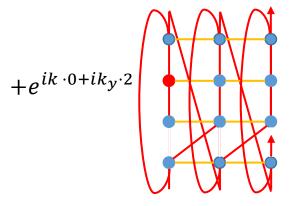
 T_{χ}

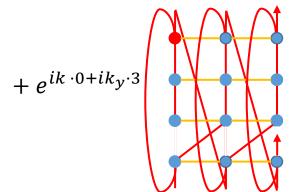
$$W = 4$$
 for example

• Helix

$$T_{y} \left| \Phi(B)_{k_{x},k_{y}} \right\rangle = e^{ik \cdot 0 + ik_{y} \cdot 0}$$

$$+e^{ik\cdot 0+ik_y\cdot 1}$$



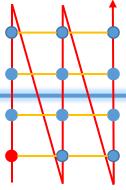


Graph summation



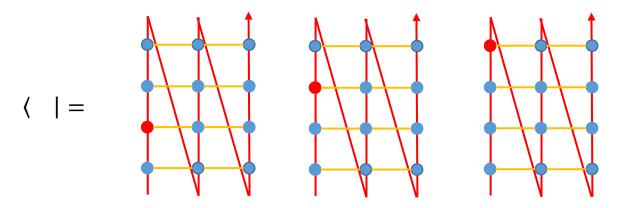
Graph summation

 $| \rangle = e^{ik \cdot 0 + ik_y \cdot 0}$

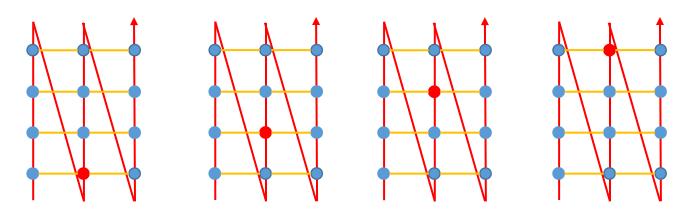


W = 4 for example

$$S^{+_1} = e^{ik_x \cdot 0 + ik_y \cdot 1} = + e^{ik_x \cdot 0 + ik_y \cdot 2} + e^{ik_x \cdot 0 + ik_y \cdot 3} + e^{ik_x \cdot 0 + ik_y \cdot 3} = e^{ik_x \cdot 0 + ik_y \cdot 1} = e^{ik_x \cdot 0 + ik_y \cdot 0} = e^{i$$



$$+e^{ik_x\cdot 1+ik_y\cdot 0}\pm^3+e^{ik_x\cdot 1+ik_y\cdot 1}\pm^4+e^{ik_x\cdot 1+ik_y\cdot 2}\pm^5+e^{ik_x\cdot 1+ik_y\cdot 3}\pm^6$$



Graph summation

$$S^{+_{1}} = \left(e^{ik_{x}\cdot0+ik_{y}\cdot1} \pm + e^{ik_{x}\cdot0+ik_{y}\cdot2} \pm + e^{ik_{x}\cdot0+ik_{y}\cdot3} \pm^{2} + e^{ik_{x}\cdot1+ik_{y}\cdot0} \pm^{3}\right) \cdot \left(\pm + e^{ik_{x}\cdot1} \pm^{4} + e^{ik_{x}\cdot2} \pm^{8} + \cdots\right)$$

$$\equiv \left(e^{ik_{x}\cdot0+ik_{y}\cdot1} \pm + e^{ik_{x}\cdot0+ik_{y}\cdot2} \pm + e^{ik_{x}\cdot0+ik_{y}\cdot3} \pm^{2} + e^{ik_{x}\cdot1+ik_{y}\cdot0} \pm^{3}\right) S_{4}^{+}$$

$$S^{+} = S^{+_{1}} + S^{+_{2}} + S^{+_{3}} + S^{+_{4}}$$

$$= \left(\left(3e^{ik_{x}\cdot0+ik_{y}\cdot1} + e^{ik_{x}\cdot1-ik_{y}\cdot3}\right) \pm + \left(2e^{ik_{x}\cdot0+ik_{y}\cdot2} + 2e^{ik_{x}\cdot1-ik_{y}\cdot2}\right) \pm + \left(e^{ik_{x}\cdot0+ik_{y}\cdot3} + 3e^{ik_{x}\cdot1-ik_{y}\cdot1}\right) \pm^{2} + 4e^{ik_{x}\cdot1+ik_{y}\cdot0} \pm^{3}\right) S_{4}^{+}$$

Same way:

$$S^{-} = S^{-1} + S^{-2} + S^{-3} + S^{-4}$$

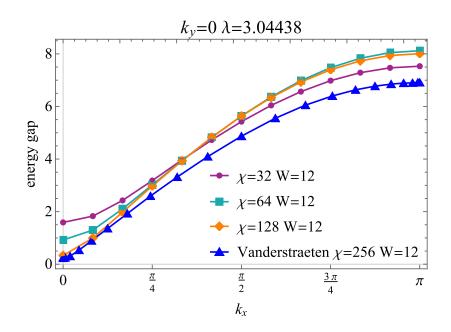
$$= \left(\left(3e^{ik_{x} \cdot 0 - ik_{y} \cdot 1} + e^{-ik_{x} \cdot 1 + ik_{y} \cdot 3} \right) \pm + \left(2e^{ik_{x} \cdot 0 - ik_{y} \cdot 2} + 2e^{-ik_{x} \cdot 1 + ik_{y} \cdot 2} \right) \pm \right.$$

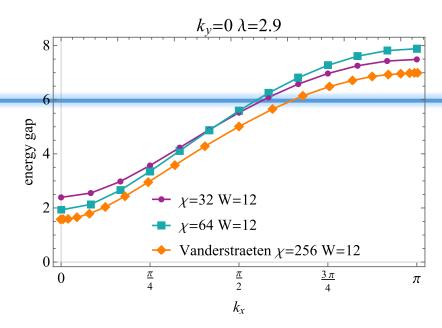
$$+ \left. \left(e^{ik_{x} \cdot 0 - ik_{y} \cdot 3} + 3e^{-ik_{x} \cdot 1 + ik_{y} \cdot 1} \right) \pm \left. 2 + 4e^{-ik_{x} \cdot 1 + ik_{y} \cdot 0} \pm \right. \right) S_{4}^{-}$$

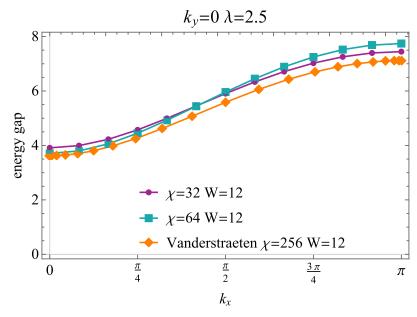
$$S_4^- = \left(\Xi + e^{-ik_{\chi}\cdot 1} \pm^4 + e^{-ik_{\chi}\cdot 2} \pm^8 + \cdots \right)$$

result

• 2D TFIsing $k_v = 0$

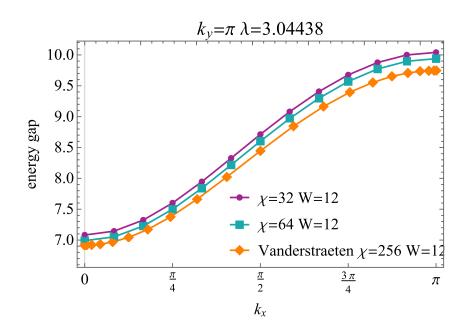


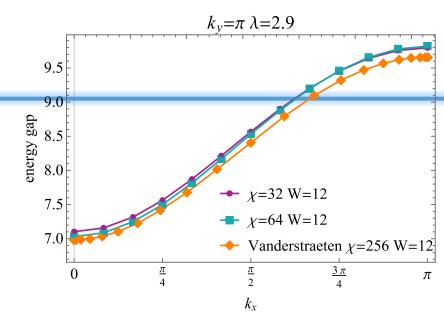


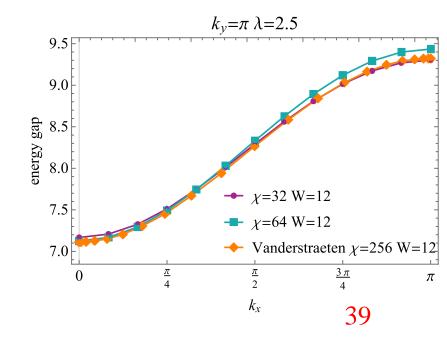


result

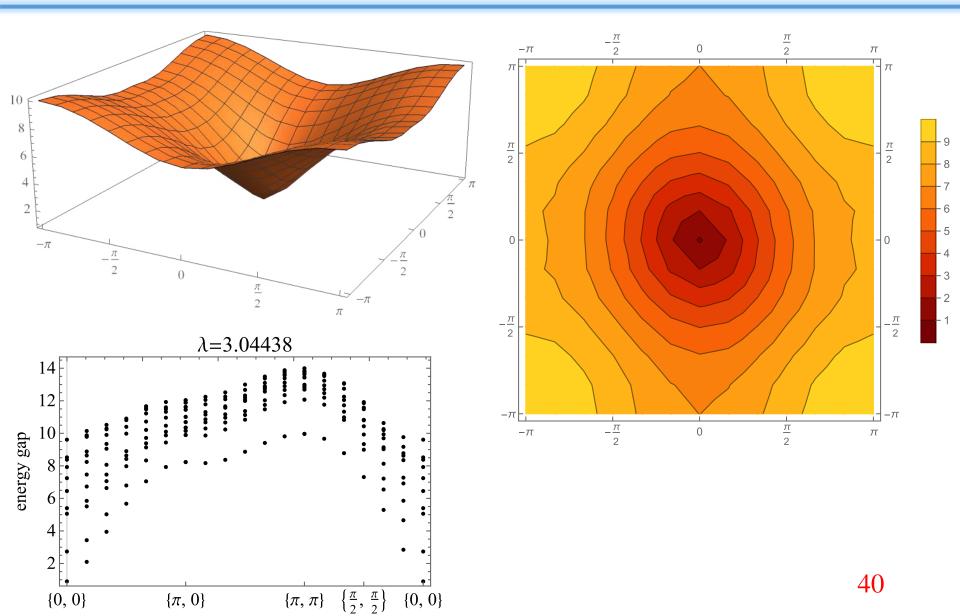
• 2D TFIsing $k_y = \pi$







result



outlook

- 1D anti-Heisenberg, Large unit cell
- 2D anti-Heisenberg
- Kitaev

Thank you for listening!

Q&A?