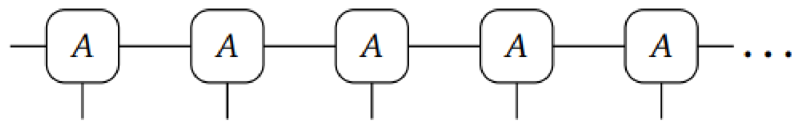
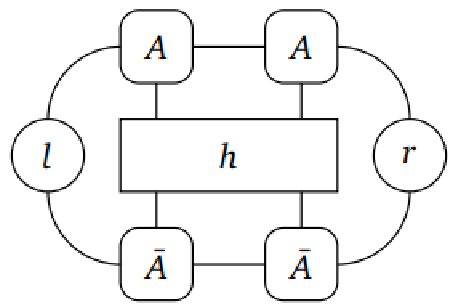
AD_excitation

Xingyu Zhang
2022.11.4

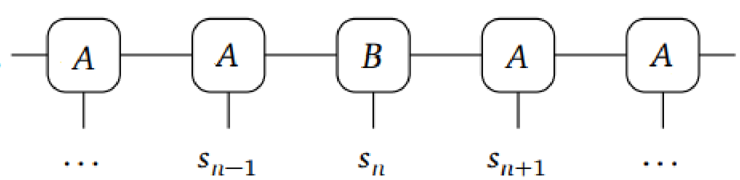
background

- Ground state

$|\Psi(A)\rangle = \ldots$ 

$\langle\Psi(\bar{A})|\, h \,|\Psi(A)\rangle =$ 

- Quasiparticle ansatz(single-mode approximation)

$|\Phi(B)_k\rangle = \sum_n \mathrm{e}^{ikn} \ldots$ 

Steps summary and difficulties

graph summation

$\downarrow$

$$\frac{\partial}{\partial B^{\dagger}}[\langle\Phi(B)_{k}|\mathcal{H}|\Phi(B)_{k}\rangle-\omega_{k}(\langle\Phi(B)_{k}|\Phi(B)_{k}\rangle-1)]=0$$

$\downarrow$ Only depend on B

$$H_{eff}(k)B=\omega N_{eff}B$$

$\downarrow$ Orthogonal Parameterization of $\Phi(B)$

$$H_{beff}(k)X=\omega N_{beff}X$$

$\downarrow$ ordinary eigenvalue problem

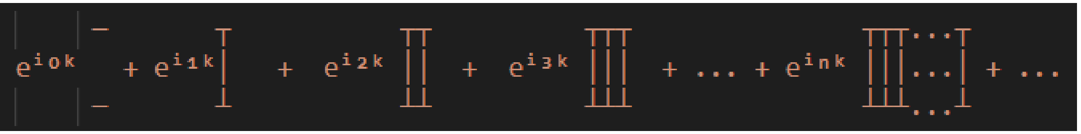
$$H_{Nbeff}(k)X=\omega X$$

Correct graph summation

- Correct series summation

$s1$ is series summation of

$s2$ is series summation of



They are divergent

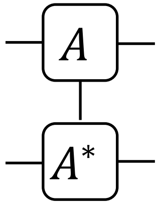
$$\begin{tikzcd} X \arrow[r] \arrow[rrr, bend right] & B \arrow[r, "f"] & HB \arrow[r] & Hx \end{tikzcd}$$

```
1. Bu, Bd* and H on the same site:

 ┌──Bu───A──┐
 │  │    │  │
L_n ├─ H ─┤ R_n
 │  │    │  │
 └──A*───Bd*┘

2. Bu and Bd* are on the same site but away from the site of H

 ┌──Bu─┬──A────A──┐
 │  │  │  │    │  │
L_n │ s1  ├─ H ─┤ R_n
 │  │  │  │    │  │
 └──Bd*┴──A*───A*─┘

3. one of Bu and Bd* on the same site of H

 ┌──Bu─┬──A────A──┐
 │  │  │  │    │  │
L_n │ s2  ├─ H ─┤ R_n (removed cased by gauge)
 │  │  │  │    │  │
 └──A*─┴──Bd*──A*─┘

 ┌──A────A──┬─Bu──┐
 │  │    │  │ │   │
L_n ├─ H ─┤ s2 │  R_n
 │  │    │  │ │   │
 └──Bd*──A*─┴─A*──┘

4. Bu and Bd* are on the different sites and away from the site of H on the same side

 ┌──Bu─┬──A──┬──A────A──┐
 │  │  │  │  │  │    │  │
L_n │ s2  │ s1  ├─ H ─┤ R_n  (removed cased by gauge)
 │  │  │  │  │  │    │  │
 └──A*─┴──Bd*┴──A*───A*─┘

 ┌──A────A──┬──Bu─┬──A──┐
 │  │    │  │  │  │  │  │
L_n ├─ H ─┤ s1  │ s2  │ R_n
 │  │    │  │  │  │  │  │
 └──A*───A*─┴──A*─┴──Bd*┘

5. Bu and Bd* are on the different sites and away from the site of H on the different side

 ┌──Bu─┬──A────A──┬──A──┐
 │  │  │  │    │  │  │  │
L_n │ s2  ├─ H ─┤ s2  │ R_n (removed cased by gauge)
 │  │  │  │    │  │  │  │
 └──A*─┴──A*───A*─┴──Bd*┘
```

Geometric Sums of Transfer Matrices(1/3)

- Geometric Sums

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

$T =$ 

$T^0 = \mathbb{1}$

- decomposition

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

$(j|k) = \delta_{jk}$

$\lambda_0 = 1 \qquad |\lambda_{j>0}| < 1$

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

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

divergent

Geometric Sums of Transfer Matrices(2/3)

- projectors

$$P = |0)(0| \qquad\qquad Q = \mathbb{1} - |0)(0|$$

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

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

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

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

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

x

$I + I + II + III \cdots IIII$

$P \quad T - P$

$(I - X)(\ ) + (I - X)(\ ) + (I - X)(\ )^2$

$I) =)$

$(I = ($

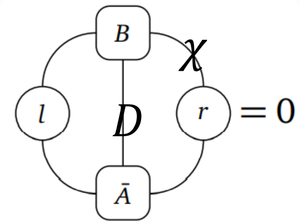
$(I - X)(\ )(I - X)(\ ) = II - XI - IX + X = II - X$

$(I - X)^n = I^n - X$


Bu
A A
Bd
Bu
Bd
A A
Bu
Bd
e

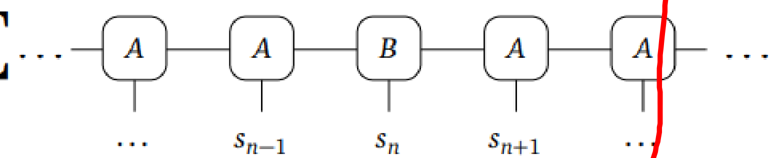
Orthogonal Parameterization of $\Phi(B)$(1/2)

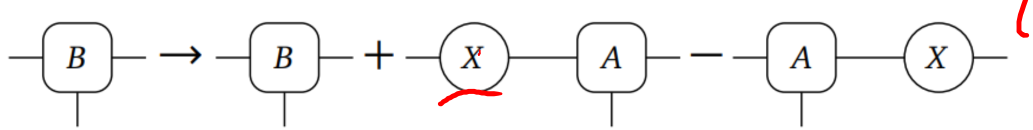
- $\Phi(B)$ is Orthogonal to $\psi(A)$



- Gauge Invariant of Tangent vector

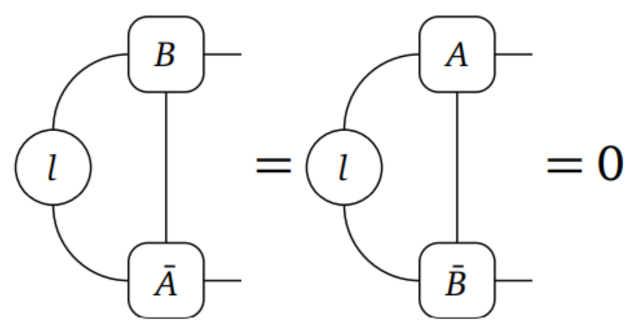
$$|\Phi(B;A)\rangle = B^i \frac{\partial}{\partial A_i}|\Psi(A)\rangle = \sum_n$$





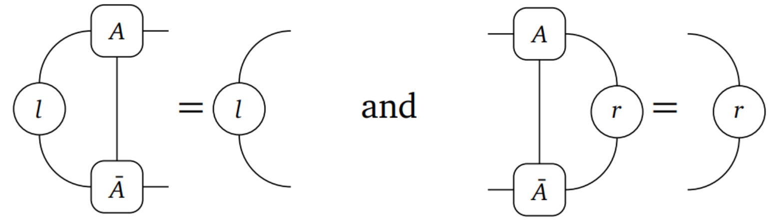
Parameters $D\chi^2 \rightarrow D\chi^2 - 1 \rightarrow D\chi^2 - \chi^2$

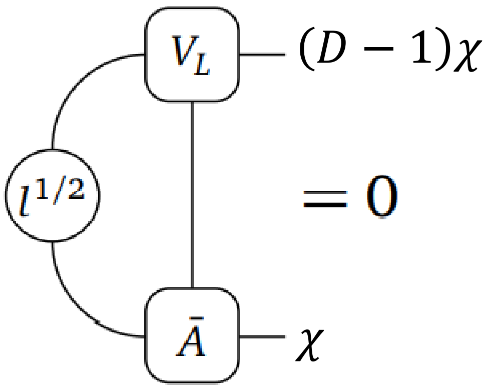
- Left gauge-fixing condition

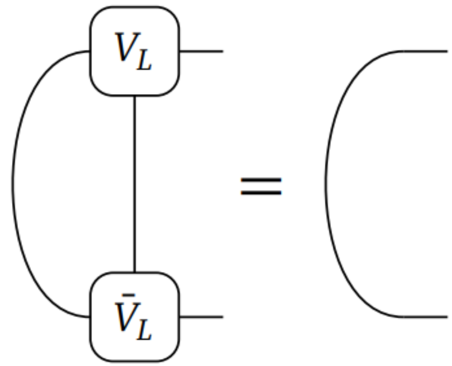


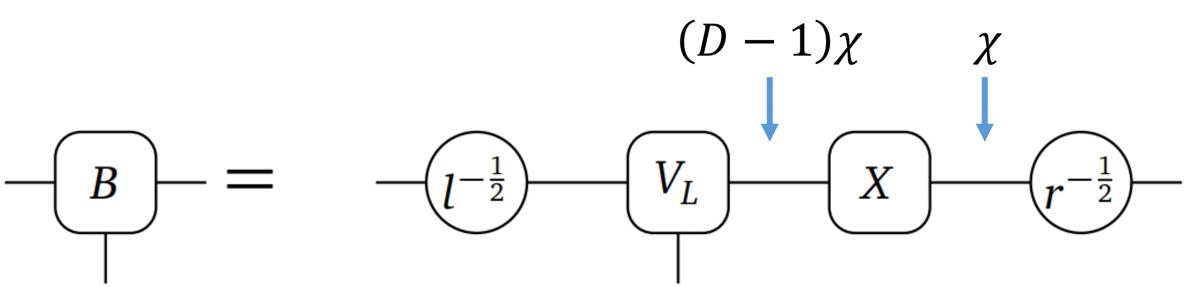
Orthogonal Parameterization of $\Phi(B)$(2/2)

- parameterization





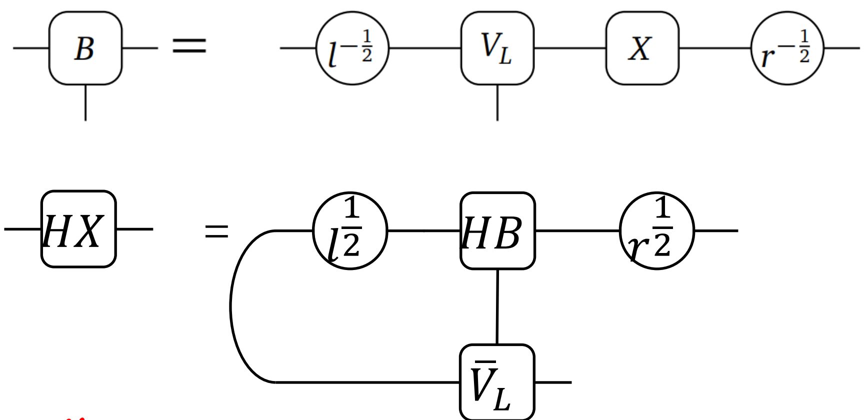


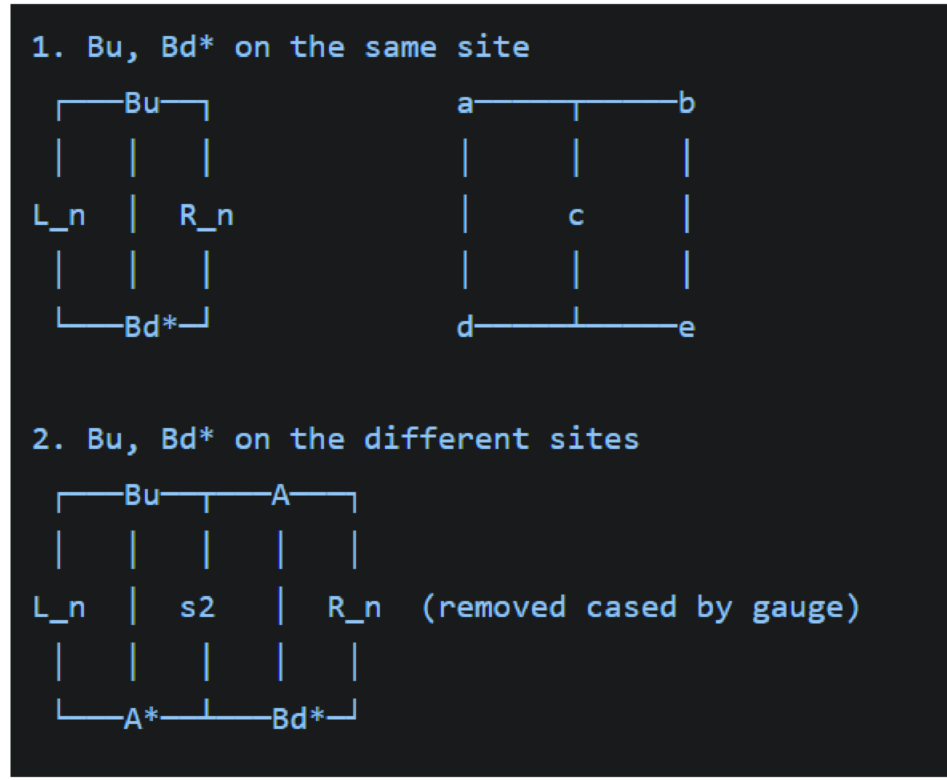


test

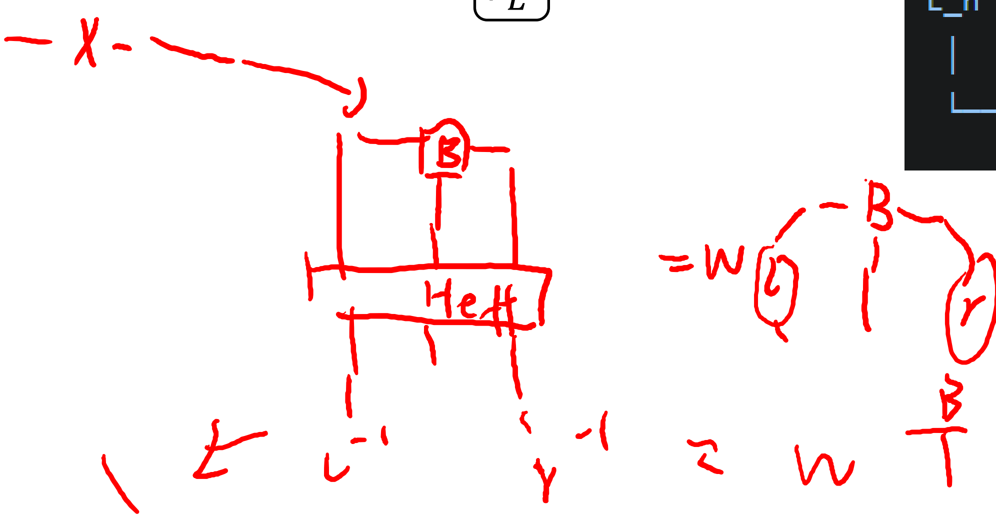
ordinary eigenvalue problem

- $N_{eff} \rightarrow N_{beff}$





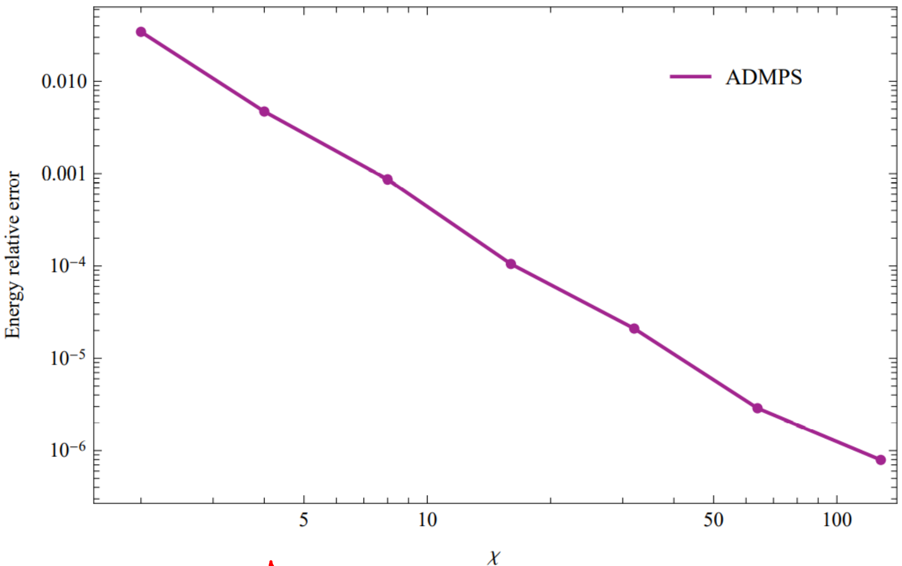
```
1. Bu, Bd* on the same site

 ┌───Bu──┐              a──────┬──────b
 |   |   |              |      |      |
L_n  |  R_n             |      c      |
 |   |   |              |      |      |
 └───Bd*─┘              d──────┴──────e


2. Bu, Bd* on the different sites

 ┌───Bu──┬───A───┐
 |   |   |   |   |
L_n  |   s2  |  R_n   (removed cased by gauge)
 |   |   |   |   |
 └───A*──┴───Bd*─┘
```

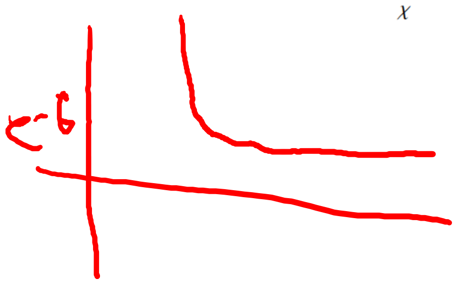


Ground state by AD

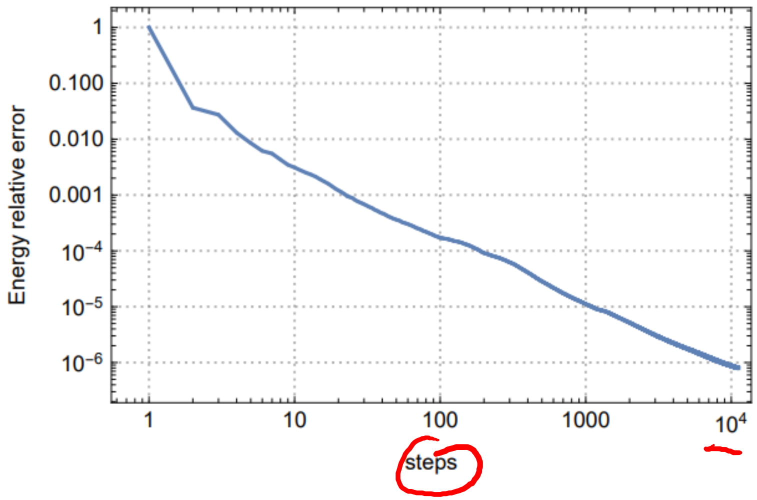
- Heisenberg $S = 1/2$

error exponentially-dependent on χ

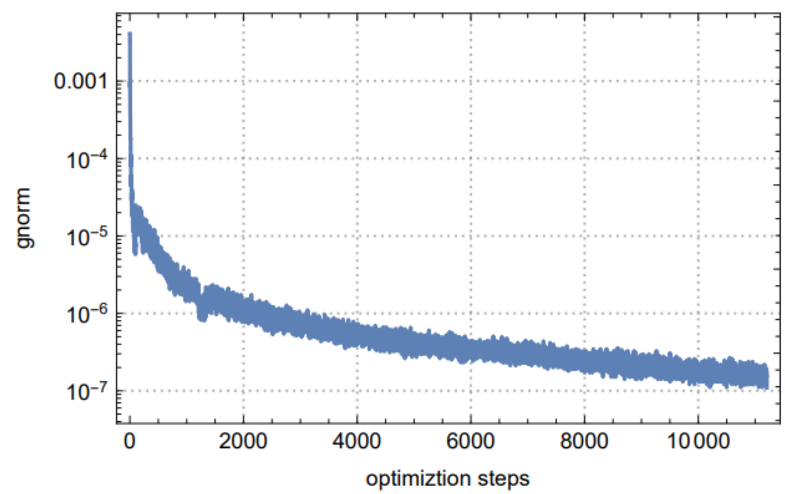




E−steps χ=128

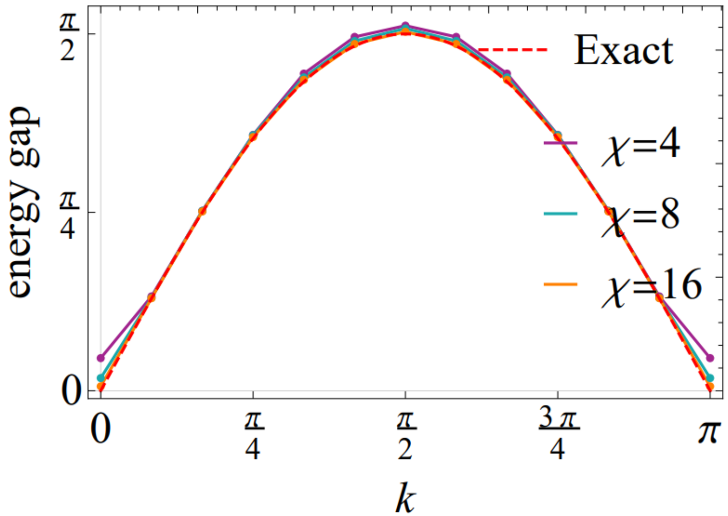


gnrom−steps χ=128

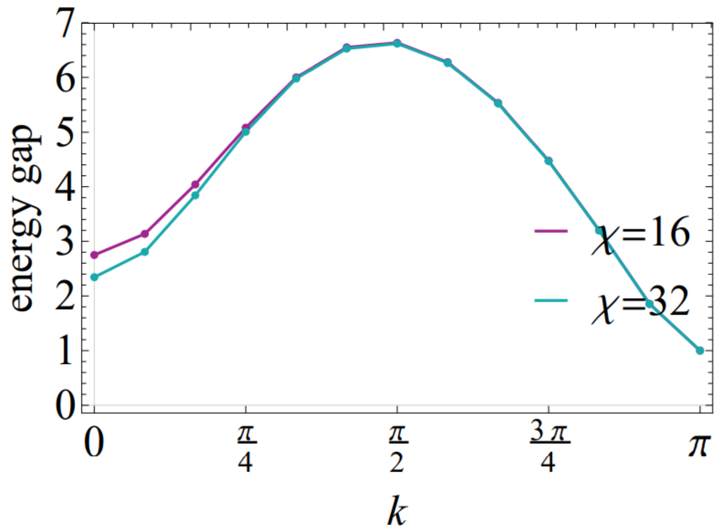


gap

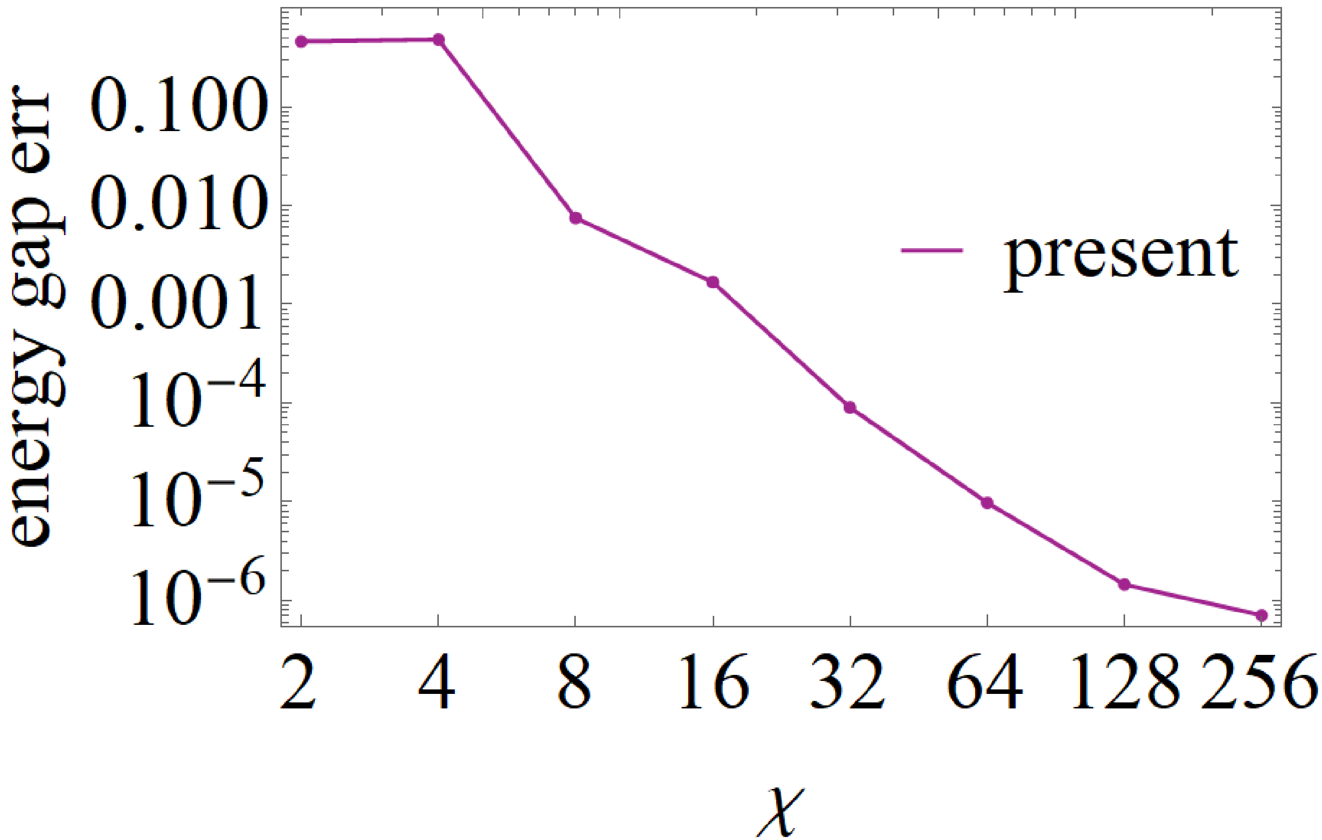
- Heisenberg $S = 1/2$



- Heisenberg $S = 1$



$k = \pi$ Haldane gap error



10-8

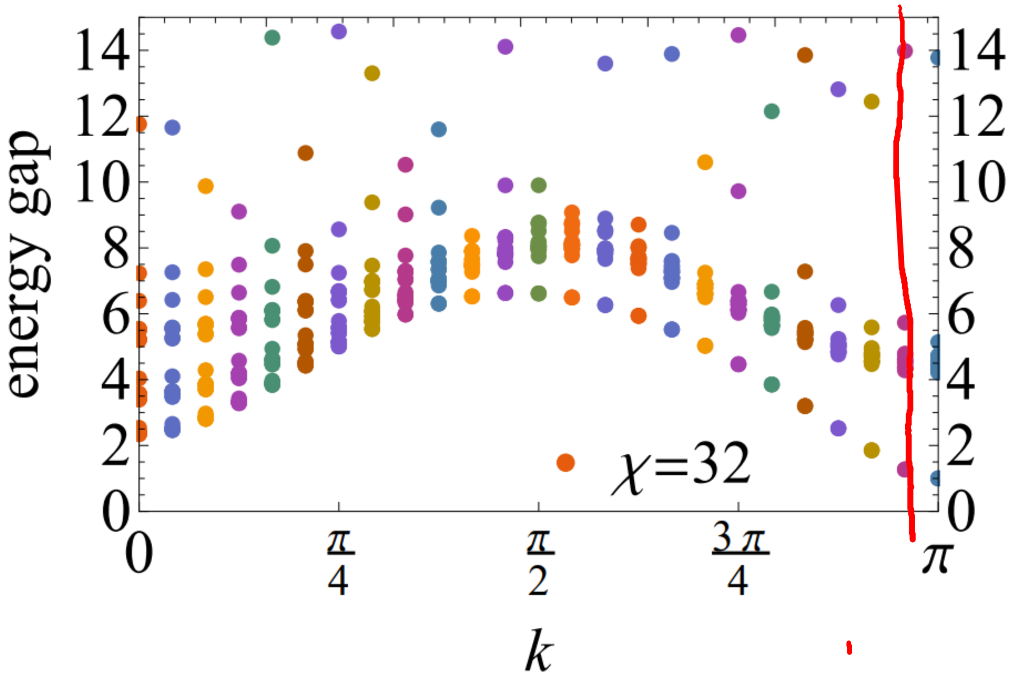
208

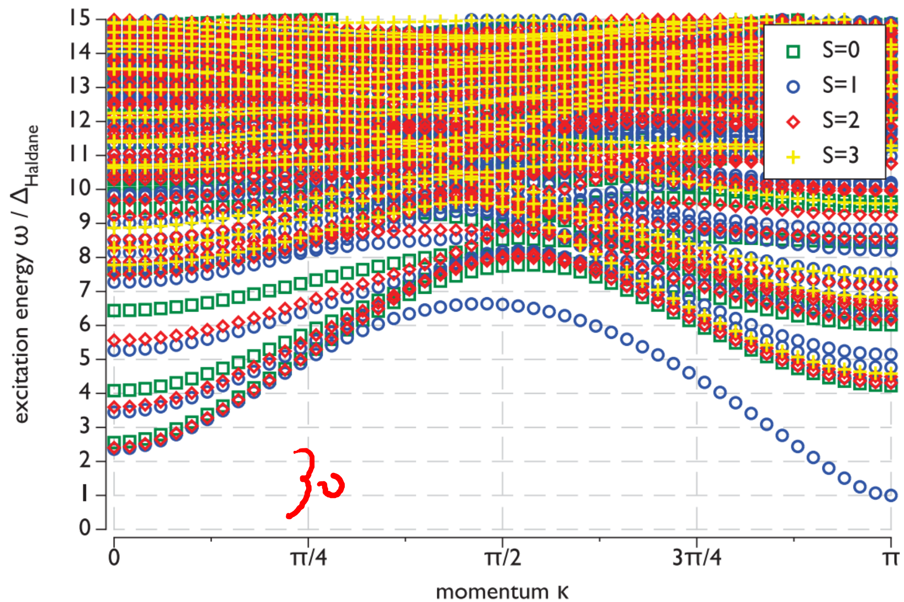
For $\chi = 256$

AD for ground state ~ 8h 10000 steps

Eigsolve for excitation state ~ 500s

Heisenberg $S = 1$ excitation spectrum

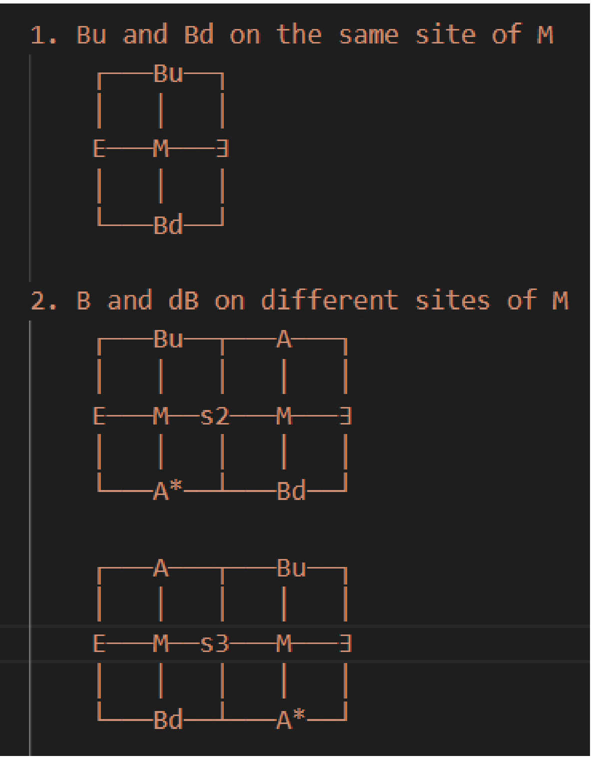




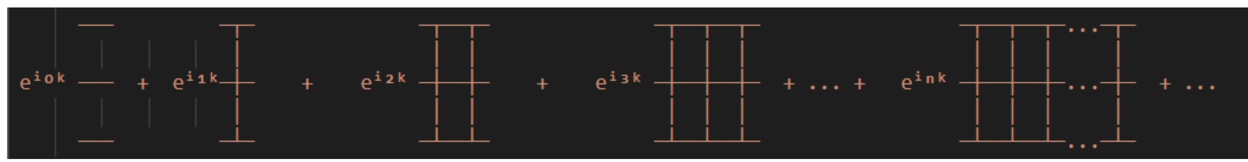
https://github.com/XingyuZhang2018/AD_Excitation/blob/main/project/result.pdf

result.pdf

MPO graph summation



s2



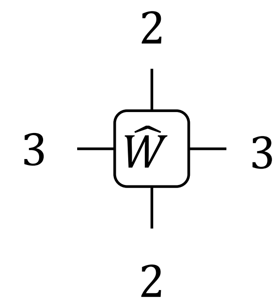
MPO

- TFIsing

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

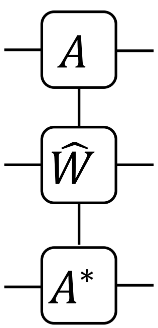
$$\hat{W} = \begin{bmatrix} \mathbb{1} & 0 & 0 \\ -JX & \lambda\mathbb{1} & 0 \\ -hZ & X & \mathbb{1} \end{bmatrix}$$

$\lambda < 1$



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

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



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

Overlap(E, Ǝ) = 0   E王Ǝ = 0

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

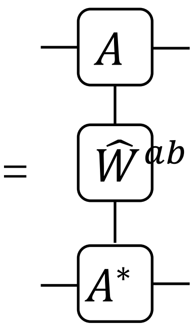
Fixed point equations

- Left and right environment EƎ

$$\text{C}_a = \text{C}_a \text{⌶}^{aa} + \text{Ꞓ}_a \qquad \text{Ꞓ}_a = \textstyle\sum_{b>a} \text{C}_b\, \text{⌶}^{ba}$$

$$\text{Ↄ}_a = \text{⌶}^{aa}\text{Ↄ}_a + \text{Э}_a \qquad \text{Э}_a = \textstyle\sum_{b<a} \text{⌶}^{\mathrm{ab}}\, \text{Ↄ}_b$$

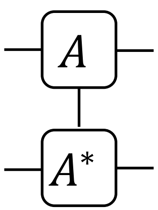
$\text{⌶}^{ab} =$



- $\text{⌶}^{aa} = 0$

$$\text{C}_a = \text{Ꞓ}_a$$
$$\text{Ↄ}_a = \text{Э}_a$$

$\text{⌶} =$



- $\text{⌶}^{aa} = \lambda_a \text{⌶}$

$$\text{C}_a = \lambda_a \text{C}_a \text{⌶} + \text{Ꞓ}_a \qquad \text{C}_a(1 - \lambda_a \text{⌶}) = \text{Ꞓ}_a$$
$$\text{Ↄ}_a = \lambda_a \text{⌶}\text{Ↄ}_a + \text{Э}_a \qquad (1 - \lambda_a \text{⌶})\text{Ↄ}_a = \text{Э}_a$$

- $\text{⌶}^{aa} = \text{⌶}$

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

$$\text{C}_a(1 - \text{⌶}) = \text{Ꞓ}_a$$
$$(1 - \text{⌶})\text{Ↄ}_a = \text{Э}_a$$

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

$$\text{C}_a(1 - \text{⌶} - \text{ɔc}) = \text{Ꞓ}_a - \text{Ꞓ}_a\text{ɔc}$$
$$(1 - \text{⌶} - \text{ɔc})\text{Ↄ}_a = \text{Э}_a - \text{ɔc}\text{Э}_a$$
$$\text{energy} = \text{c}\text{Э}_w = \text{Ꞓ}_1 \text{ɔ}$$

(一 上 一)

$e - e'$

$$\frac{(一 下 \neq (一}{下) \neq 一)}$$

(王)

k

(卅)

e

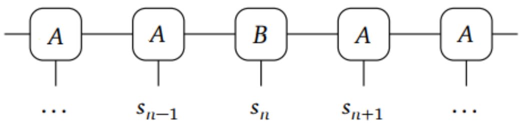
$w =$

2D excitation spectrum on helix

Xingyu Zhang
2023.1.5

Review and contents

$$|\Phi(B)_k\rangle = \sum_n e^{ikn} \ldots$$



single-mode approximation → 1D excitation spectrum

Graph summation → Eigen equation

Orthogonal Parameterization

Two site Hamiltonian

MPO (much simpler! quasi fixed points) → 2D excitation spectrum

1D to 2D

cylinders

helix

Large unit cell; k_y is not a good quantum number

Single unit cell; k_y is a good quantum number

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,‡]
[1] *Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China.*
[2] *School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China.*
[3] *Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China.*
[4] *Beijing Academy of Quantum Information Sciences, Beijing, China.*

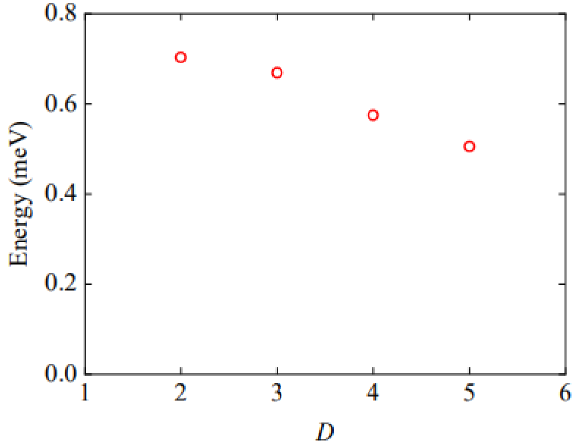
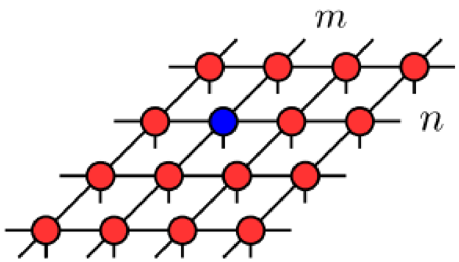


FIG. S2. **Minimal spectral gap as a function of bond dimension** D**.** The lowest spectral gap of the XXZ model occurs at the K point (see. Fig. S1) in the Brillouin zone. The gap values are obtained by contracting the effective Hamiltonian tensor network states of the excited states using the corner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

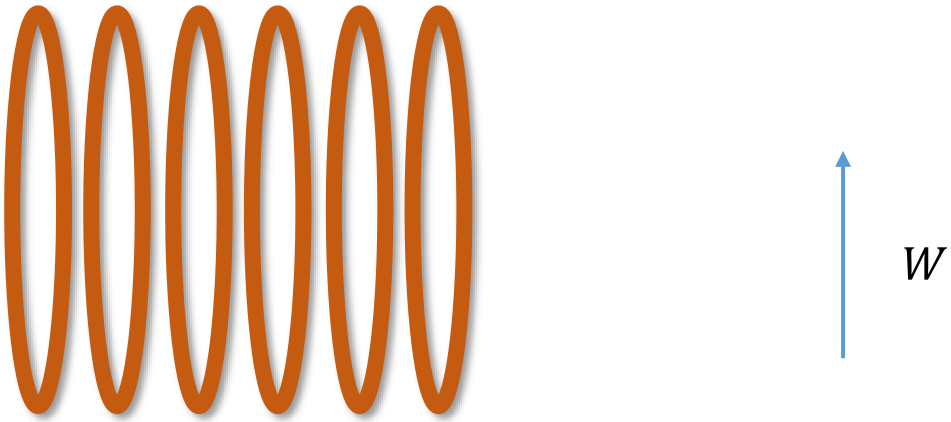
$$|\Phi_{\kappa_x\kappa_y}(B)\rangle = \sum_{m,n} \mathrm{e}^{i(\kappa_x m + \kappa_y n)}$$



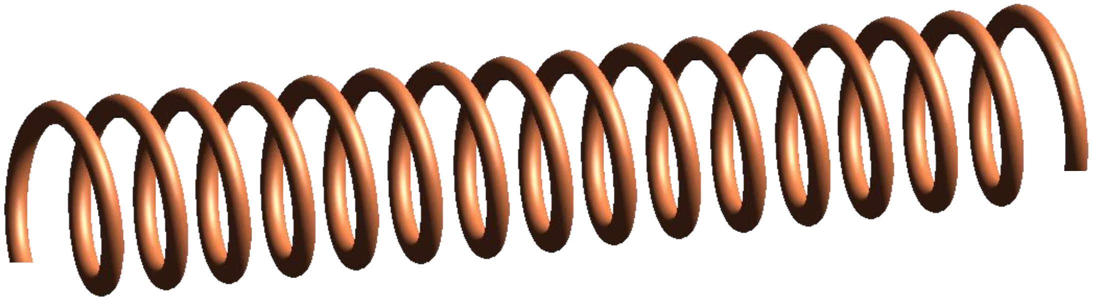
- High computational cost
- No innovation point

1D→2D map

- Cylinder



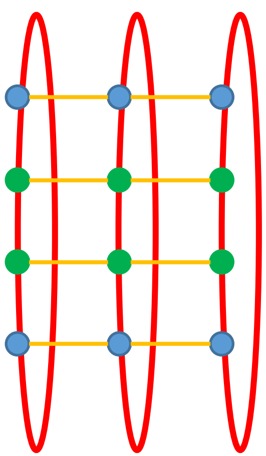
- Helix

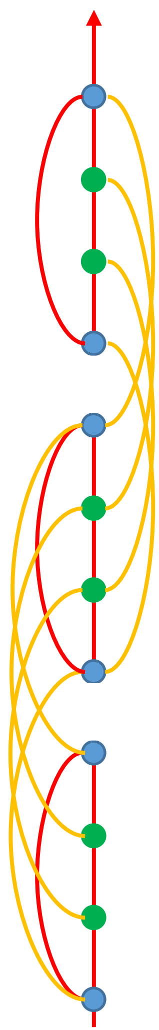


1D→2D map

$W = 4$ for example

- Cylinder





NN

1,3,4 A_1

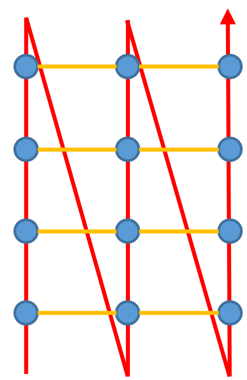
1, 4 A_2

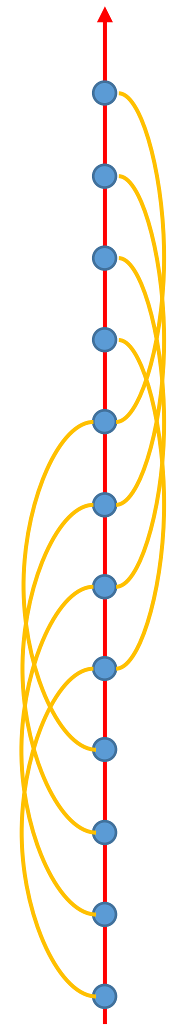
1, 4 A_2

1,3,4 A_1

Unit cell length=4

- Helix





NN

1, 4 A

1, 4 A

1, 4 A

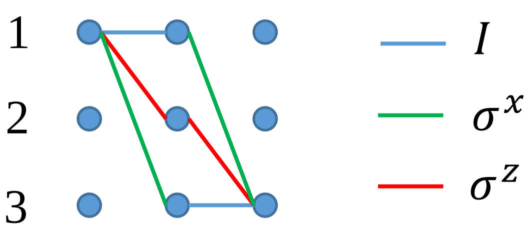
1, 4 A

Single unit!

MPO from matrix product (MP) diagram

- 1D TFIsing

$$H = \sum_i -\sigma_i^z \sigma_{i+1}^z - \lambda \sigma_i^x$$
$$= -\sigma_1^z \sigma_2^z I_3 I_4 \dots - \sigma_1^x I_2 I_3 I_4$$
$$-I_1 \sigma_2^z \sigma_3^z I_4 \dots - I_1 \sigma_2^x I_3 I_4$$
$$-I_1 I_2 \sigma_3^z \sigma_4^z \dots - I_1 I_2 \sigma_3^x I_4$$

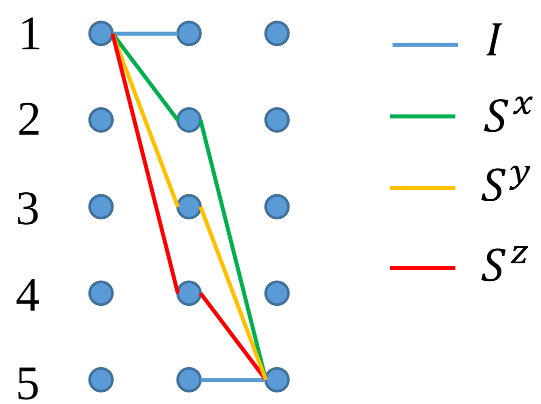


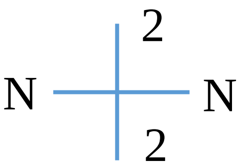
$$M = \begin{bmatrix} I & -\sigma^z & -\sigma^x \\ 0 & 0 & \sigma^z \\ 0 & 0 & I \end{bmatrix}$$

$N = 3$

- 1D Heisenberg

$$H = \sum_i S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z$$





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

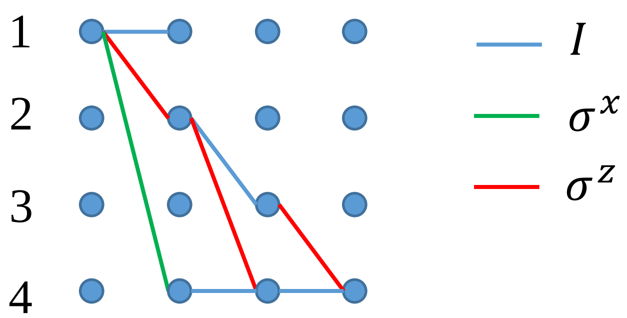
$N = 5$

PHYSICAL REVIEW B 89, 214203 (2014)

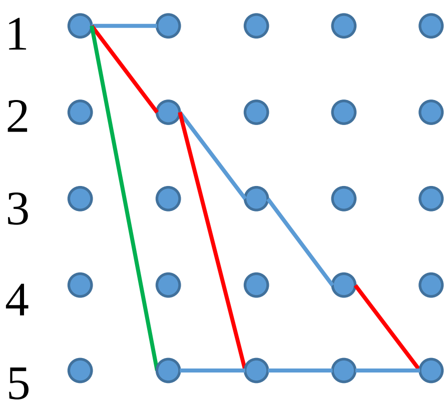
MPO from matrix product (MP) diagram

- TFIsing

NN NN-2



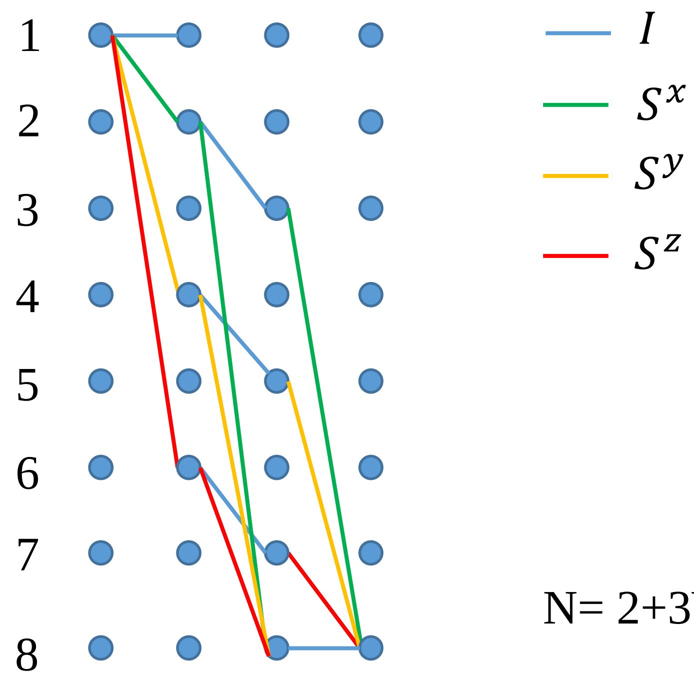
NN NN-3



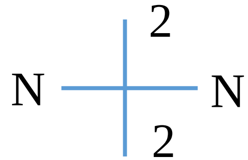
N=2+W

- Heisenberg

NN NN-2



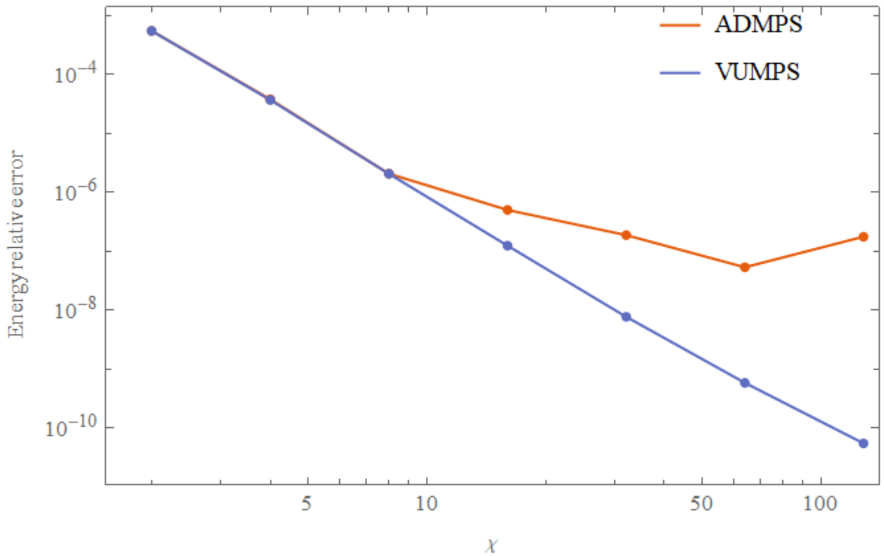
N= 2+3W



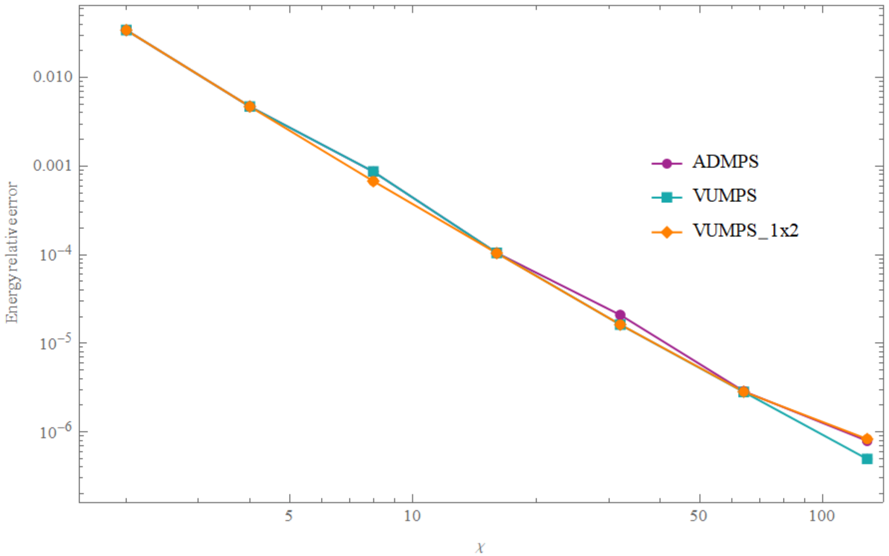
Ground state vumps

- 1D TFIsing NN

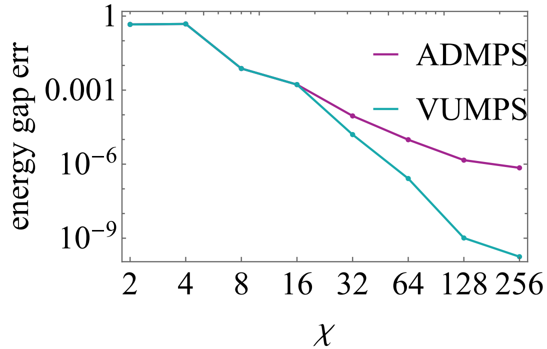
$\lambda_c = 1$



- 1D Heisenberg NN



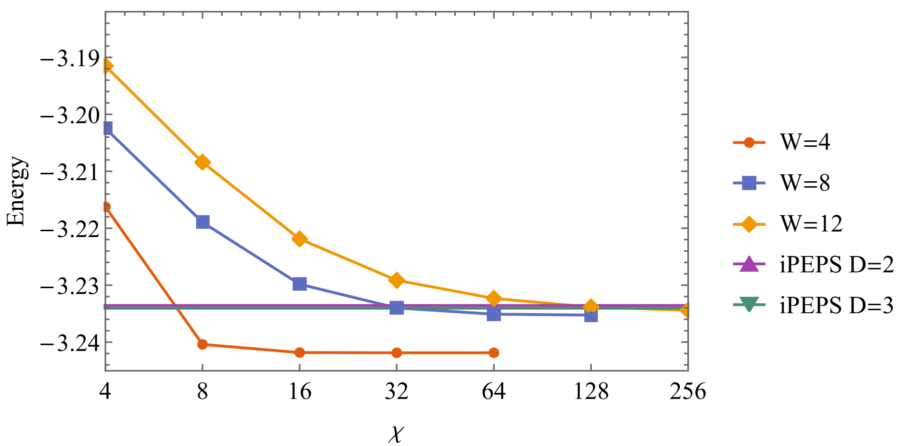
$S = 1$ Haldane gap

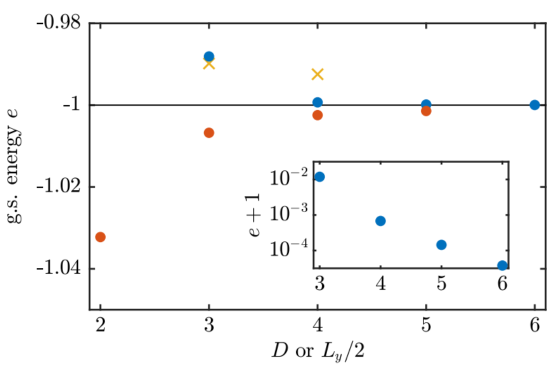


Ground state vumps

- 2D TFIsing

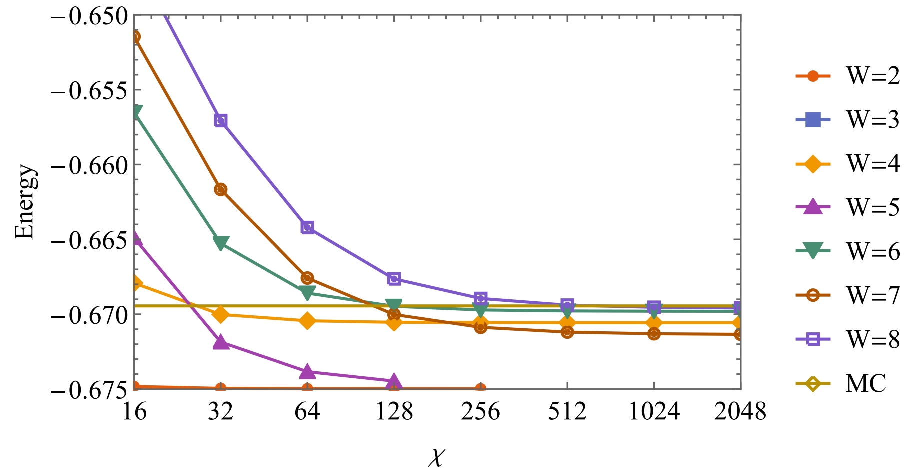
$\lambda_c = 3.04438$

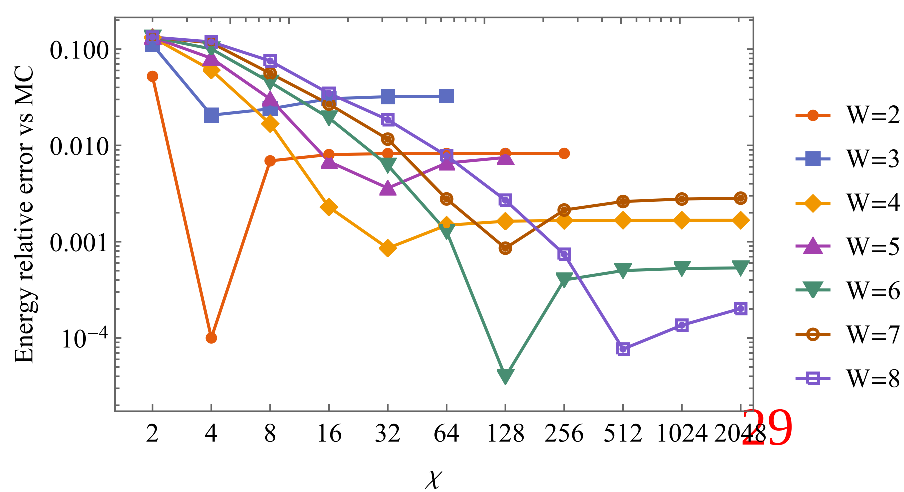




- Different approach with D v.s. W
- Nonmonotonicity with W and χ

- 2D Heisenberg NN

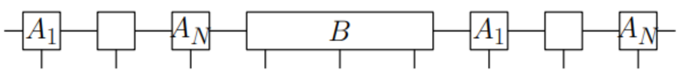




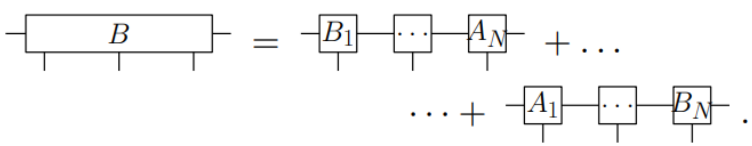
excitation spectrum

- Cylinder

$$|\Phi_{p_x}(B)\rangle = \sum_n \mathrm{e}^{ip_x n} T_x^n$$

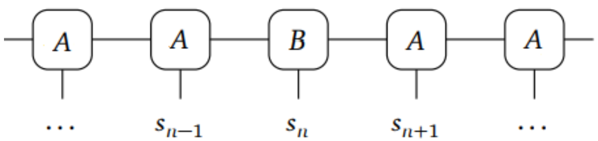


with



- Helix

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



No k_y because k_y is not a good quantum number

k_y is a good quantum number

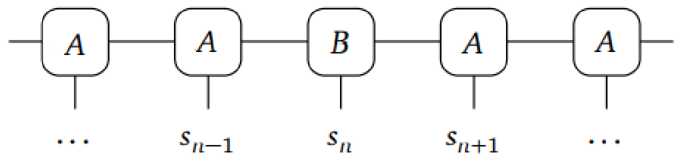
Recover by directly calculating

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

arXiv:2102.10982v2

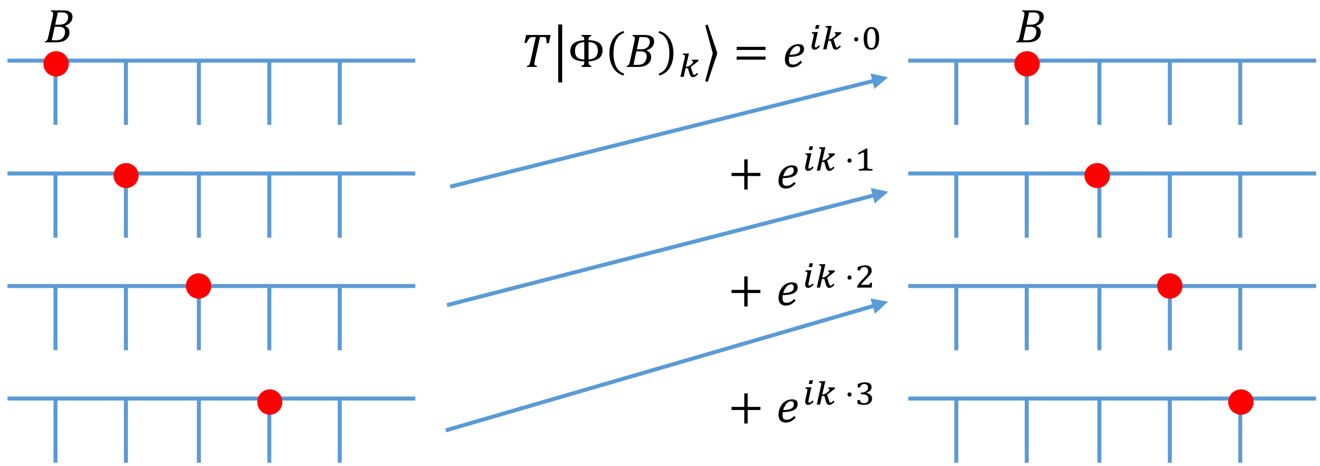
translation operator

$$|\Phi(B)_k\rangle = \sum_n e^{ikn} \ldots$$



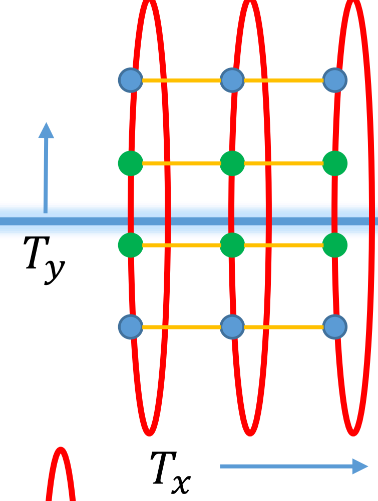
$$\left|\Phi(B)_k\right\rangle = e^{ik\cdot 0} + e^{ik\cdot 1} + e^{ik\cdot 2} + e^{ik\cdot 3}$$

$$T\left|\Phi(B)_k\right\rangle = e^{ik\cdot 0} + e^{ik\cdot 1} + e^{ik\cdot 2} + e^{ik\cdot 3}$$



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

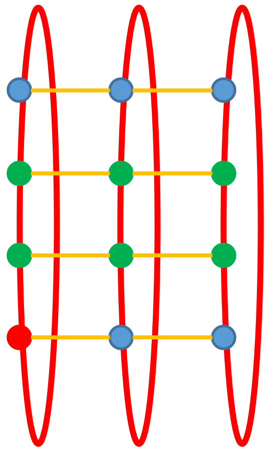
translation operator T_y



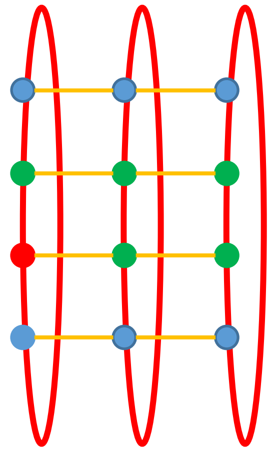
$W = 4$ for example

- Cylinder

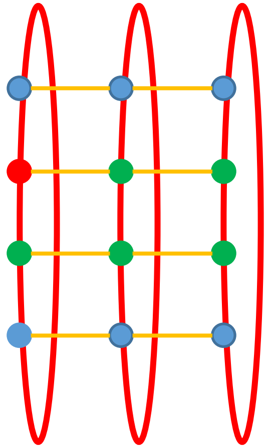
$T_y \left| \Phi(B)_{k_x,k_y} \right\rangle = e^{ik_x \cdot 0 + ik_y \cdot 0}$



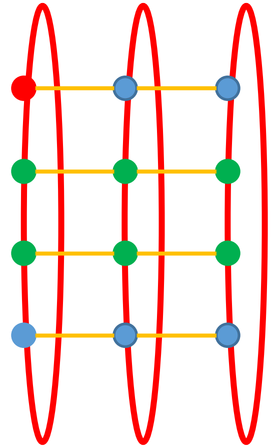
$+\, e^{ik_x \cdot 0 + ik_y \cdot 1}$



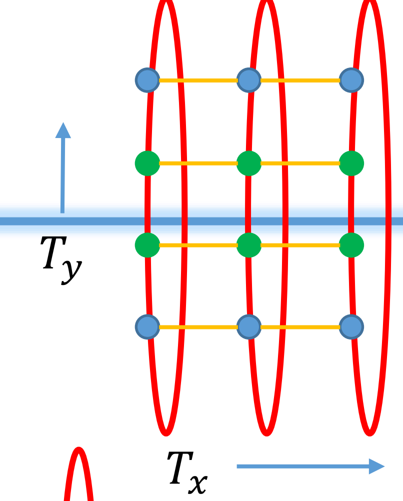
$+ e^{ik_x \cdot 0 + ik_y \cdot 2}$



$+\, e^{ik_x \cdot 0 + ik_y \cdot 3}$



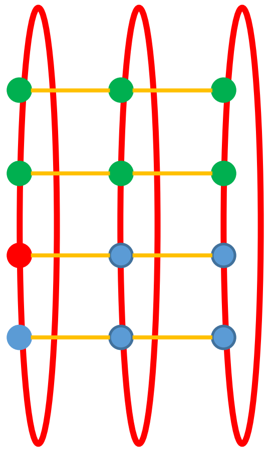
translation operator T_y



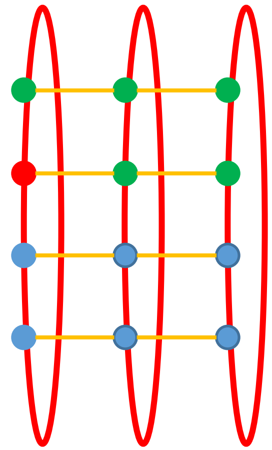
$W = 4$ for example

- Cylinder

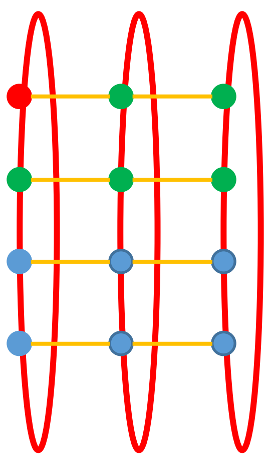
$T_y\left|\Phi(B)_{k_x,k_y}\right\rangle = e^{ik_x\cdot 0+ik_y\cdot 0}$



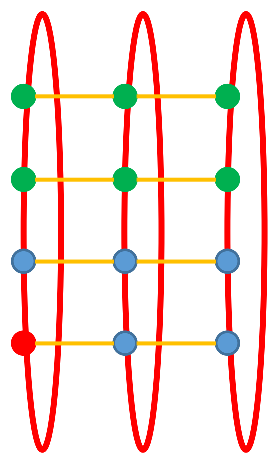
$+\, e^{ik_x\cdot 0+ik_y\cdot 1}$

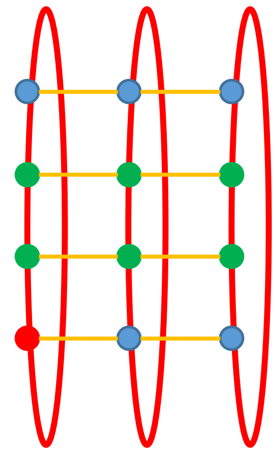


$+e^{ik_x\cdot 0+ik_y\cdot 2}$



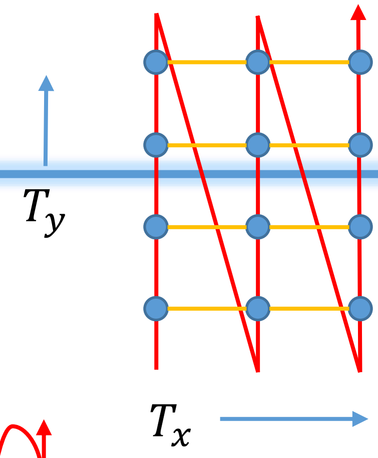
$+\, e^{ik_x\cdot 0+ik_y\cdot 3}$





k_y is not a good quantum number!

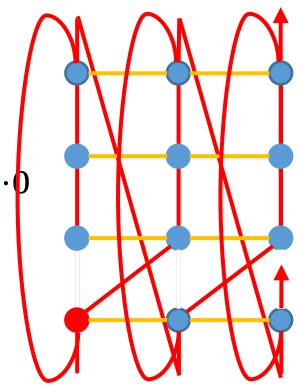
translation operator T_y



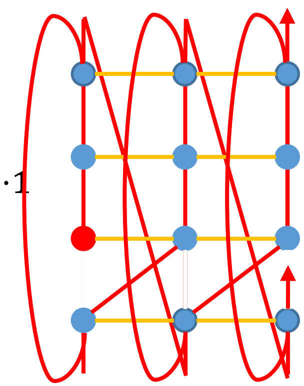
$W = 4$ for example

- Helix

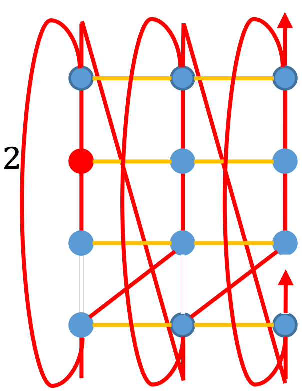
$T_y\left|\Phi(B)_{k_x,k_y}\right\rangle = e^{ik_x\cdot 0+ik_y\cdot 0}$



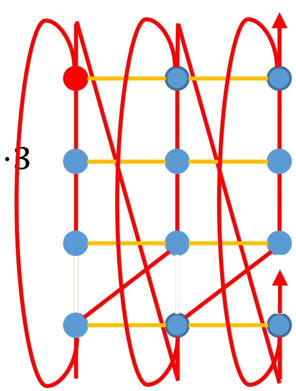
$+\, e^{ik_x\cdot 0+ik_y\cdot 1}$



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



$+\, e^{ik_x\cdot 0+ik_y\cdot 3}$



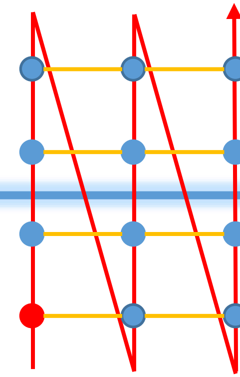
k_y is a good quantum number!

Graph summation

```
1. Bu and Bd on the same site of M
    ┌───Bu──┐
    │   │   │
    E───M───Ǝ
    │   │   │
    └───Bd──┘
2. B and dB on different sites of M
    ┌───Bu──┬───A───┐
    │   │   │   │   │
    E───M──s2───M───Ǝ
    │   │   │   │   │
    └───A*──┴───Bd──┘
    ┌───A───┬───Bu──┐
    │   │   │   │   │
    E───M──s3───M───Ǝ
    │   │   │   │   │
    └───Bd──┴───A*──┘
    s2 = sum of `eⁱᵏ 王` series:
       ───           ─┬─            ─┬──┬─            ─┬──┬──┬─              ─┬──┬──┬──...─┬─
        │   │   │     │              │  │              │  │  │                │  │  │      │
 eⁱ⁰ᵏ  ───   +  eⁱ¹ᵏ ─┼─    +   eⁱ²ᵏ ─┼──┼─    +   eⁱ³ᵏ ─┼──┼──┼─  + ... + eⁱⁿᵏ ─┼──┼──┼──...─┼─  + ...
        │   │   │     │              │  │              │  │  │                │  │  │      │
       ───           ─┴─            ─┴──┴─            ─┴──┴──┴─              ─┴──┴──┴──...─┴─
```

Graph summation

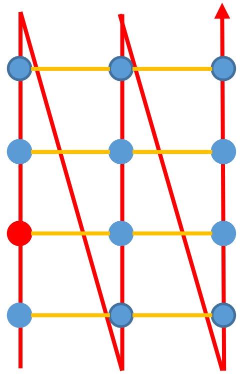
$| \quad \rangle = e^{ik\cdot 0+ik_y\cdot 0}$

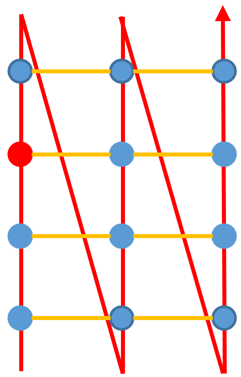


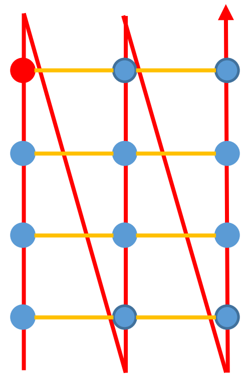
$W = 4$ for example

$S^{+}{}_{1} = e^{ik_x\cdot 0+ik_y\cdot 1}$三 $+\ e^{ik_x\cdot 0+ik_y\cdot 2}$王 $+\ e^{ik_x\cdot 0+ik_y\cdot 3}$王^{2}

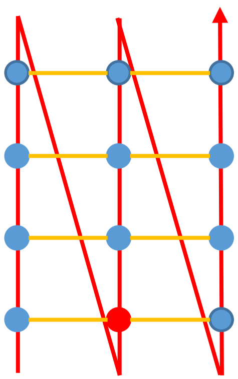
$\langle \quad | =$

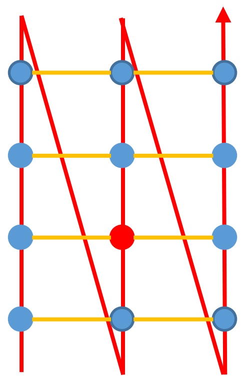


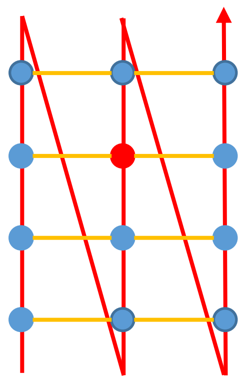


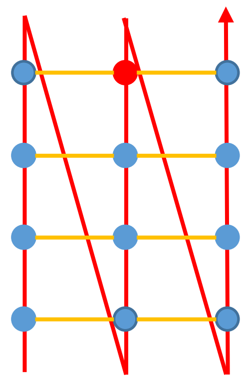


$+e^{ik_x\cdot 1+ik_y\cdot 0}$王^{3} $+\ e^{ik_x\cdot 1+ik_y\cdot 1}$王^{4} $+\ e^{ik_x\cdot 1+ik_y\cdot 2}$王^{5} $+\ e^{ik_x\cdot 1+ik_y\cdot 3}$王^{6}









Graph summation

$$S^{+_1} = \left(e^{ik_x\cdot 0+ik_y\cdot 1}三 + e^{ik_x\cdot 0+ik_y\cdot 2}王 + e^{ik_x\cdot 0+ik_y\cdot 3}王^2 + e^{ik_x\cdot 1+ik_y\cdot 0}\ 王^3\right)\cdot \left(三 + e^{ik_x\cdot 1}王^4 + e^{ik_x\cdot 2}王^8 + \cdots\right)$$

$$\equiv \left(e^{ik_x\cdot 0+ik_y\cdot 1}三 + e^{ik_x\cdot 0+ik_y\cdot 2}王 + e^{ik_x\cdot 0+ik_y\cdot 3}王^2 + e^{ik_x\cdot 1+ik_y\cdot 0}\ 王^3\right)S_4^+$$

$$S^+ = S^{+_1} + S^{+_2} + S^{+_3} + S^{+_4}$$
$$= \left(\left(3e^{ik_x\cdot 0+ik_y\cdot 1} + e^{ik_x\cdot 1-ik_y\cdot 3}\right)三 + \left(2e^{ik_x\cdot 0+ik_y\cdot 2} + 2e^{ik_x\cdot 1-ik_y\cdot 2}\right)王 + \left(e^{ik_x\cdot 0+ik_y\cdot 3}+3e^{ik_x\cdot 1-ik_y\cdot 1}\right)王^2 + 4e^{ik_x\cdot 1+ik_y\cdot 0}\ 王^3\right)S_4^+$$

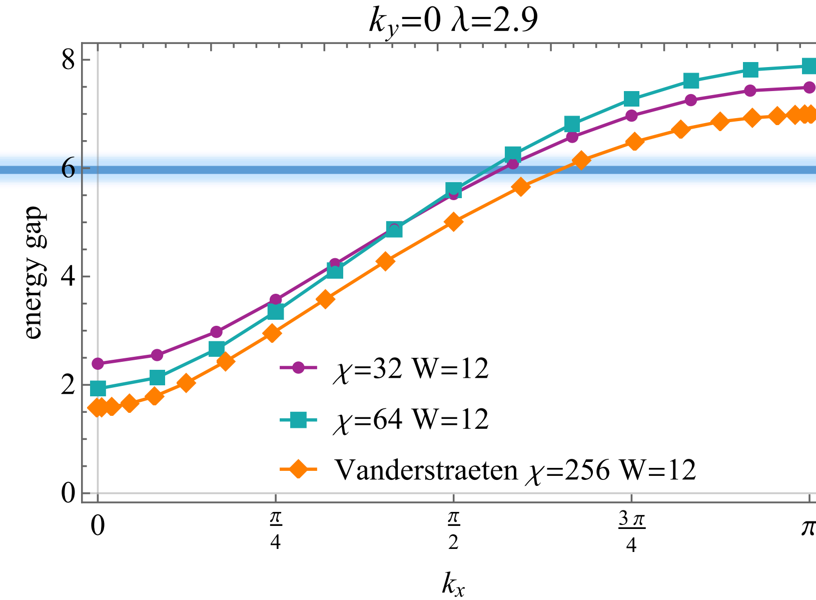
Same way:

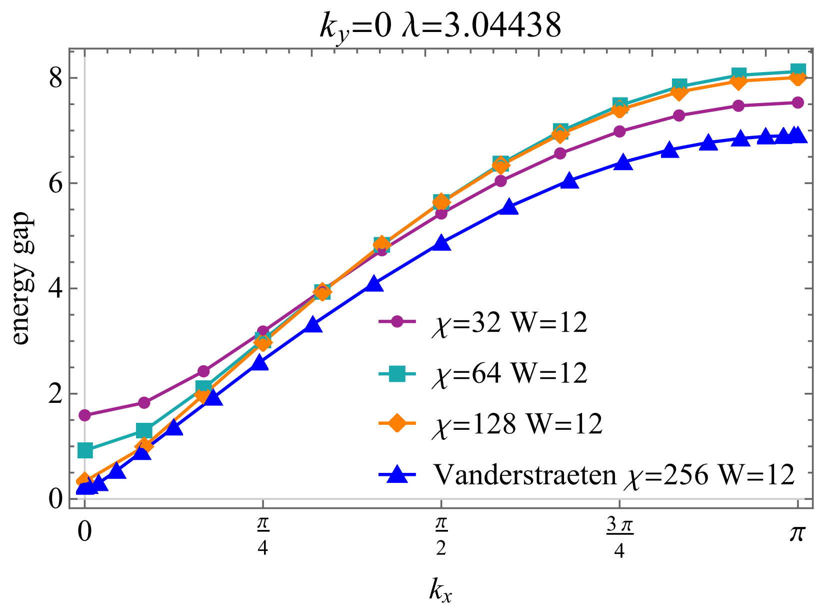
$$S^- = S^{-_1} + S^{-_2} + S^{-_3} + S^{-_4}$$
$$= \left(\left(3e^{ik_x\cdot 0-ik_y\cdot 1} + e^{-ik_x\cdot 1+ik_y\cdot 3}\right)三 + \left(2e^{ik_x\cdot 0-ik_y\cdot 2} + 2e^{-ik_x\cdot 1+ik_y\cdot 2}\right)王 + \left(e^{ik_x\cdot 0-ik_y\cdot 3}+3e^{-ik_x\cdot 1+ik_y\cdot 1}\right)王^2 + 4e^{-ik_x\cdot 1+ik_y\cdot 0}\ 王^3\right)S_4^-$$

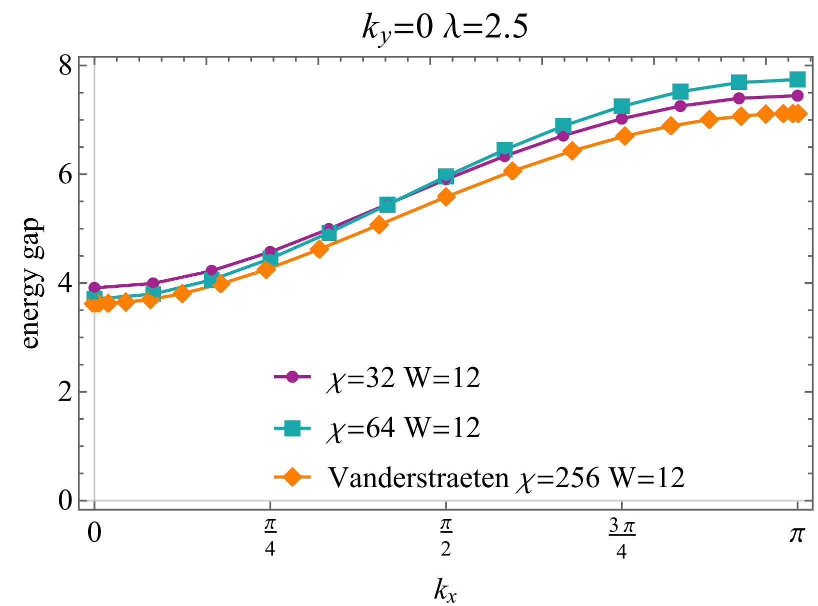
$$S_4^- = \left(三 + e^{-ik_x\cdot 1}王^4 + e^{-ik_x\cdot 2}王^8 + \cdots\right)$$

result

- 2D TFIsing $k_y = 0$

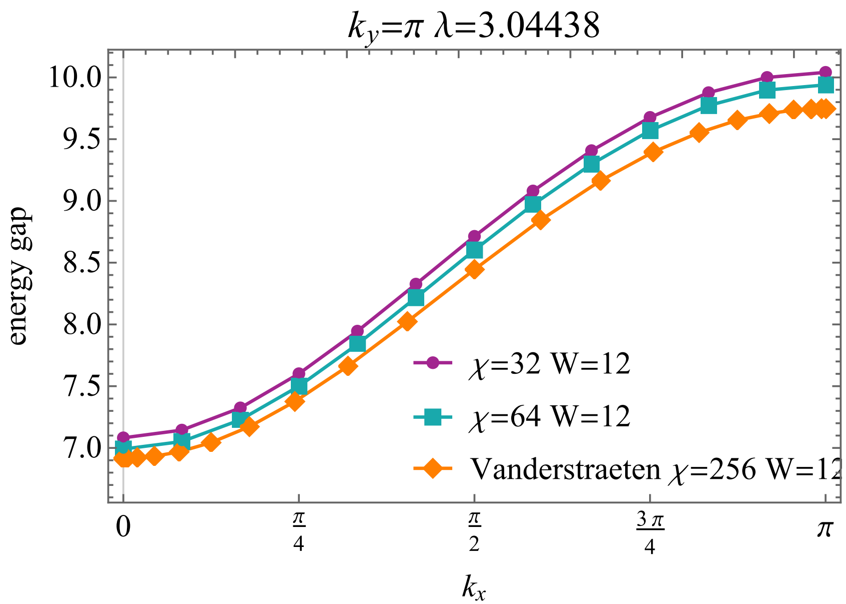


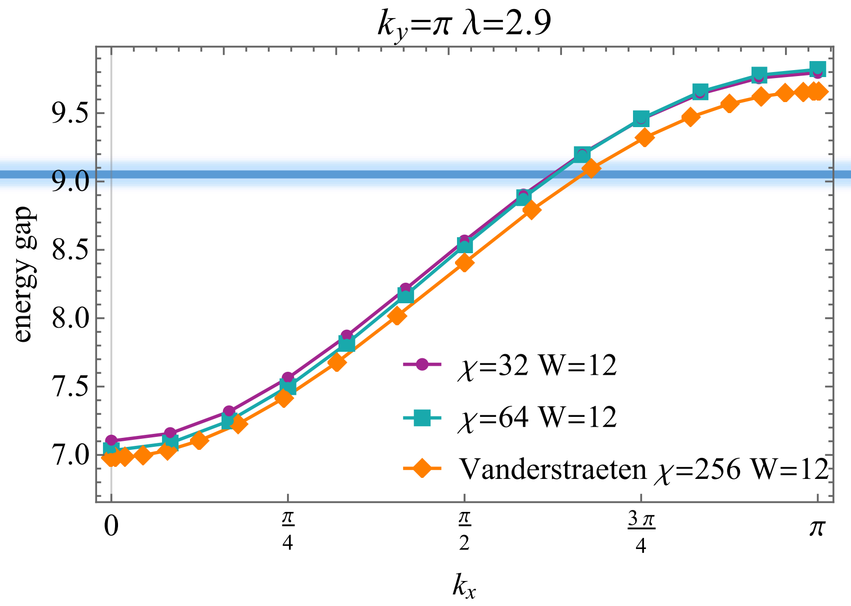


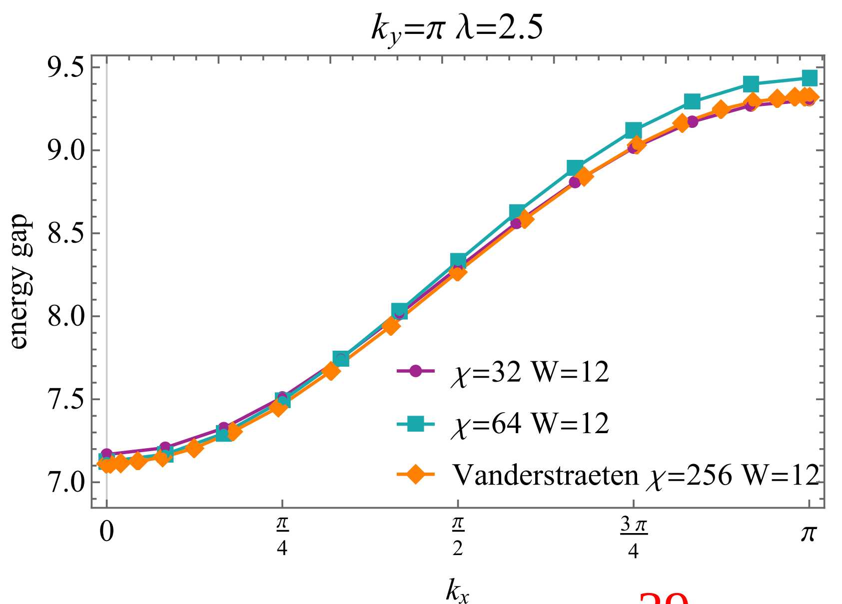


result

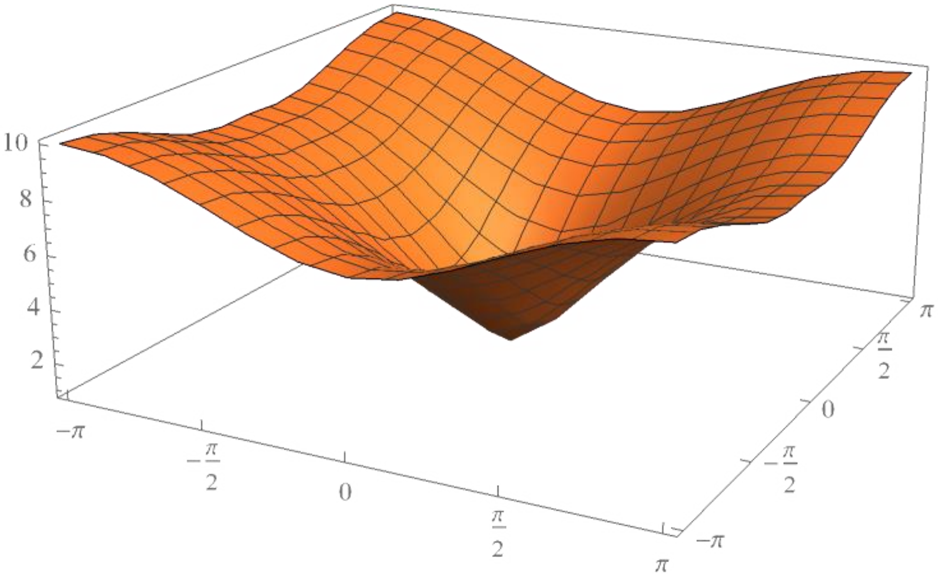
- 2D TFIsing $k_y = \pi$



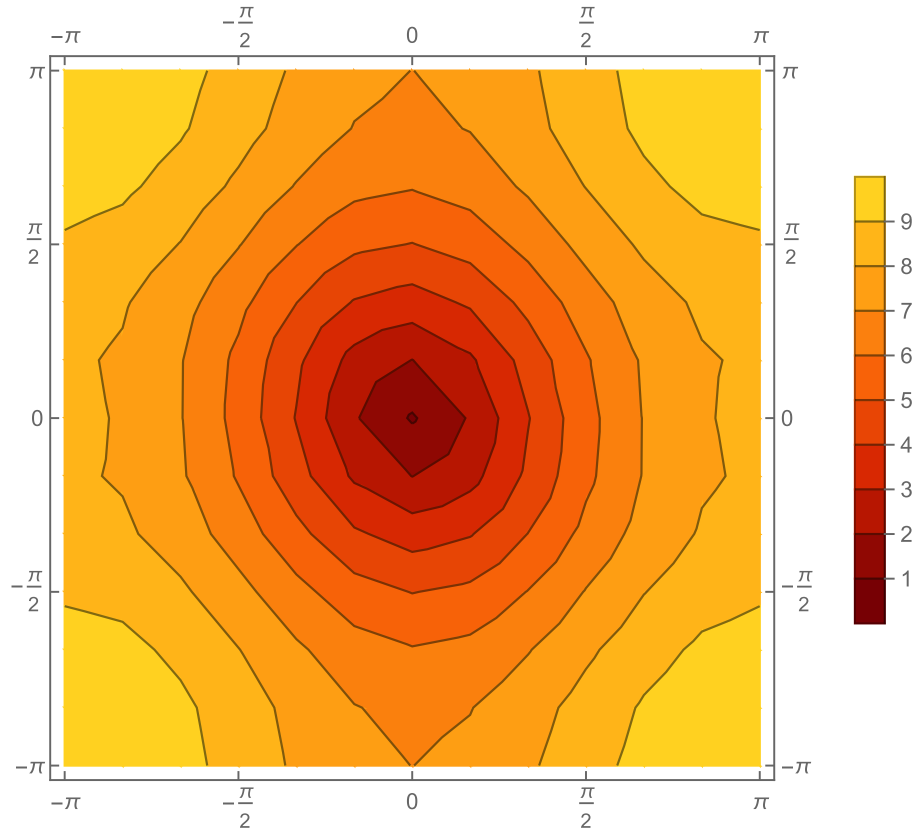




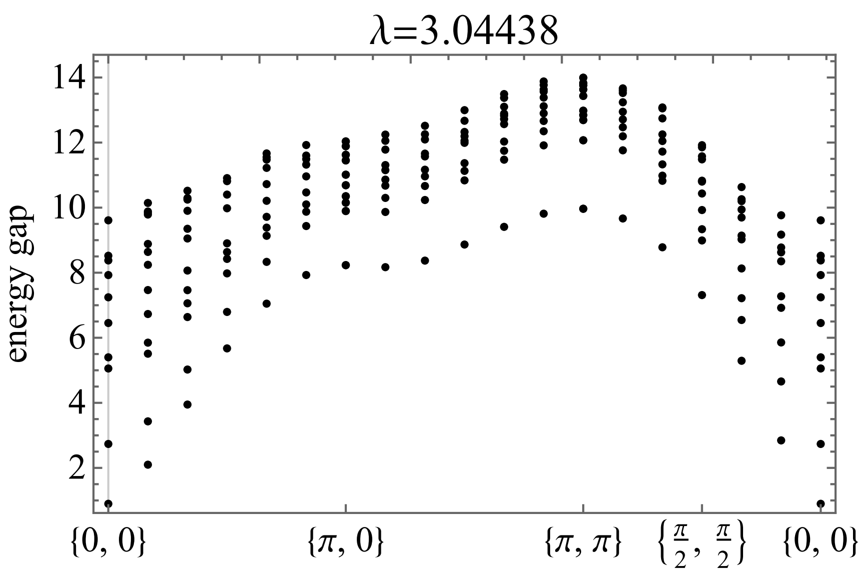
result



10
8
6
4
2
$-\pi$
$-\frac{\pi}{2}$
0
$\frac{\pi}{2}$
π



$-\pi$
$-\frac{\pi}{2}$
0
$\frac{\pi}{2}$
π
1
2
3
4
5
6
7
8
9



λ=3.04438
energy gap
14
12
10
8
6
4
2
{0, 0}
{π, 0}
{π, π}
$\{\frac{\pi}{2}, \frac{\pi}{2}\}$
{0, 0}

outlook

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

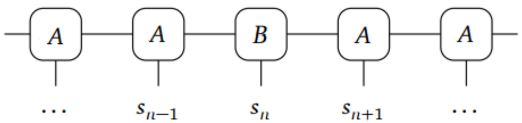
Thank you for listening!

Q&A?

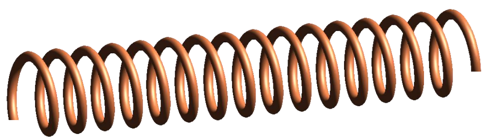
2D excitation spectrum on helix

Xingyu Zhang
2023.3.31

Review

$|\Phi(B)_k\rangle = \sum_n e^{ikn} \ldots$ 

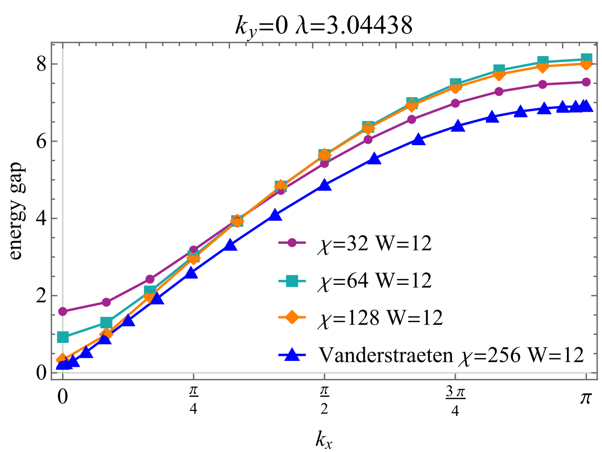
single-mode approximation → 1D excitation spectrum

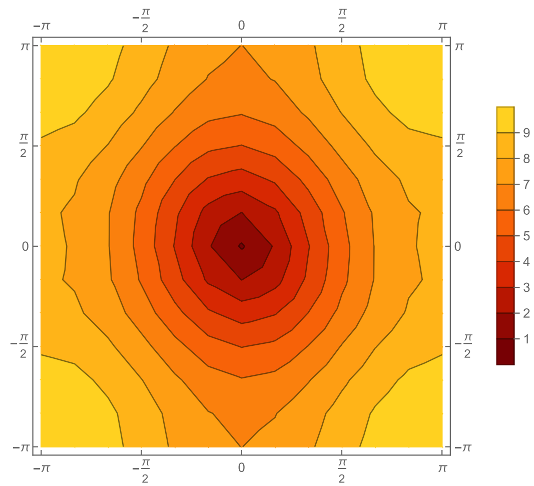


helix { Single unit cell
good quantum number

2D excitation spectrum

TFIsing result：

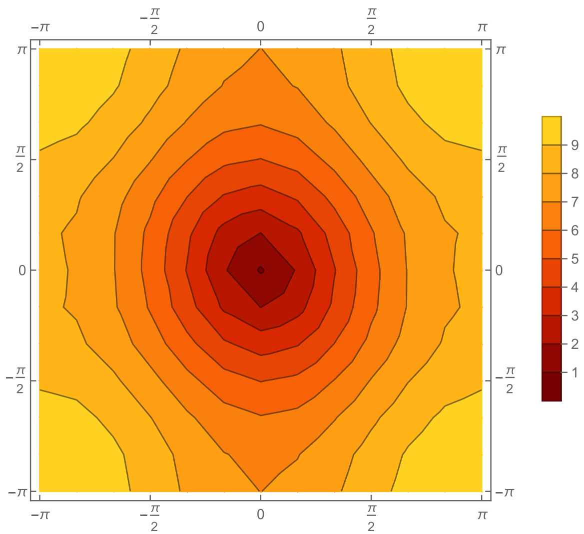


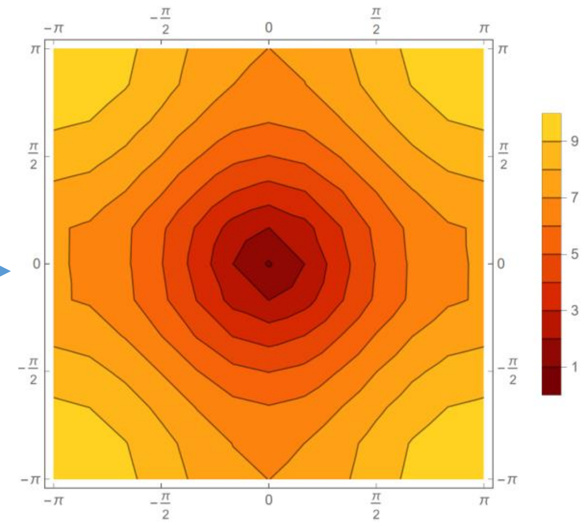


Non-symmetry by
Finite width effect

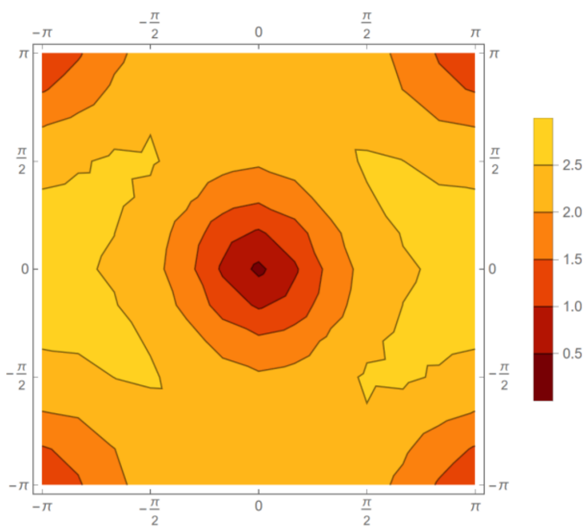
mitigate finite effect

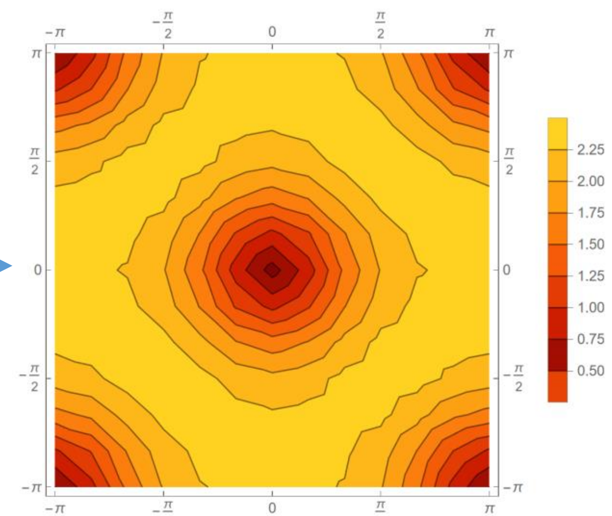
TFIsing





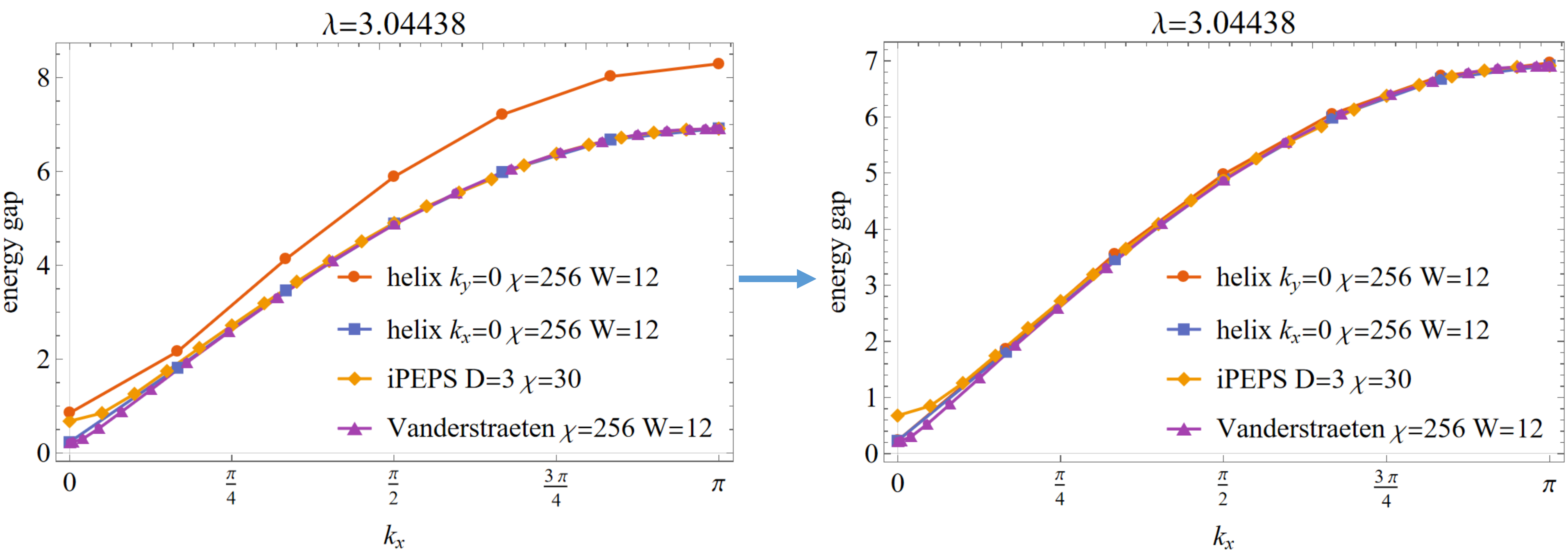
Heisenberg





$k_x = 0$ is more accurate

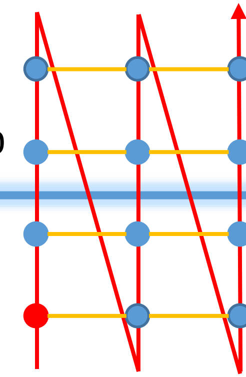
TFIsing



Graph summation

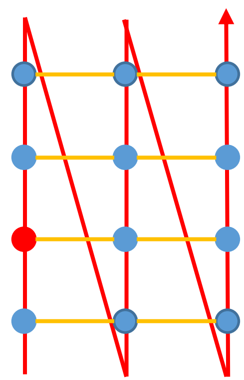
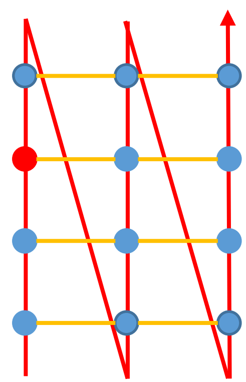
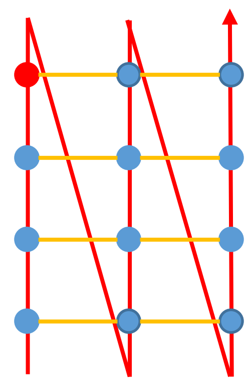
```
1. Bu and Bd on the same site of M
   │
   │   ┌───Bu──┐
   │   │   │   │
   │   E───M───Ǝ
   │   │   │   │
   │   └───Bd──┘
2. B and dB on different sites of M
   │   ┌───Bu──┬───A───┐
   │   │   │   │   │   │
   │   E───M──s2───M───Ǝ
   │   │   │   │   │   │
   │   └───A*──┴───Bd──┘
   │   ┌───A───┬───Bu──┐
   │   │   │   │   │   │
   │   E───M──s3───M───Ǝ
   │   │   │   │   │   │
   │   └───Bd──┴───A*──┘
   │   s2 = sum of `e^ik 王` series:
   │   │
   │   │  ───        ─┬─         ─┬──┬─         ─┬──┬──┬─          ─┬──┬──┬─...─┬─
   │   │   │   │   │   │          │  │           │  │  │            │  │  │     │
   e^i0k ───  +  e^i1k─┼─   +  e^i2k─┼──┼─   +  e^i3k─┼──┼──┼─ + ... + e^ink─┼──┼──┼─...─┼─  + ...
   │   │   │   │   │   │          │  │           │  │  │            │  │  │     │
   │   │  ───        ─┴─         ─┴──┴─         ─┴──┴──┴─          ─┴──┴──┴─...─┴─
```

Graph summation

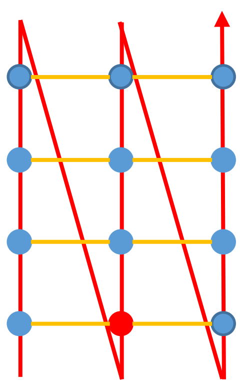
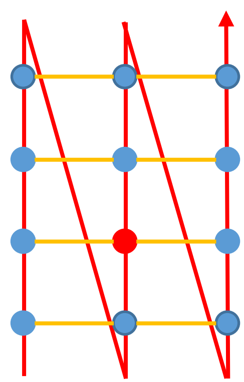
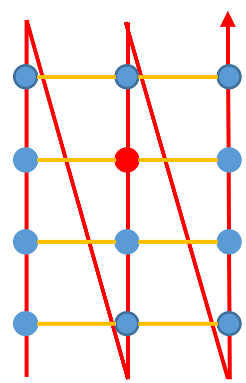
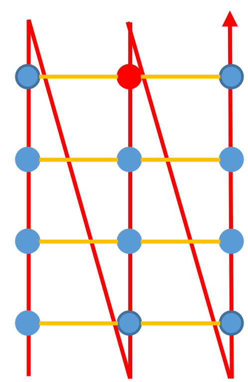
$| \quad \rangle = e^{ik \cdot 0+ik_y\cdot 0}$ 

$W = 4$ for example

$$S^{+}{}_{1} = e^{ik_x\cdot 0+ik_y\cdot 1}\text{三} + e^{ik_x\cdot 0+ik_y\cdot 2}\text{王} + e^{ik_x\cdot 0+ik_y\cdot 3}\text{王}^{2}$$

$\langle \quad | =$   

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

mitigate finite effect

The formula of the left environment general term is:

$$\sum_{j=1}^{W}\left(\frac{W-j+je^{ik_x}}{W}e^{ik_y\cdot j}\text{王}^{j-1}\right)\cdot\sum_{j=0}^{\infty}\left(e^{ik_x}\text{王}^{W}\right)^{j}$$

The right is just transformation of $(k_x,k_y)\rightarrow-(k_x,k_y)$

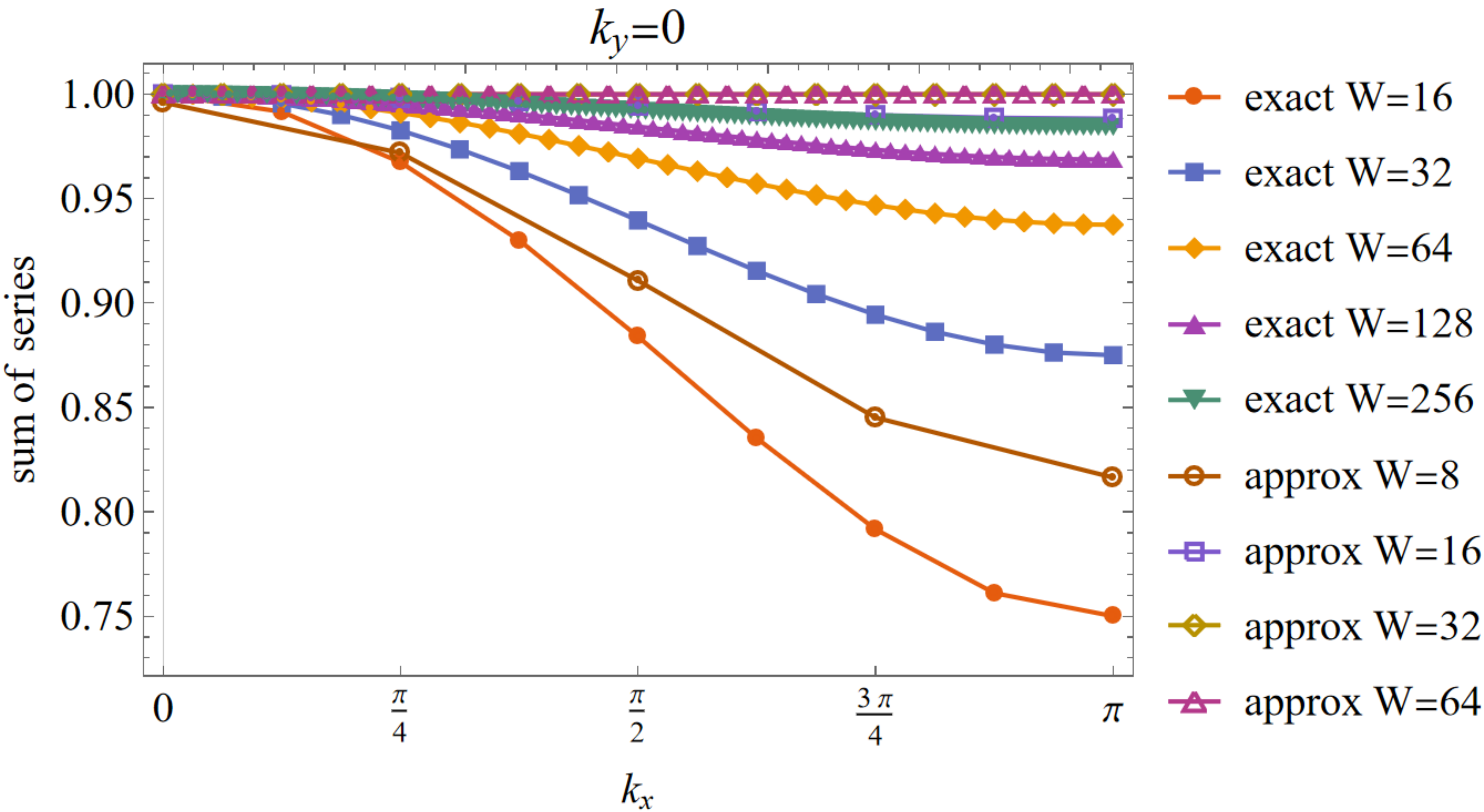
We do some approximation for the above equation:

$$\left(\sum_{j=1}^{\lceil W/2\rceil-1}\left(e^{ik_y\cdot j}\text{王}^{j-1}\right)+\frac{1+e^{ik_x}}{2}e^{ik_y\cdot\lceil W/2\rceil}\text{王}^{\lceil W/2\rceil-1}+\sum_{j=\lceil W/2\rceil+1}^{W}\left(e^{ik_x}e^{ik_y\cdot j}\text{王}^{j-1}\right)\right)\cdot$$
$$\sum_{j=0}^{\infty}\left(e^{ik_x}\text{王}^{W}\right)^{j}$$

$\lceil\rceil$ is ceil int. $W-j$ and je^{ik_x} compete with each other. We retain $W-j$ for the first $\lceil W/2\rceil-1$ terms and je^{ik_x} for the last $\lceil W/2\rceil-1$ terms, the mix them in the middle term.

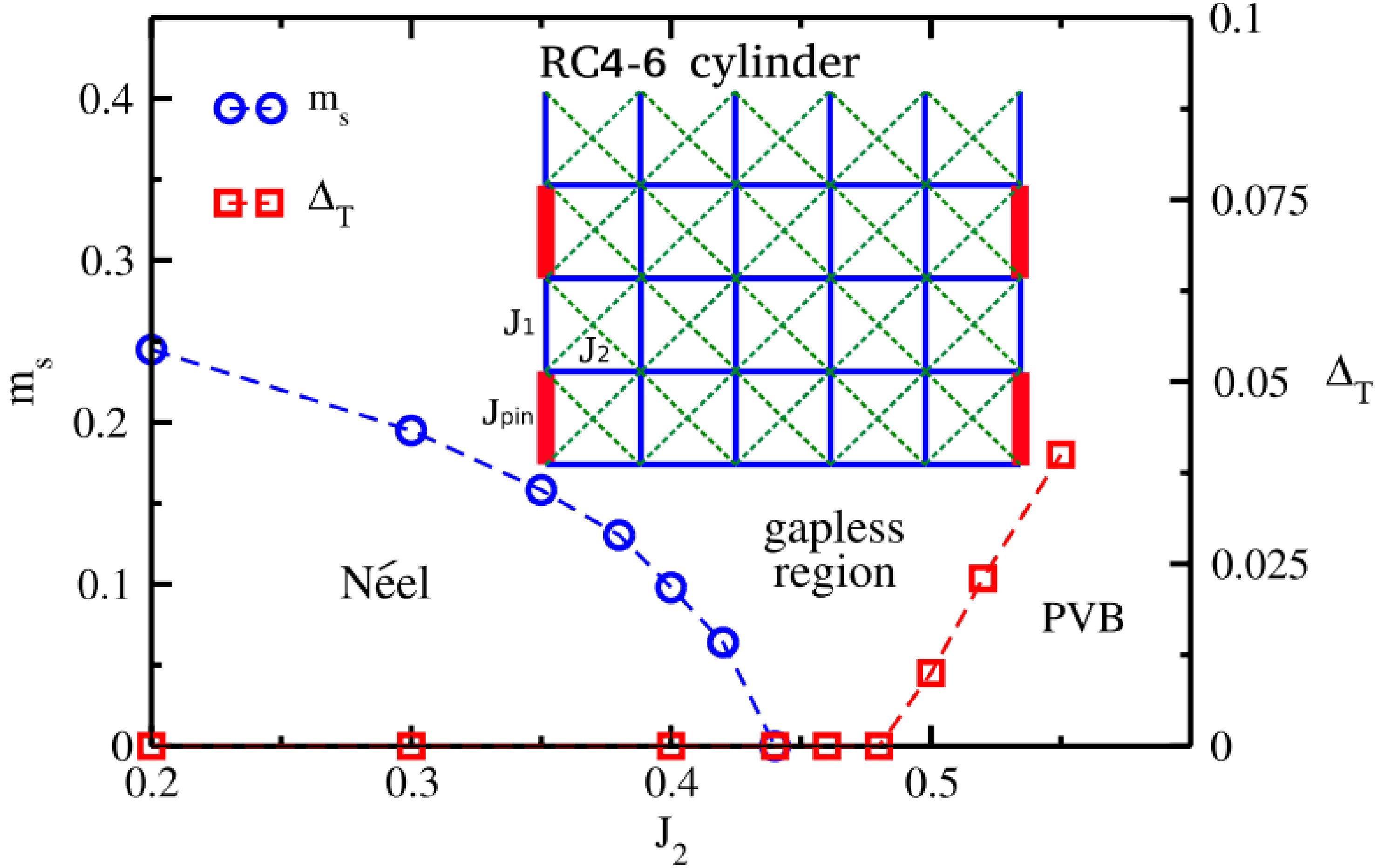
They both converge into $\dfrac{e^{ik_y}\text{王}}{1-e^{ik_y}\text{王}}\cdot\sum_{j=0}^{\infty}\left(e^{ik_x}\text{王}^{W}\right)^{j}$ when $W\rightarrow\infty$

asymptotic behavior



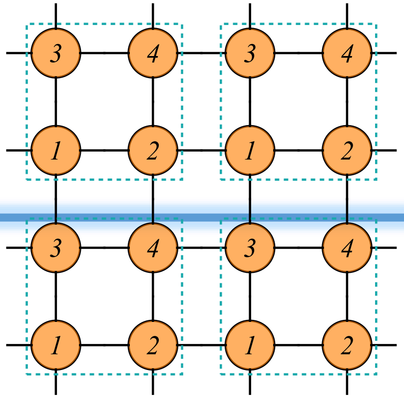
Prepare for $J_1 - J_2$ model

- $$H = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j.$$

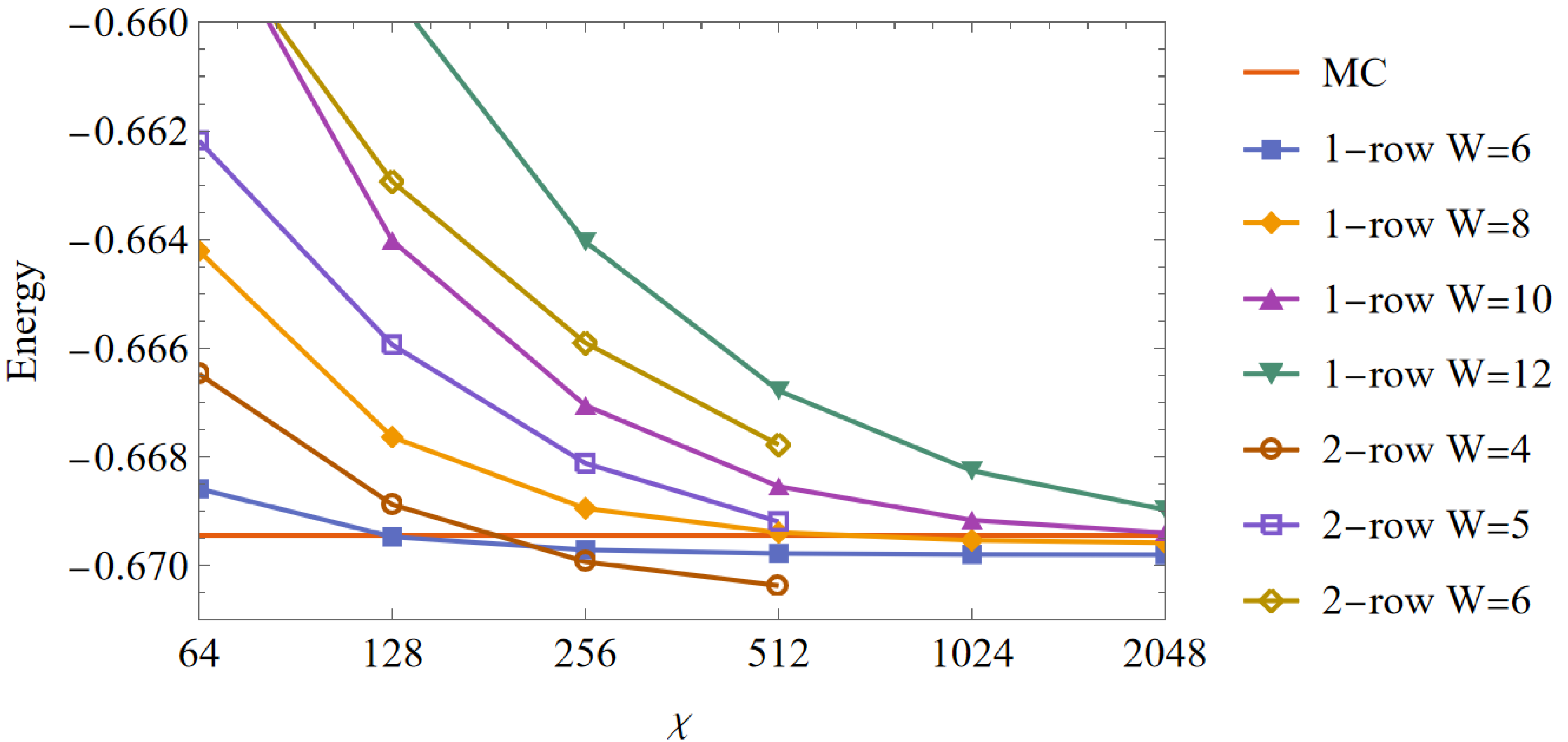


PRL 113, 027201 (2014)

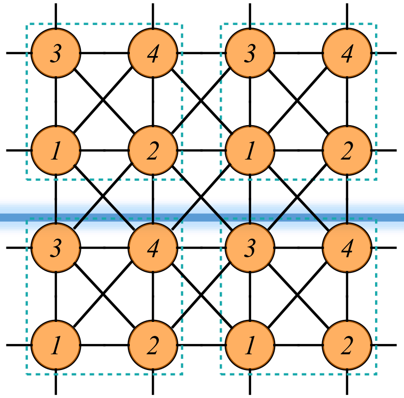
Merge 4 site ground energy



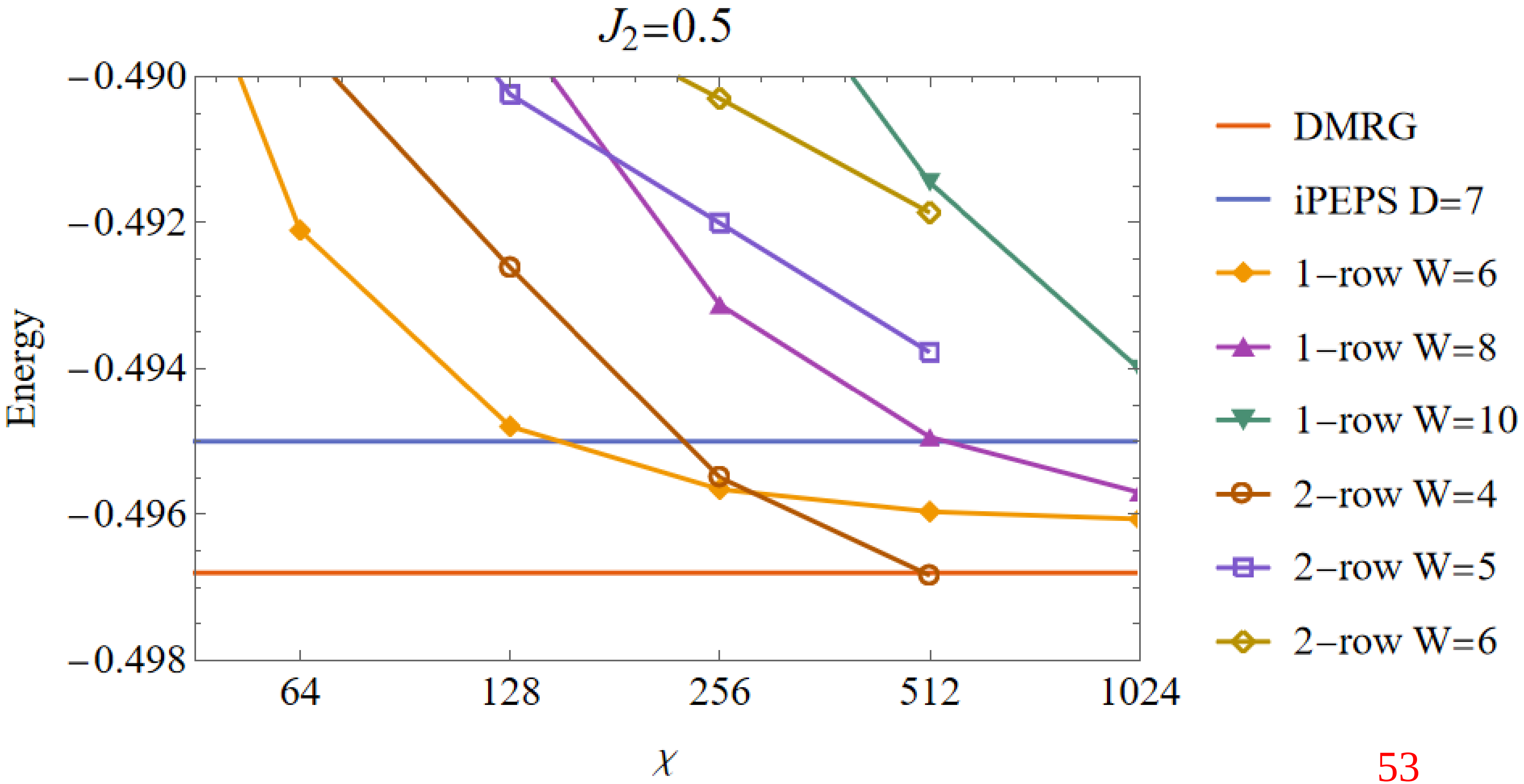
Heisenberg



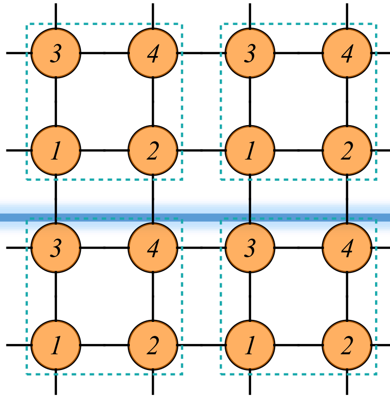
Merge 4 site ground energy

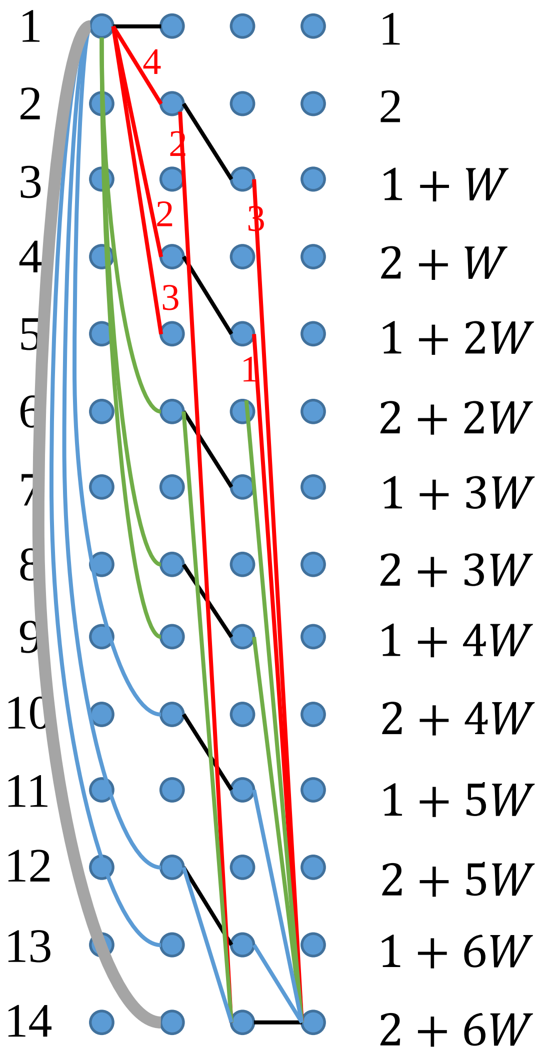


$J_1 - J_2$



MPO from MP diagram





- Heisenberg
  - On site term in cells
  - coupling between cells

$I \otimes I \otimes I \otimes I$

IS^x

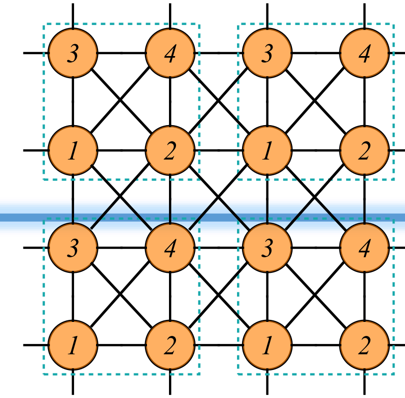
$IS^y \qquad IS_n^\alpha \equiv I \otimes S_n^\alpha \ldots I \otimes I$

IS^z

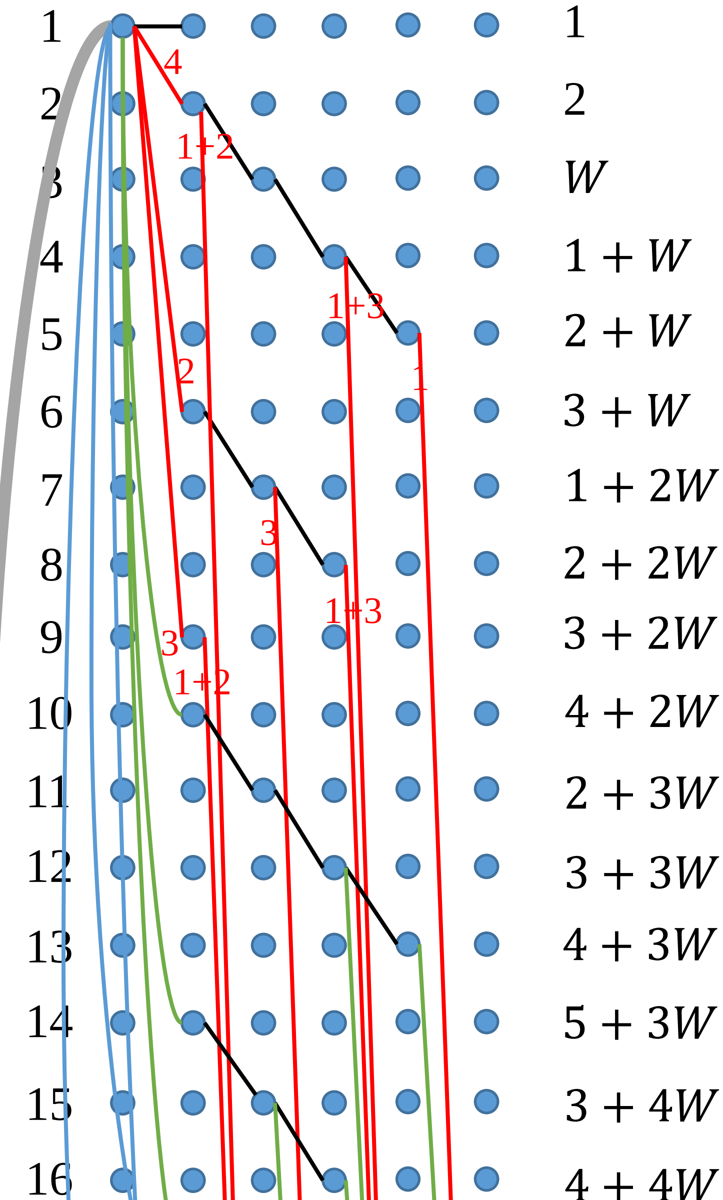
$$\sum_\alpha \begin{array}{l} S^\alpha \otimes S^\alpha \otimes I \otimes I + S^\alpha \otimes I \otimes S^\alpha \otimes I \\ + I \otimes S^\alpha \otimes I \otimes S^\alpha + I \otimes I \otimes S^\alpha \otimes S^\alpha \end{array}$$

$N = 2 + 6W$

MPO from MP diagram



- J1-J2



$I\otimes I\otimes I\otimes I$

IS^x

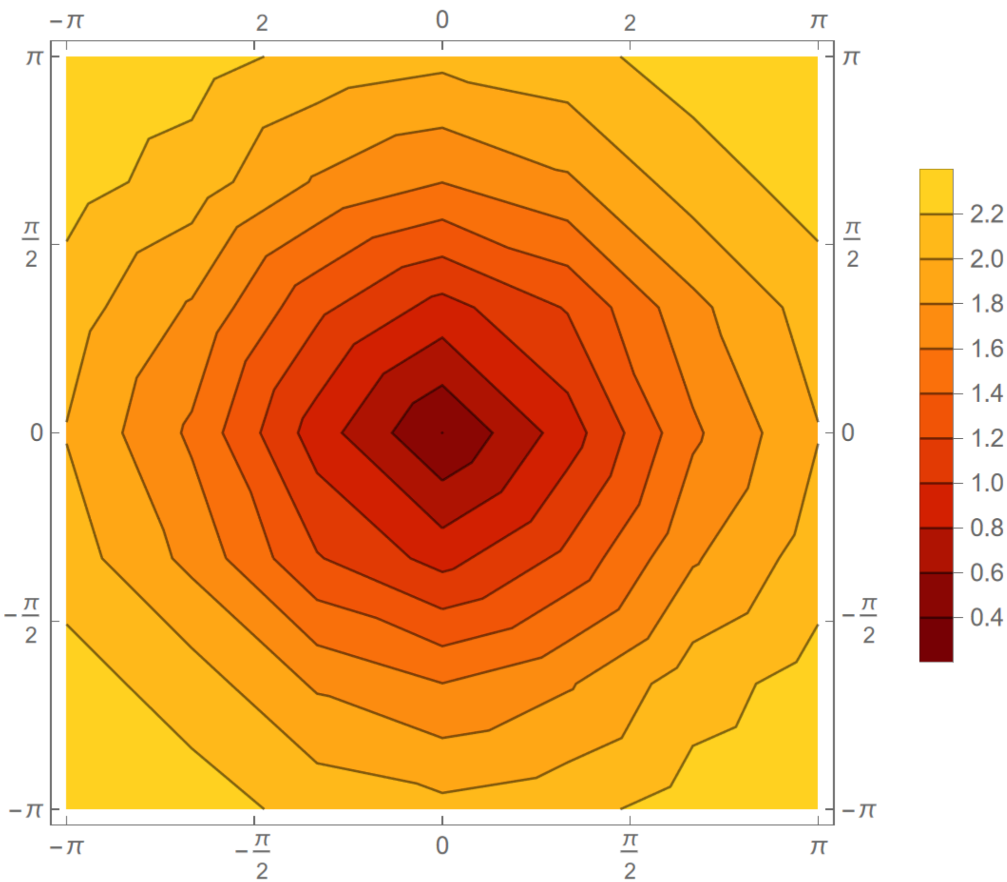
IS^y $\quad IS_n^\alpha \equiv I\otimes S_n^\alpha \ldots I\otimes I$

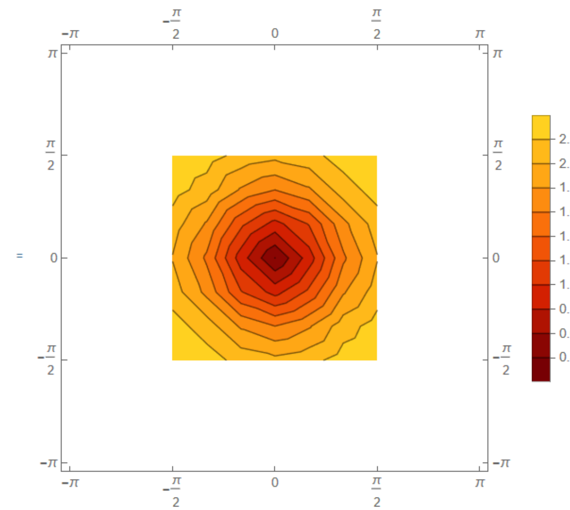
IS^z

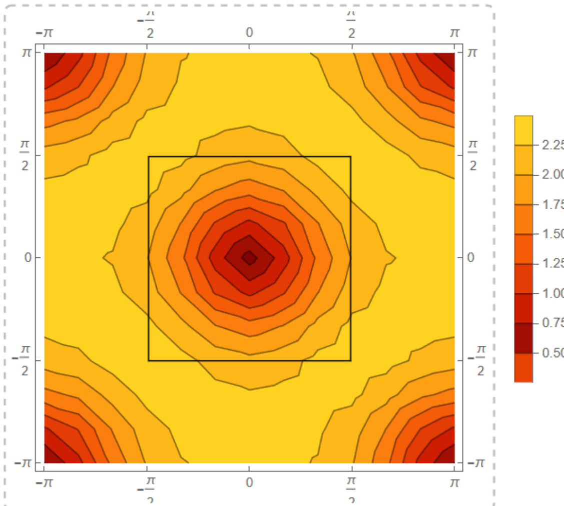
$$\sum_\alpha \begin{matrix} +J_1 S^\alpha\otimes S^\alpha\otimes I\otimes I + J_1 S^\alpha\otimes I\otimes S^\alpha\otimes I \\ +J_1 I\otimes S^\alpha\otimes I\otimes S^\alpha + J_1 I\otimes I\otimes S^\alpha\otimes S^\alpha \\ +J_2 S^\alpha\otimes I\otimes I\otimes S^\alpha + J_2\, I\otimes S^\alpha\otimes S^\alpha\otimes I \end{matrix}$$

$N = 8 + 6W$

2D Fold Brillouin zone



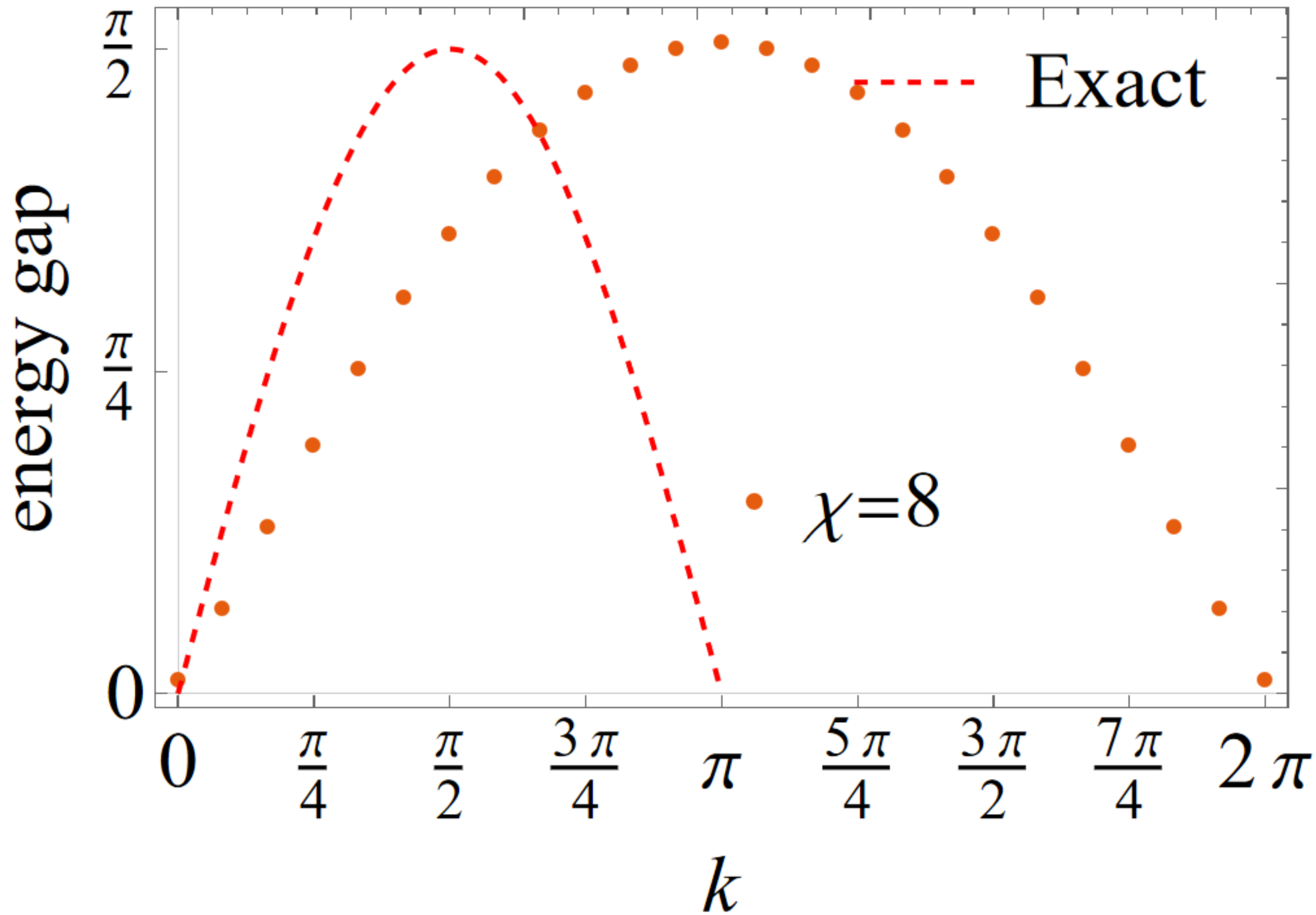




1D Fold Brillouin zone

- 1D MPS merge 2 site

Heisenberg



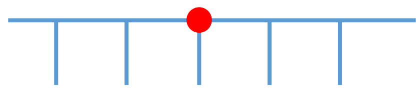
Expanded Brillouin zone

$\left|\Phi(B)_k\right\rangle = e^{ik\cdot 0}$

B

$+\, e^{ik\cdot 1}$

$+\, e^{ik\cdot 2}$



$+\, e^{ik\cdot 3}$

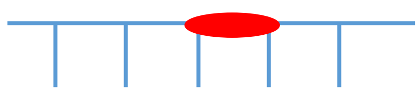
$a = 1$

$$k \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right) = (-\pi, \pi)$$

$\left|\Phi(\tilde{B})_{\tilde{k}}\right\rangle = e^{i\tilde{k}\cdot 0}$

$\tilde{B}$

$+\, e^{i\tilde{k}\cdot 1}$



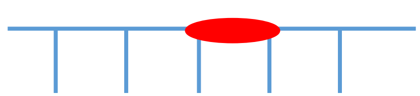
$$\tilde{a} = \frac{1}{2}$$

$$\tilde{k} \in \left(-\frac{\pi}{\tilde{a}}, \frac{\pi}{\tilde{a}}\right) = (-2\pi, 2\pi)$$

$\left|\Phi(\tilde{B})_{\tilde{k}}\right\rangle = e^{i\tilde{k}\cdot 0}$

$\tilde{B}$

$+\, e^{i\tilde{k}\cdot 2}$

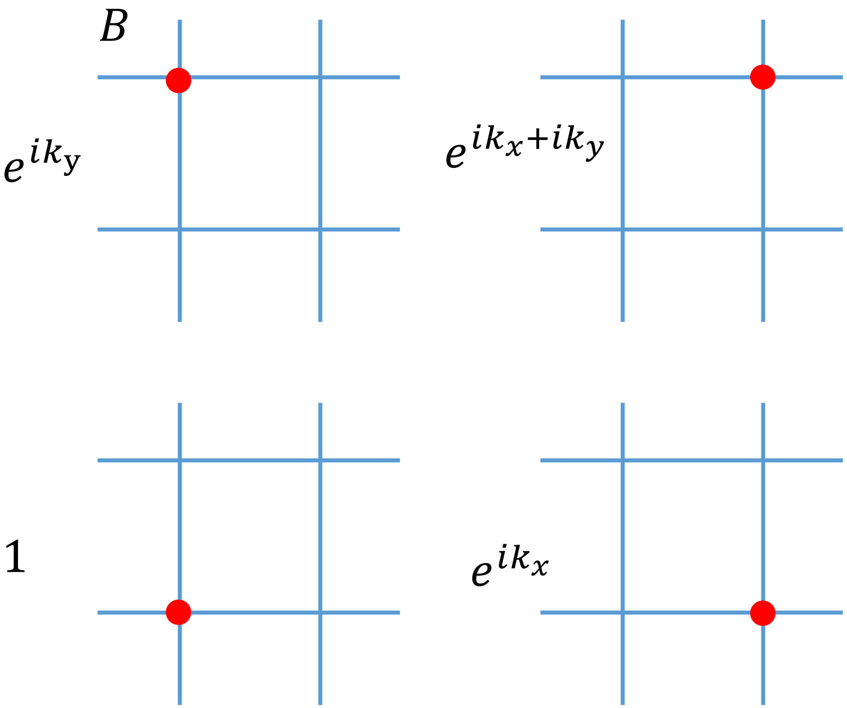


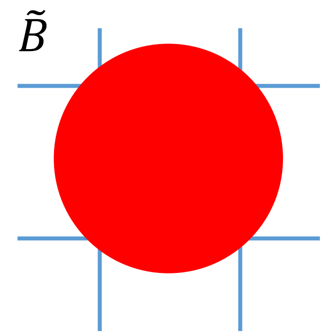
$\tilde{a} = 1$

$$\tilde{k} \in \left(-\frac{\pi}{\tilde{a}}, \frac{\pi}{\tilde{a}}\right) = (-\pi, \pi)$$

$k = 0$ and $k = \pi$ are folded on the $\tilde{k} = 0$!

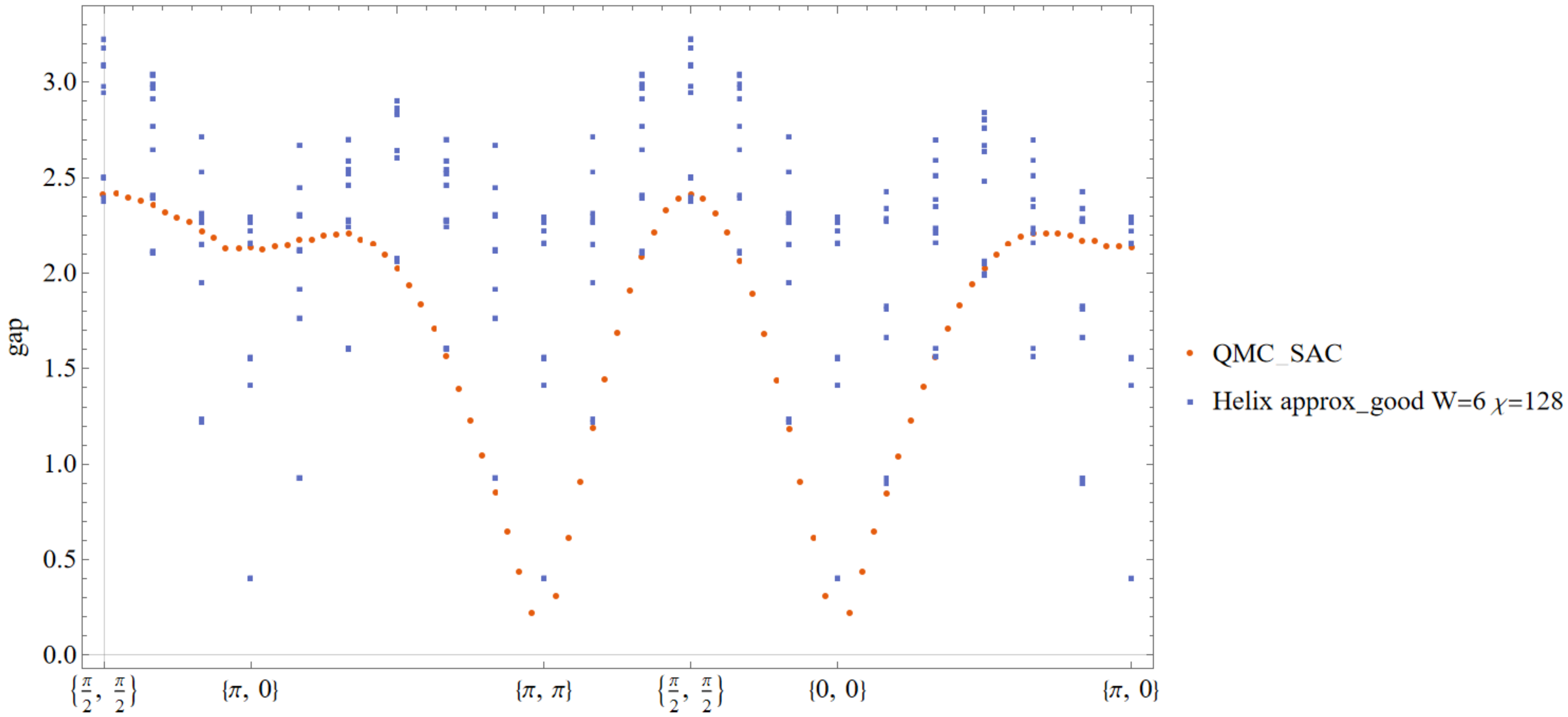
2D Fold Brillouin zone





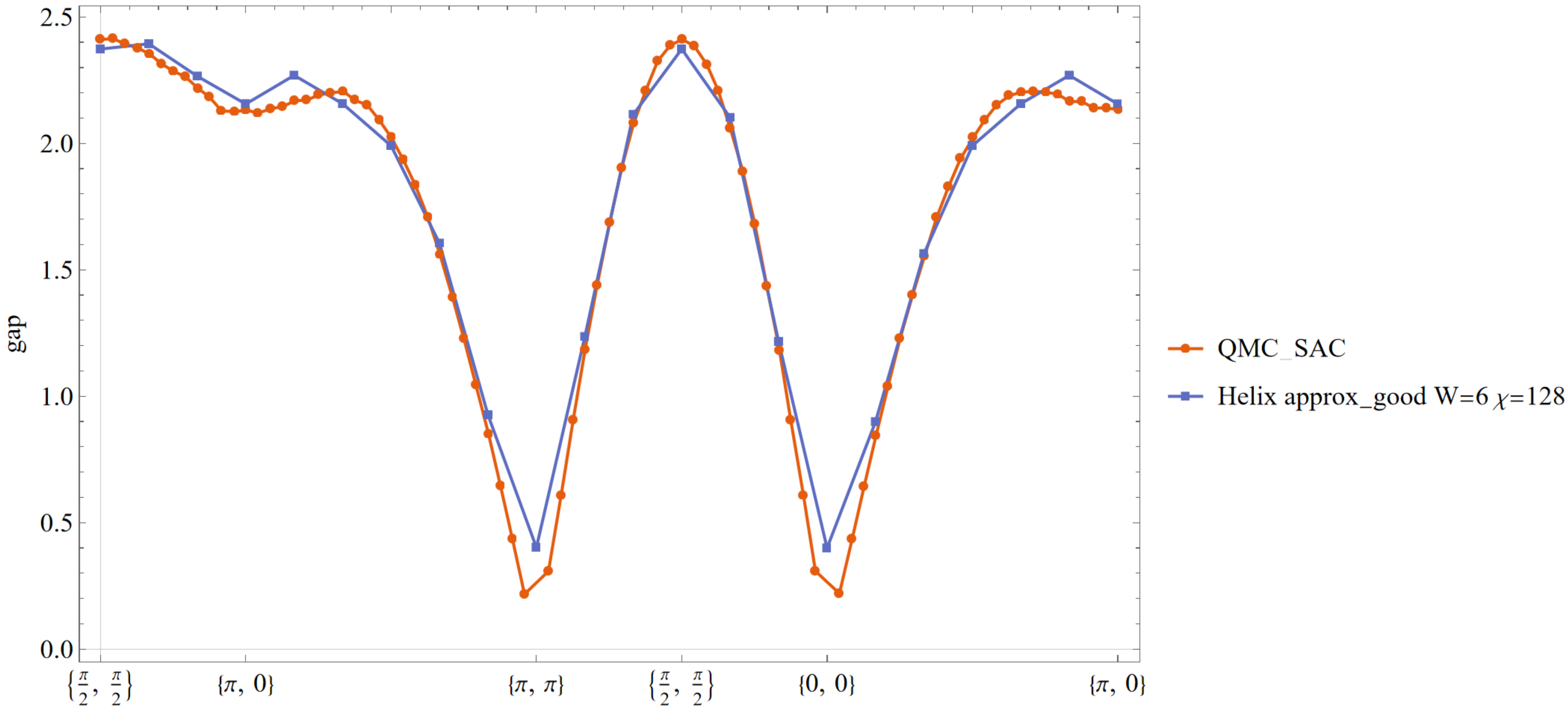
$k = (0,0), (\pi, 0), (0, \pi), (\pi, \pi)$
are folded on the $\tilde{k} = (0,0)$!

Higher energy excitation



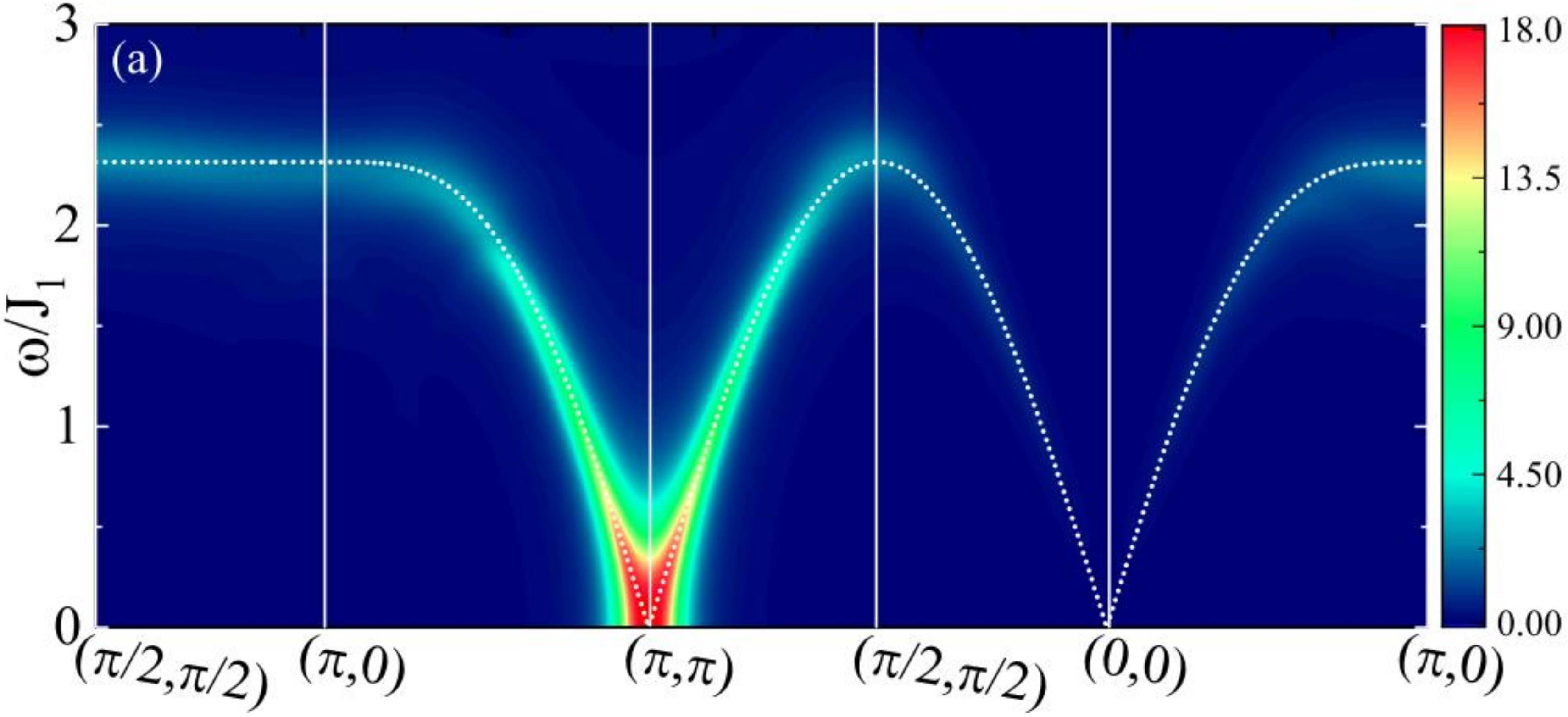
0.399593, 0.401682, 1.41092, 1.5529, 1.558,
2.15555, 2.21871, 2.26231, 2.28512, 2.29263

Select excitation state

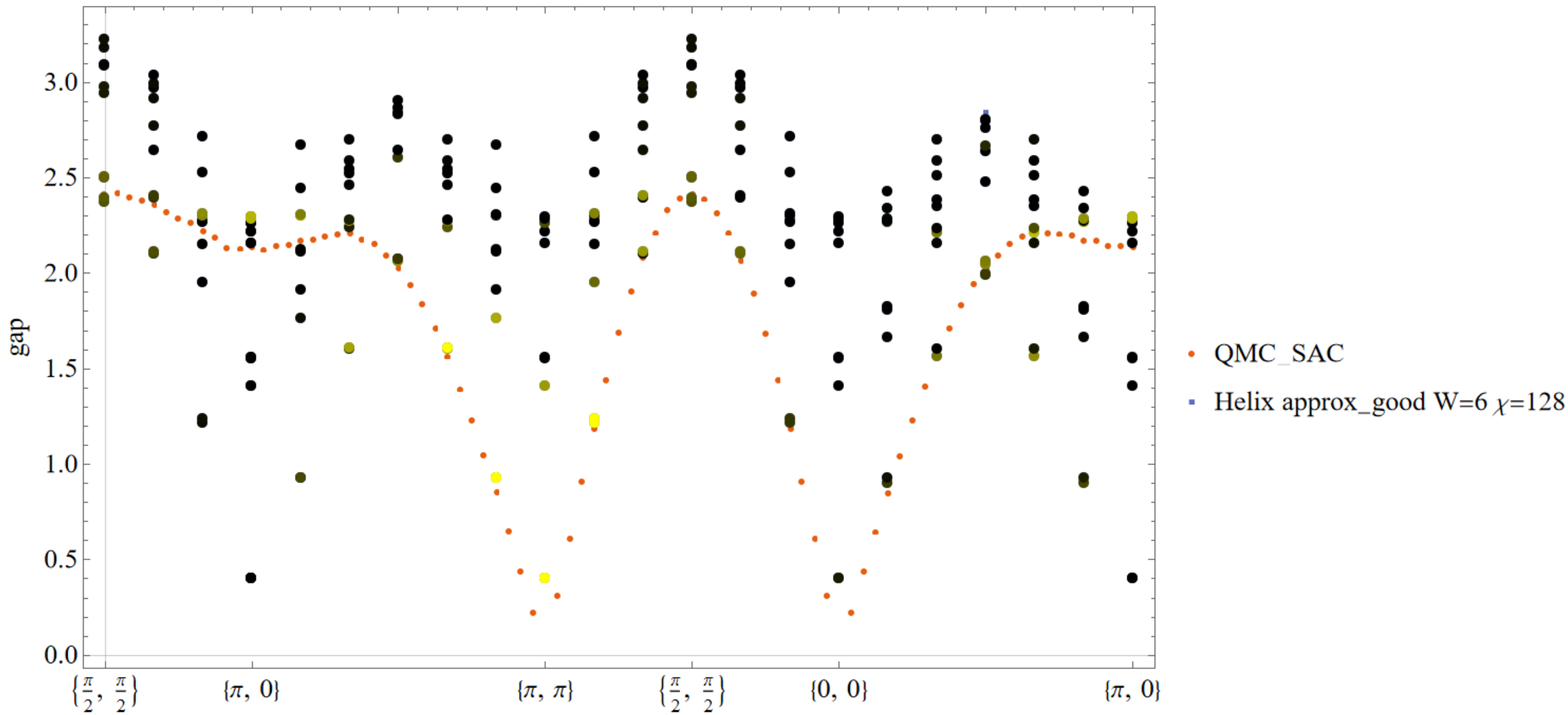


spectral weight

$$w_{\boldsymbol{k}}^{\alpha}(m) = \left|\langle \Phi_{\boldsymbol{k}}(B_m^\dagger)\left|S_{\boldsymbol{k}}^{\alpha}\right|\Psi(A)\rangle\right|^2$$



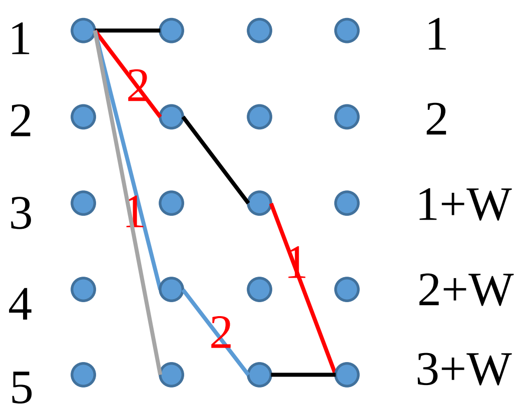
spectral weight



Summary and outlook

- mitigate finite effect by approximation of summation
- 4 site merge for computation of complex configuration
  - Find original spectral weight in folded Brillouin zone
- Outlook
  - J1-J2 excitation at (π,π) and $(\pi,0)$
  - Kitaev

MPO from MP diagram



- Kitaev

$I \otimes I$

IS^x

IS^y $\quad IS_n^\alpha \equiv I \otimes S_n^\alpha \dots I \otimes I$

IS^z

$S^y \otimes S^y$

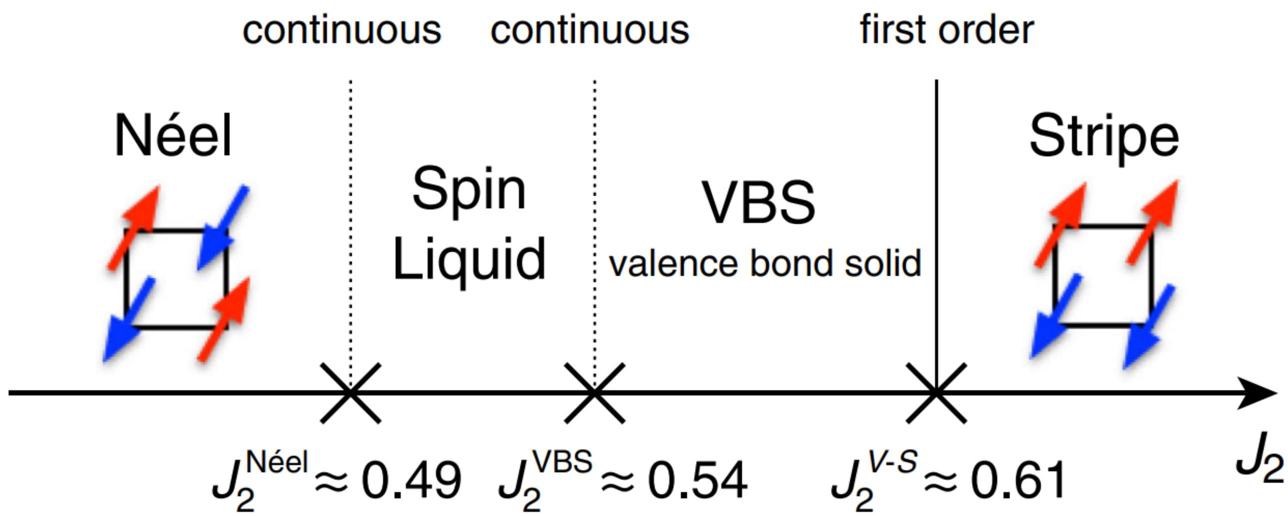
Thank you for listening!

Q&A?

Application of $J_1 - J_2$ model

2D $J_1 - J_2$ square Heisenberg model

- $H = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j.$



Yusuke Nomura, PRX 11, 031034 (2021)

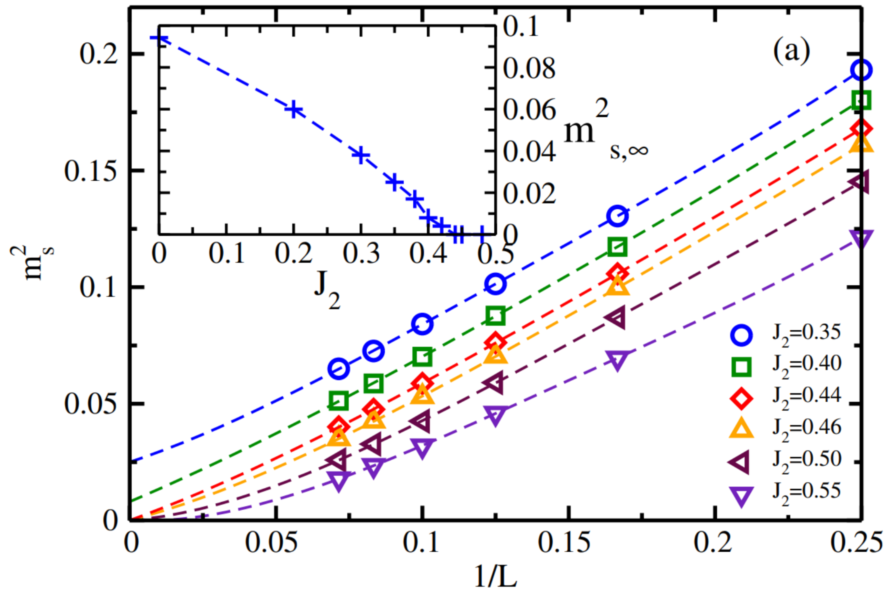
Different method and different result

Method	measure	J_{1c}^{Neel}	J_{2c}	J_{3c}^{Strip}	year
ED N=36site[1]	M, χ	0.34		0.68	1996
DMRG L=10[2]	M, singlet and triplet gaps, topological entanglement entropy	0.41		0.62	2012
VMC N=36[3]	Gap at $(\pi, 0)$ for $S = 1,2$	0.45		0.6	2013
DMRG L=14 SU(2)[4]	M, dimer correlations	0.44	0.5	0.61	2014
iPEPS D=7 FU CTMRG SU(2)[5]	M, correlation lengths	0.5			2017
DMRG L=10 U(1) SU(2)[6]	level-crossing	0.46	0.52		2018
VMC N=16×16 RBM+PP[7]	Correlation Ratio, level spectroscopy	0.49	0.54	0.61	2021
iPEPS D=7 AD CTMRG U(1)[8]	M, correlation lengths	0.45			2021

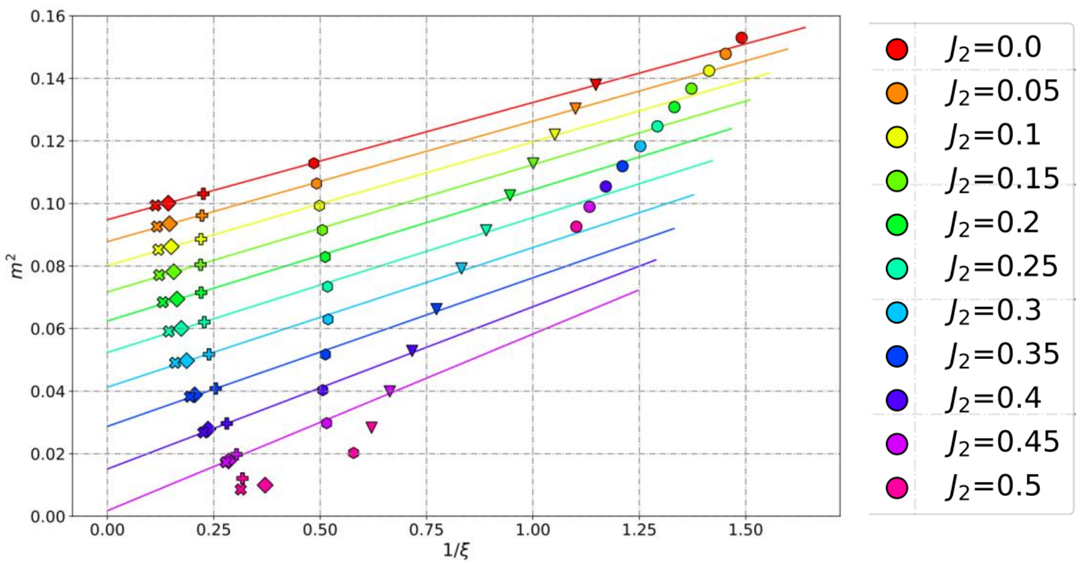
reference

[1]H-J- Schulz, j. Phys. I IYance 6 675-703(1996)
[2]Hong-Chen Jiang, PRB 86, 024424 (2012)
[3]Wen-Jun Hu, PRB 88, 060402(R) (2013)
[4]Shou-Shu Gong, PRL 113, 027201 (2014)
[5]Didier Poilblanc, PRB, 96, 014414 (2017)
[6]Ling Wang, PRL121, 107202 (2018)
[7]Yusuke Nomura, PRX 11, 031034 (2021)
[8]Juraj Hasik, SciPost Phys. 10, 012 (2021)

Extrapolations using magnetic

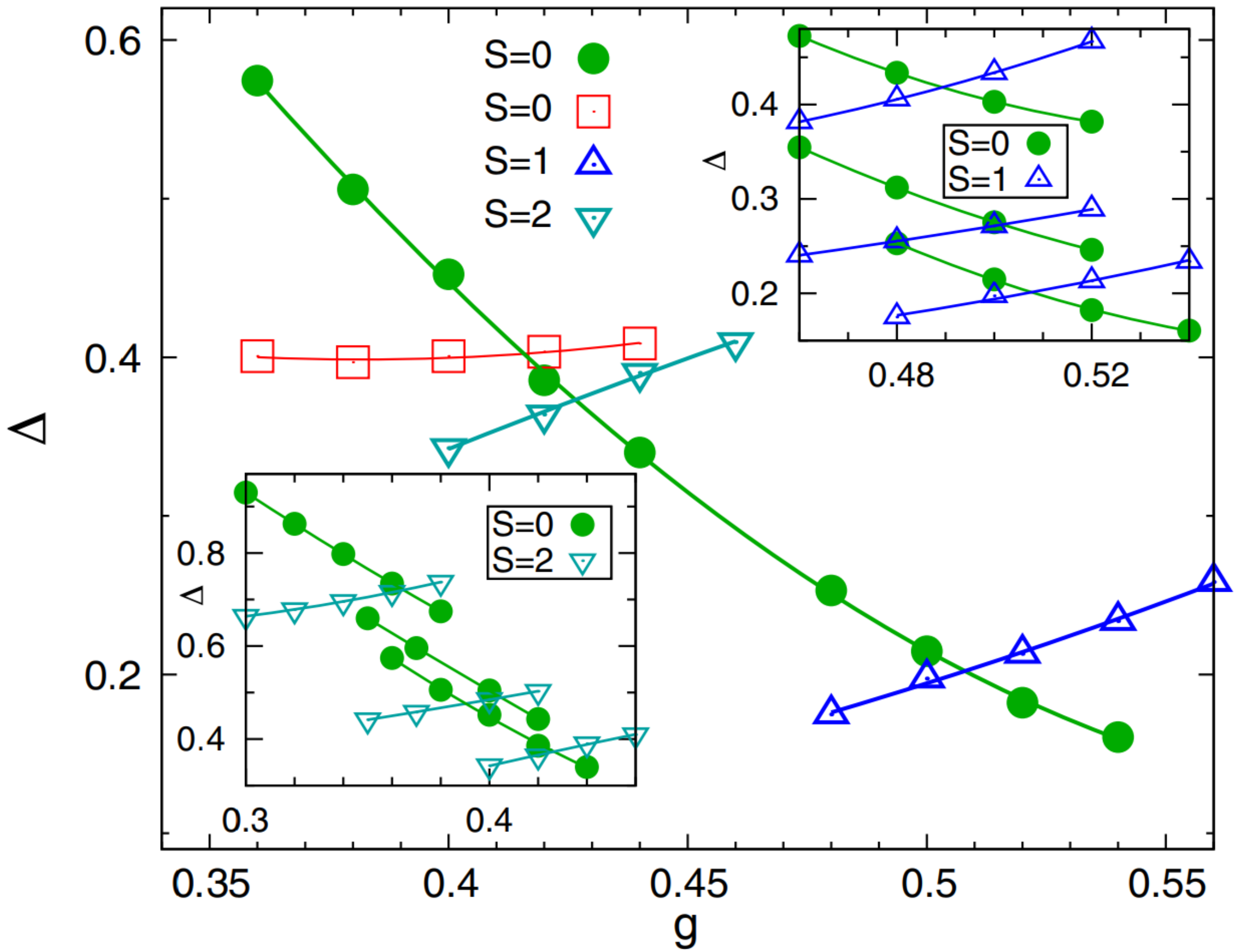


DMRG[4]



AD-U1-iPEPS[8]

level-crossing

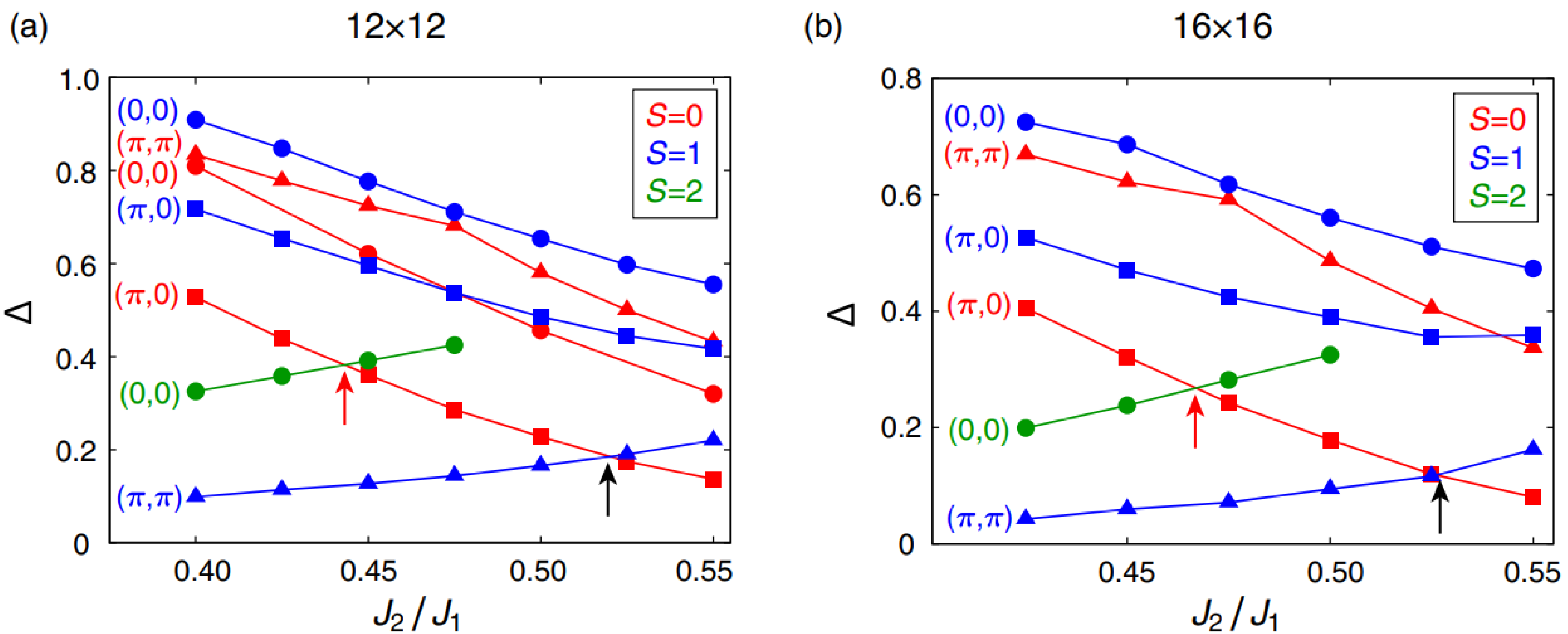


DMRG[6]

$L = 6,8,10$

$L \uparrow$ gap $\downarrow$

level spectroscopy

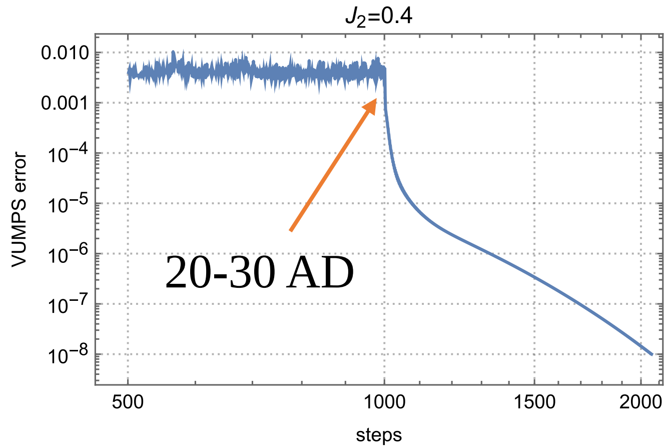


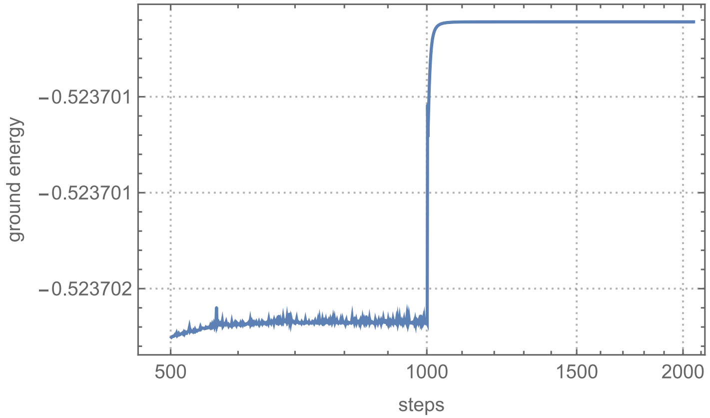
- the singlet and triplet excitations are both gapless at (0,0), (π, 0) and (π, π).

VMC[7]

Initialization for VUMPS

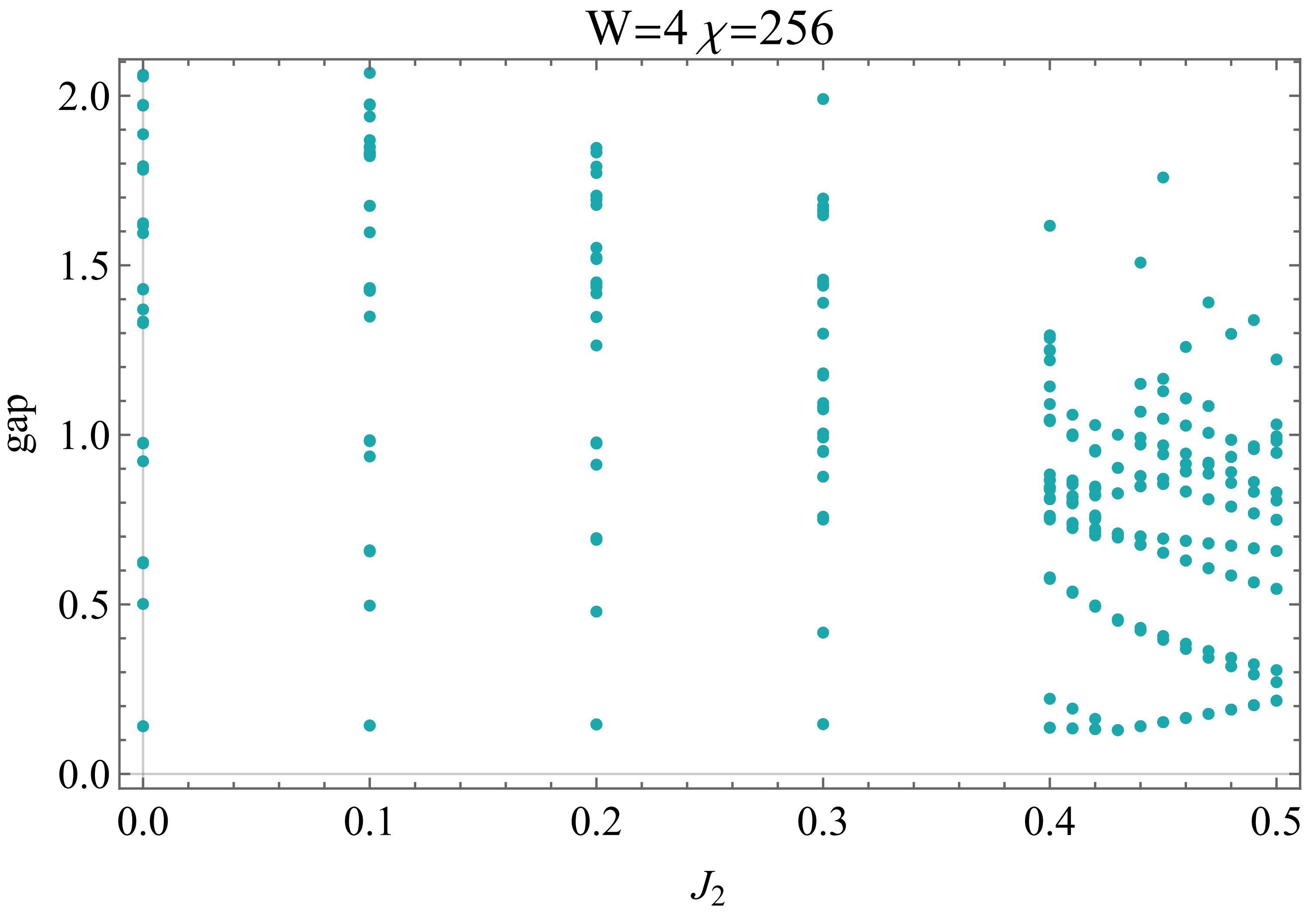
- ADMPS



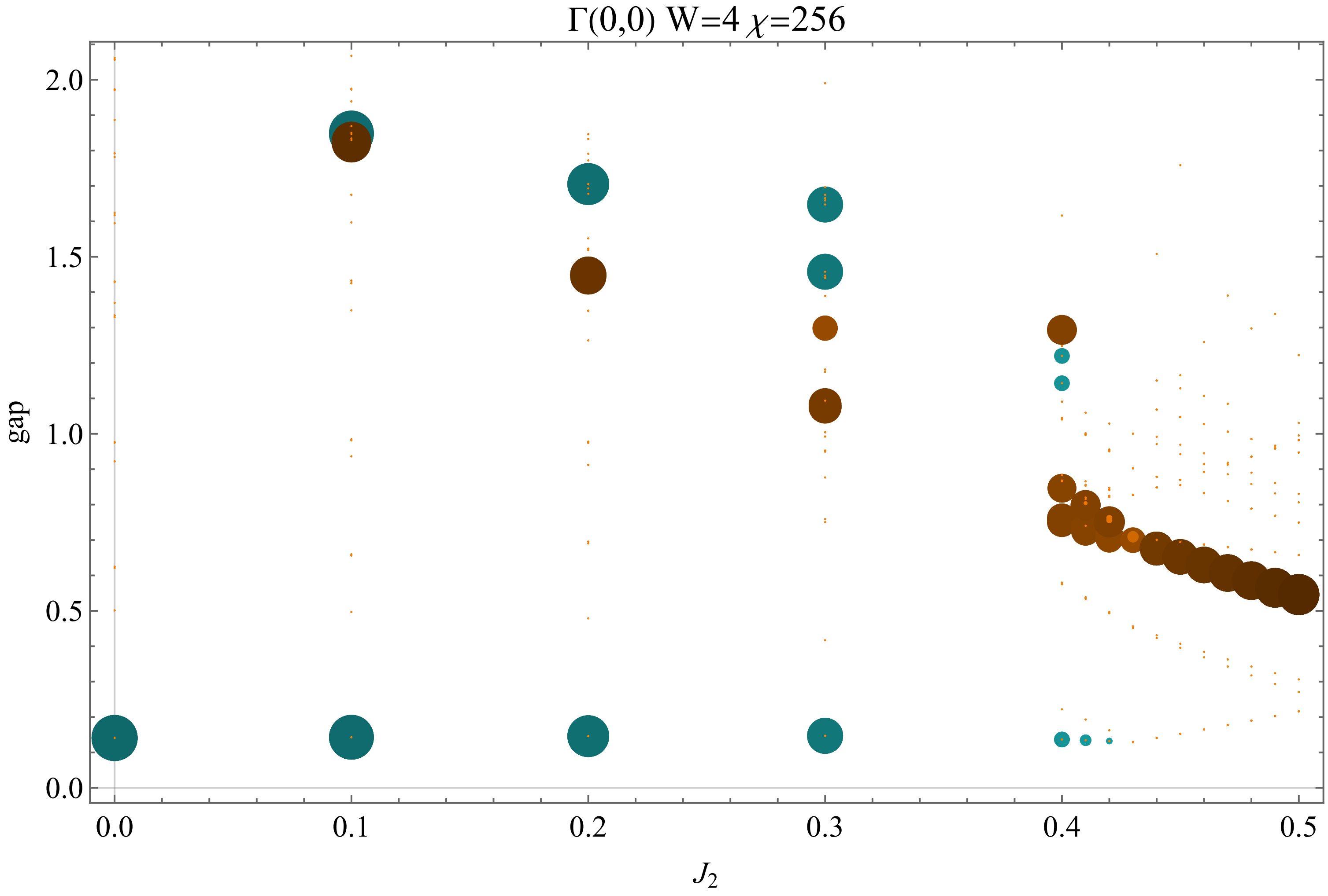


- IDMRG initial
  - Always converge
  - Slower than VUMPS
  - 10^{-12} energy difference

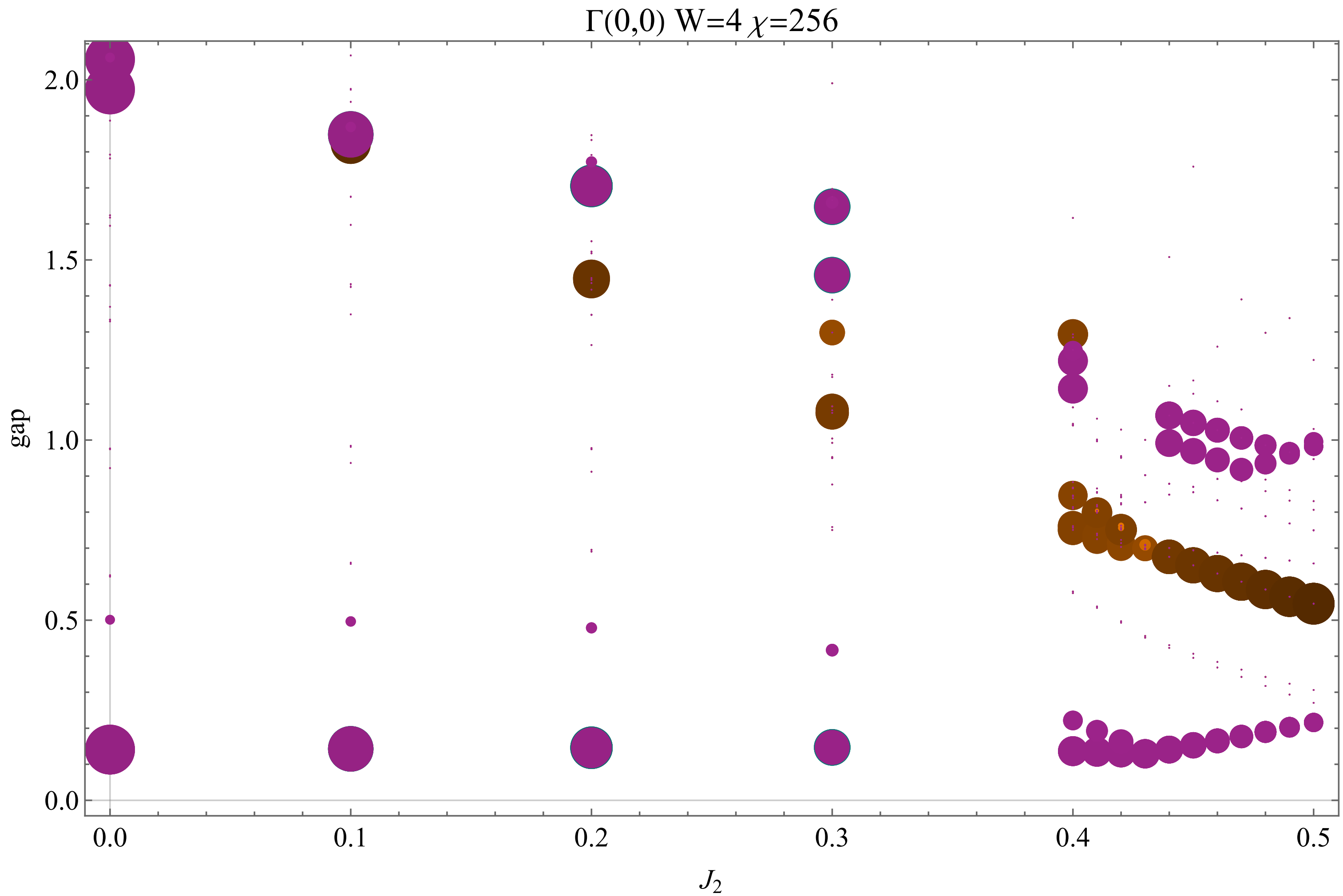
Raw spectrum



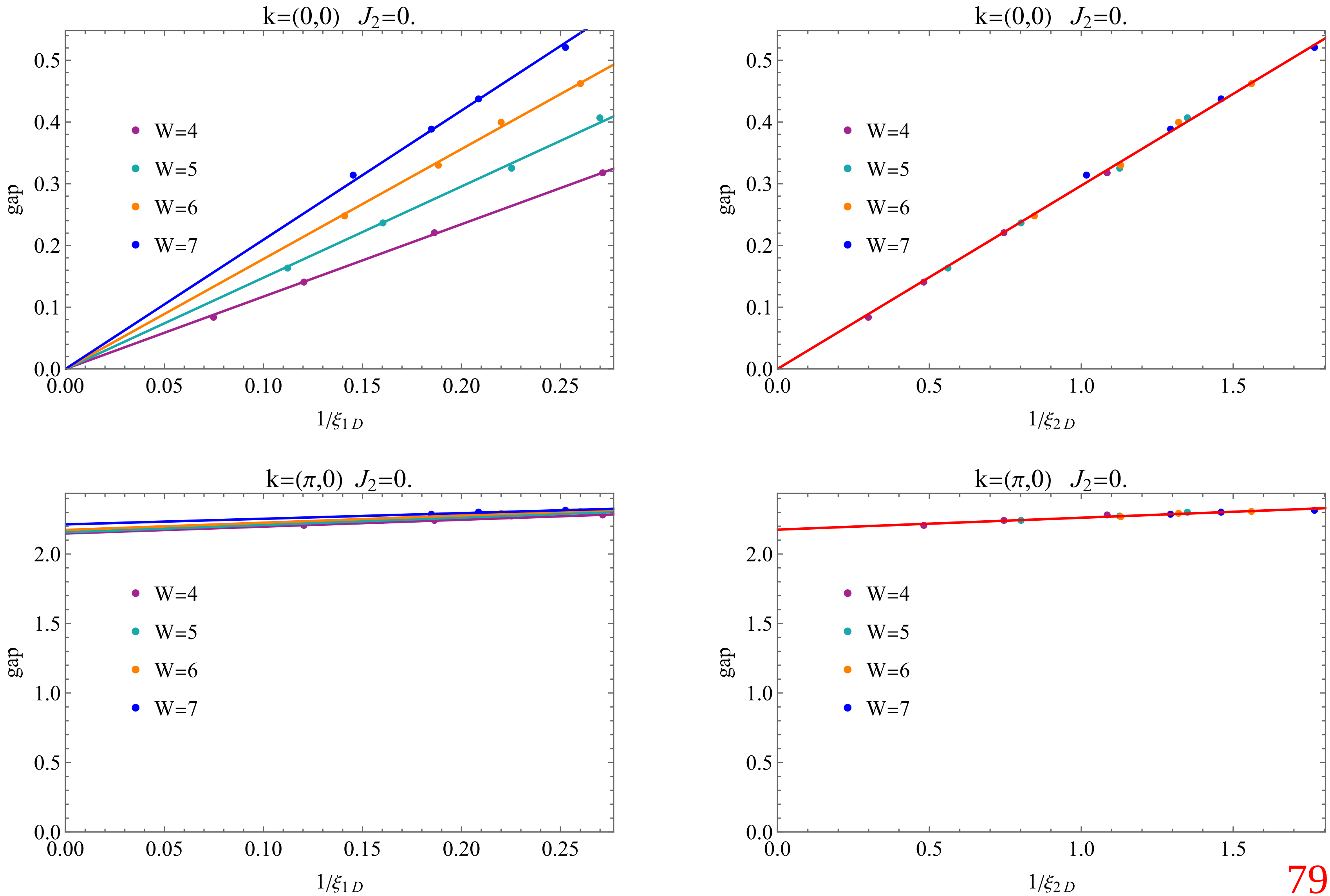
Spectral weight (0,0) and (π,0)



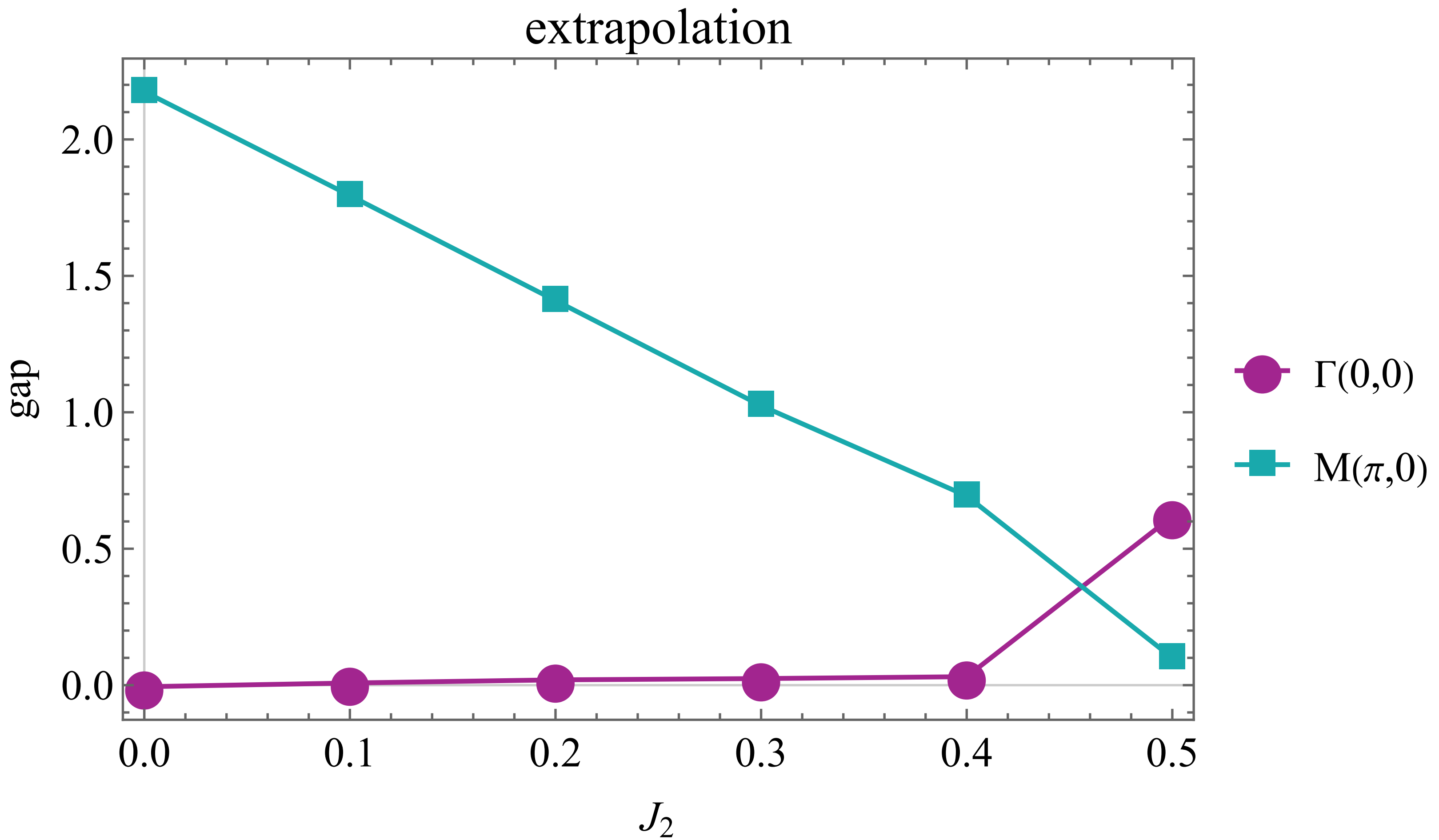
Spectral weight (0,0) and (π, π)



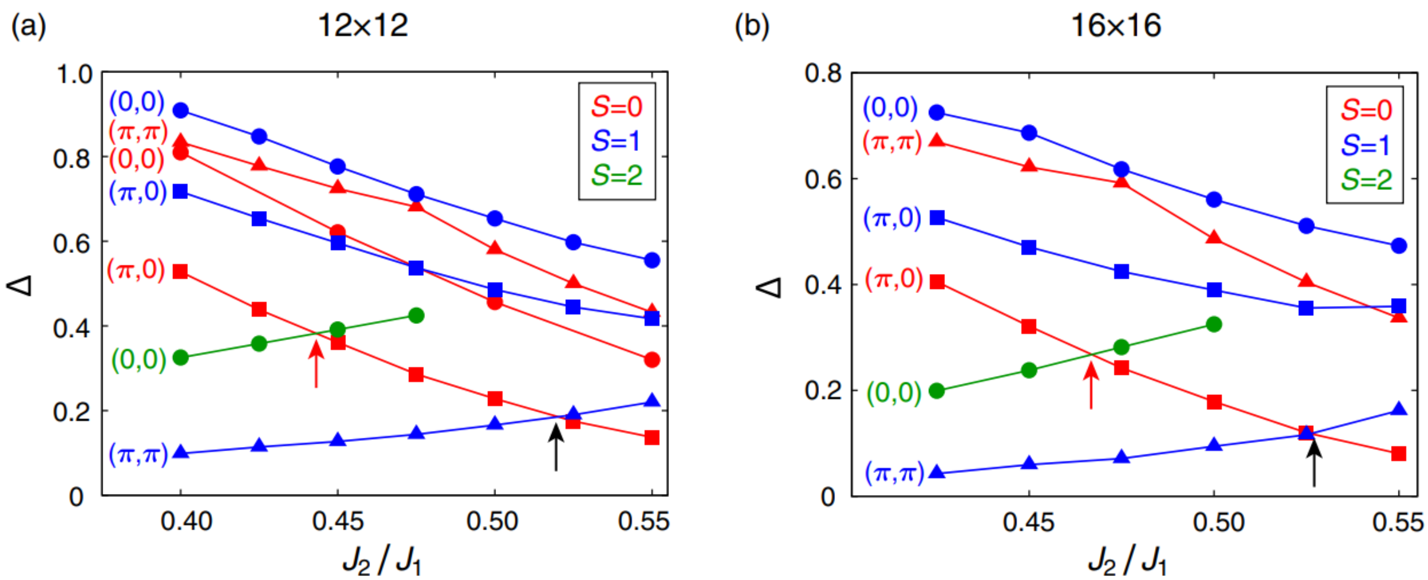
Extrapolations with correlation length

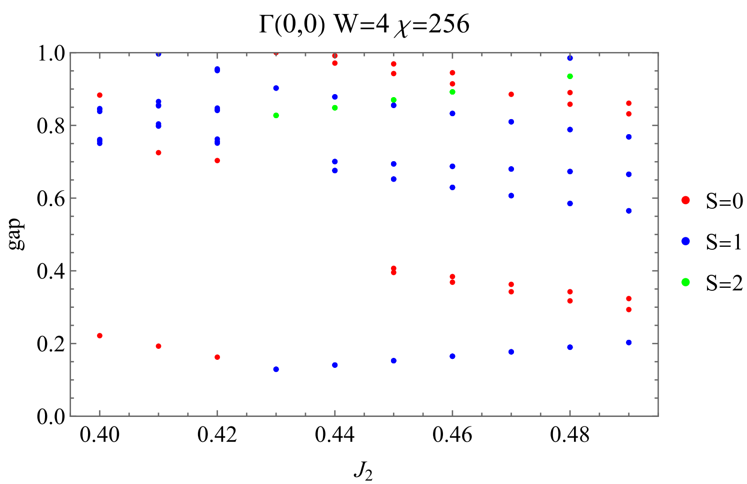


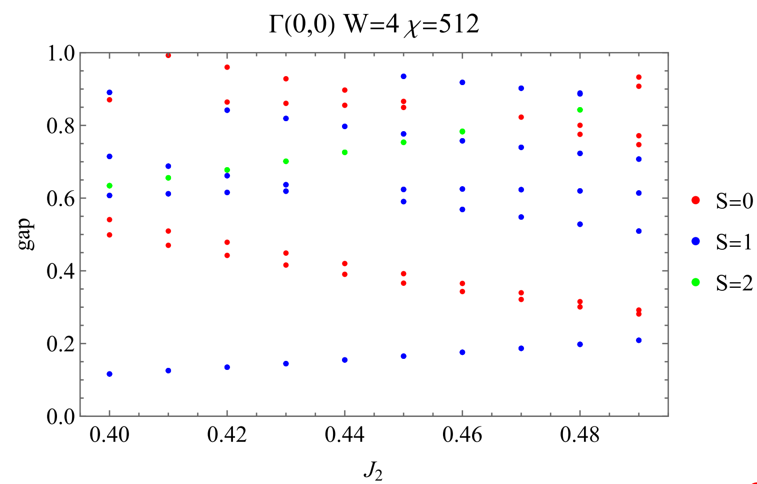
Γ and M gap



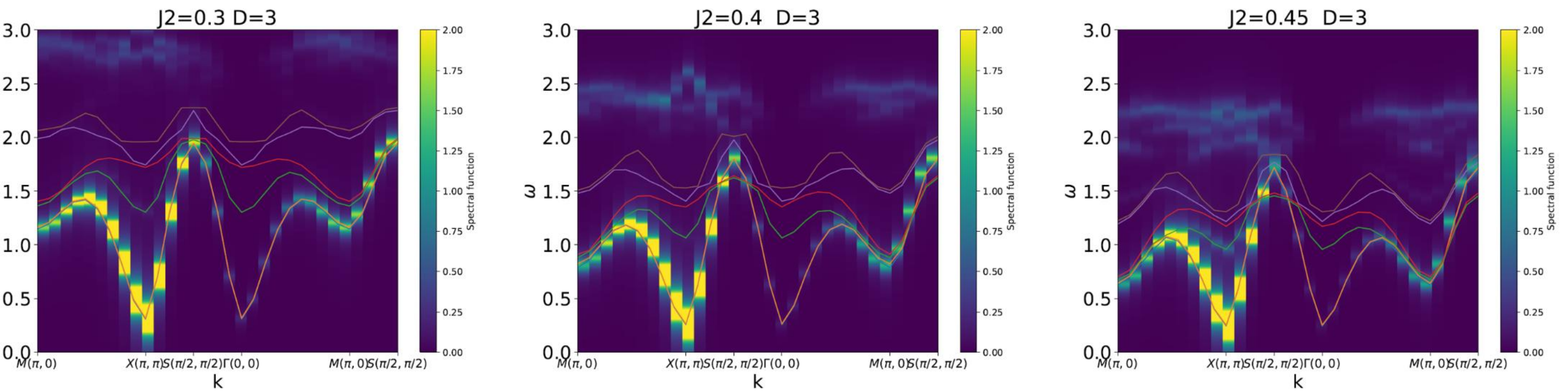
level spectroscopy

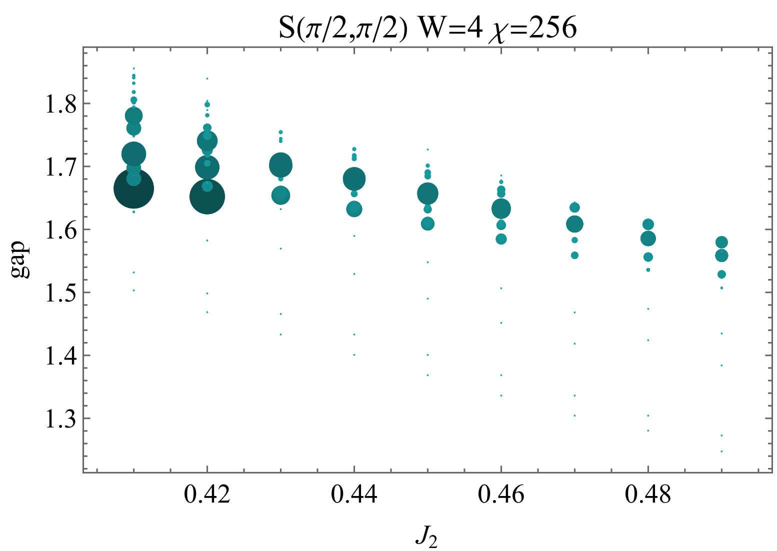






Excitation at $S(\pi/2, \pi/2)$

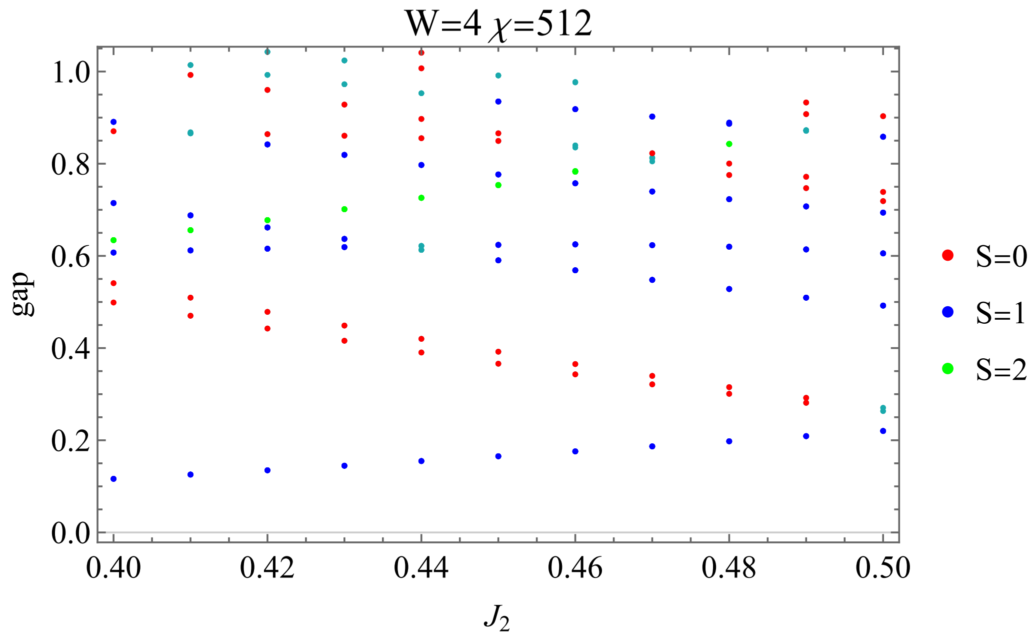




iPEPS from Yang Liu

Summary and outlook

- level-crossing is good way to detect phase transition for our method
- Calculate S from $\mathbf{S}^2$ or add SU(2) symmetry
- More story of $S(\pi/2, \pi/2)$



Thank you for listening!

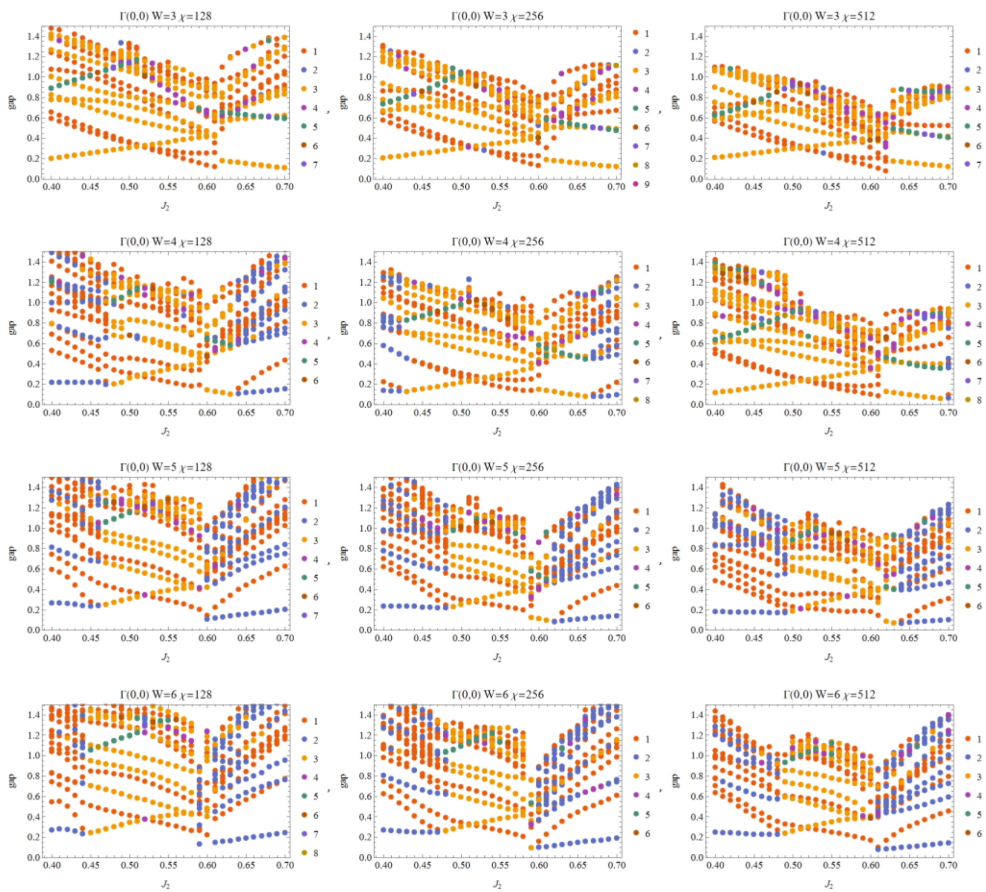
Q&A?

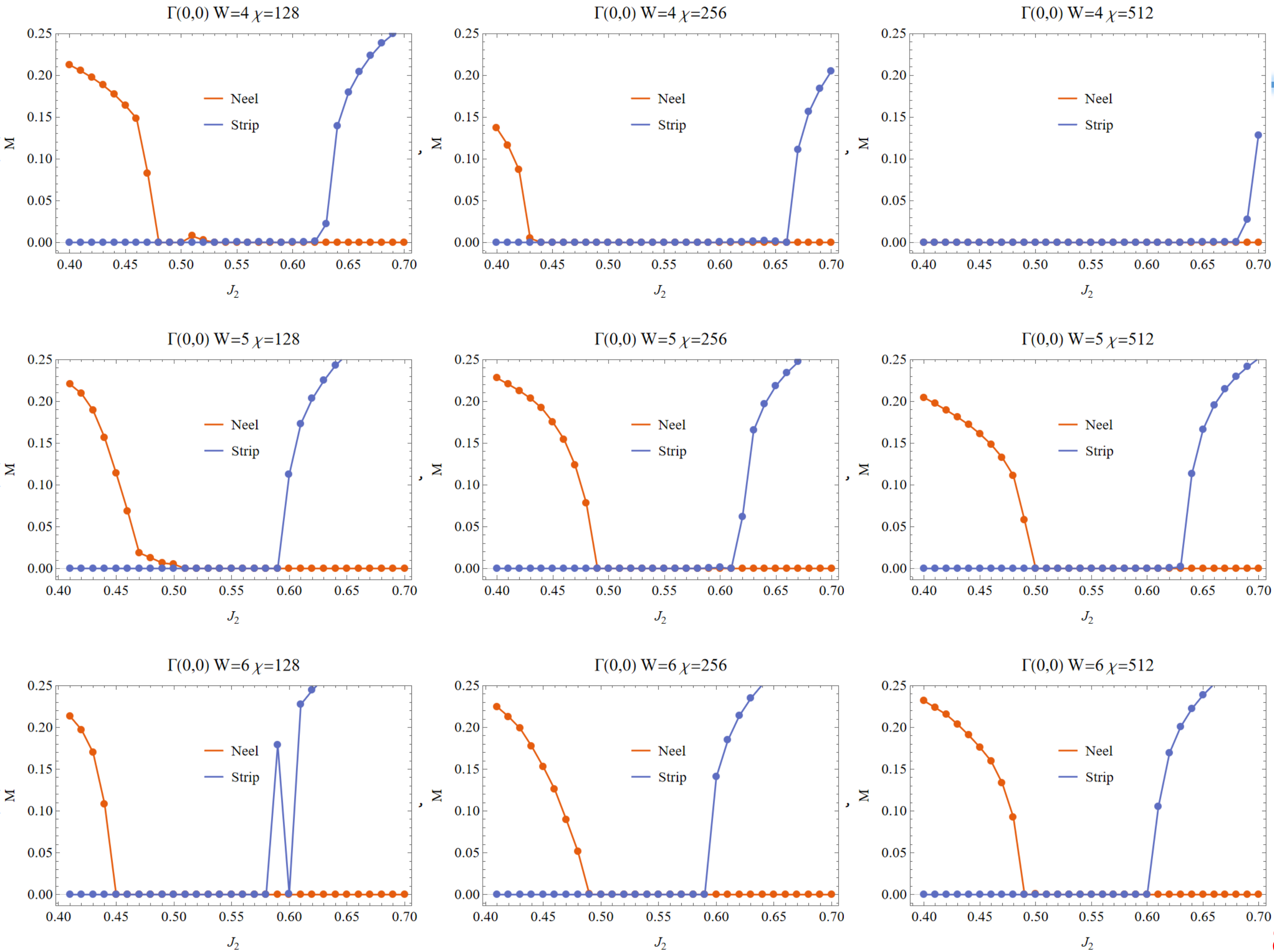
2D $J_1 - J_2$ Hensenberg model on Helix

Xingyu Zhang, Yang Liu, Run-Ze Chi, Lei Wang

Merge (0,0), $(\pi, 0)$, $(0, \pi)$ (π, π)

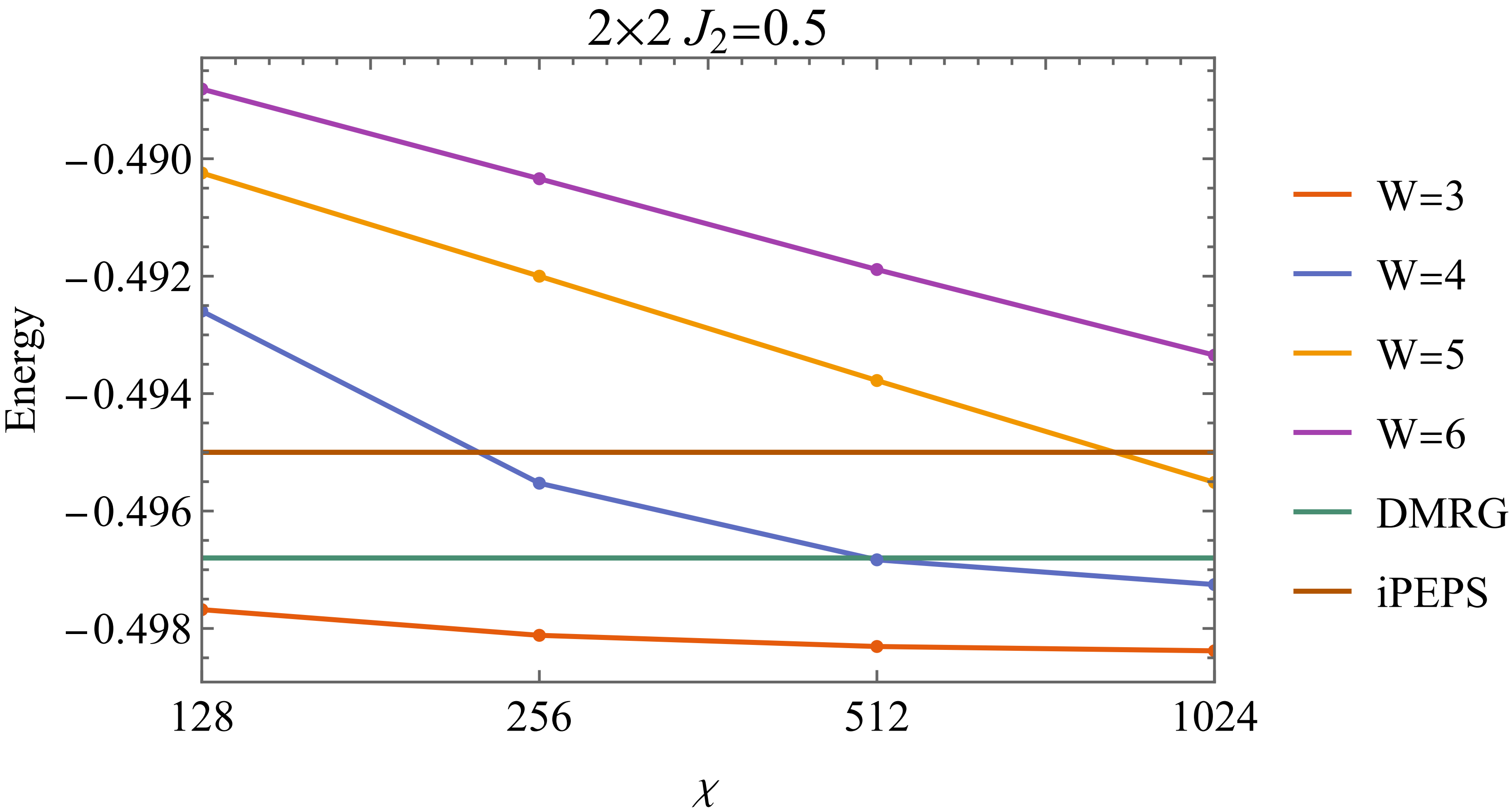
- AFM → SL → VBS → Middle → Strip
- degeneracy 2 → 3 → 1 → 3 → 2
- The Middle phase may be a illusion by insufficient χ / W (not converge/finite size)





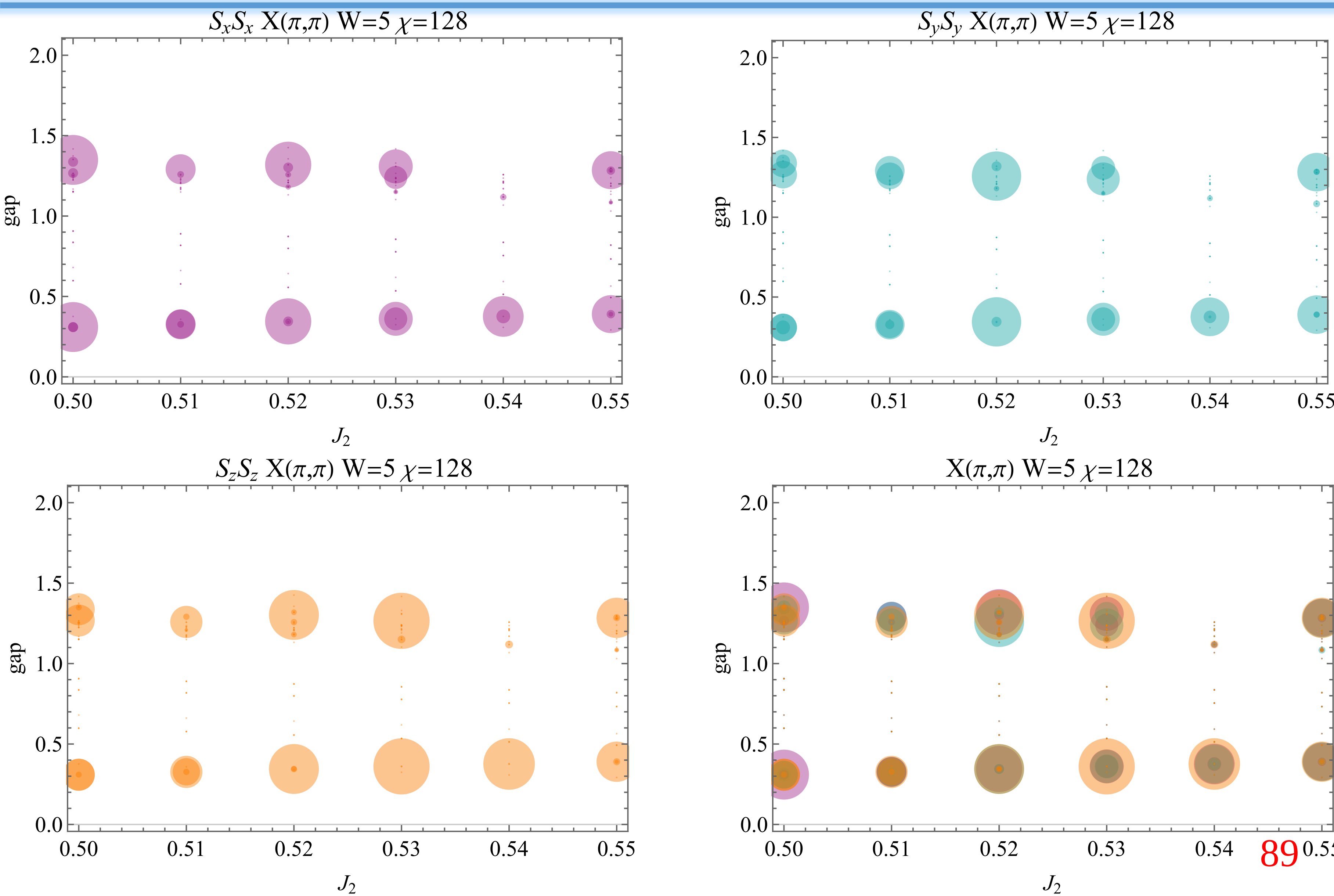
Γ(0,0) W=4 χ=128
Γ(0,0) W=4 χ=256
Γ(0,0) W=4 χ=512
Γ(0,0) W=5 χ=128
Γ(0,0) W=5 χ=256
Γ(0,0) W=5 χ=512
Γ(0,0) W=6 χ=128
Γ(0,0) W=6 χ=256
Γ(0,0) W=6 χ=512
Neel
Strip
M
J_2
0.00
0.05
0.10
0.15
0.20
0.25
0.40
0.45
0.50
0.55
0.60
0.65
0.70

Energy-χ



2×2 J_2=0.5
Energy
−0.490
−0.492
−0.494
−0.496
−0.498
128
256
512
1024
χ
W=3
W=4
W=5
W=6
DMRG
iPEPS

Quadruple degeneracy at 0.52

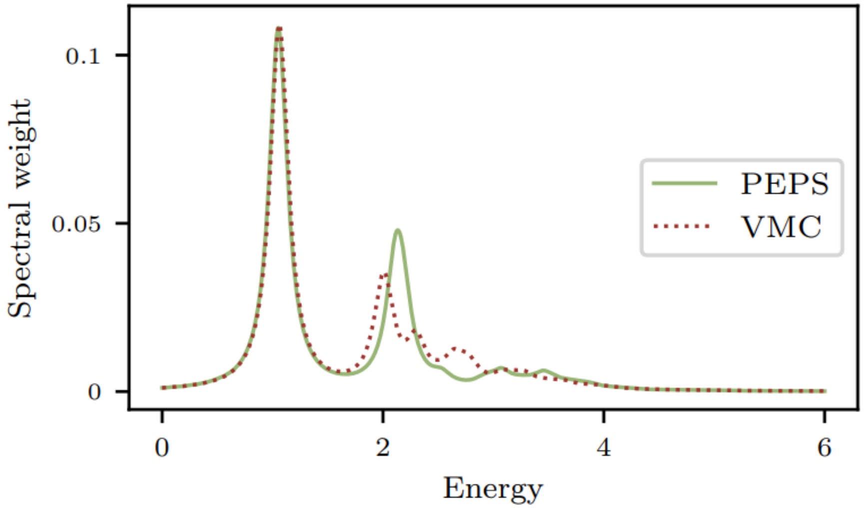


Quadruplet degeneracy at 0.52

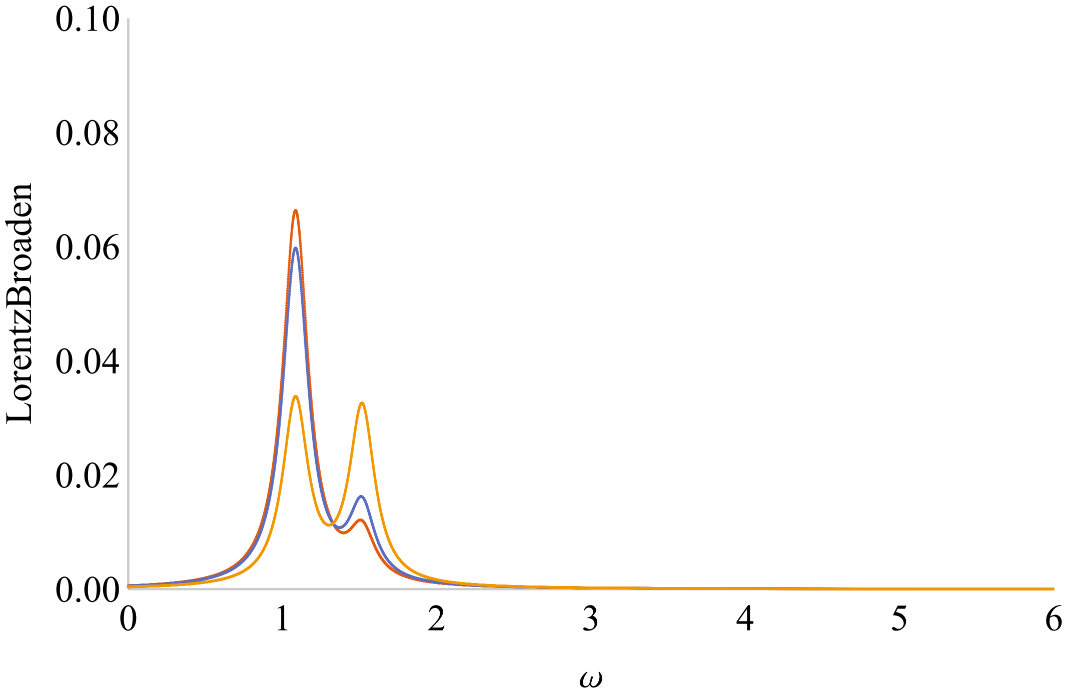
(π, π)	$S_x S_x$	$S_y S_y$	$S_z S_z$
No.1	8.268e-16	3.807e-15	3.989e-14
No.2	0.0208	0.1775	0.0224
No.3	0.0348	0.0074	0.1781
No.4	0.1647	0.0357	0.0199

Spectral weight

convolute with a Lorentzian with broadening factor $\delta = 0.1$.



W=5 χ=512 J_2=0.3



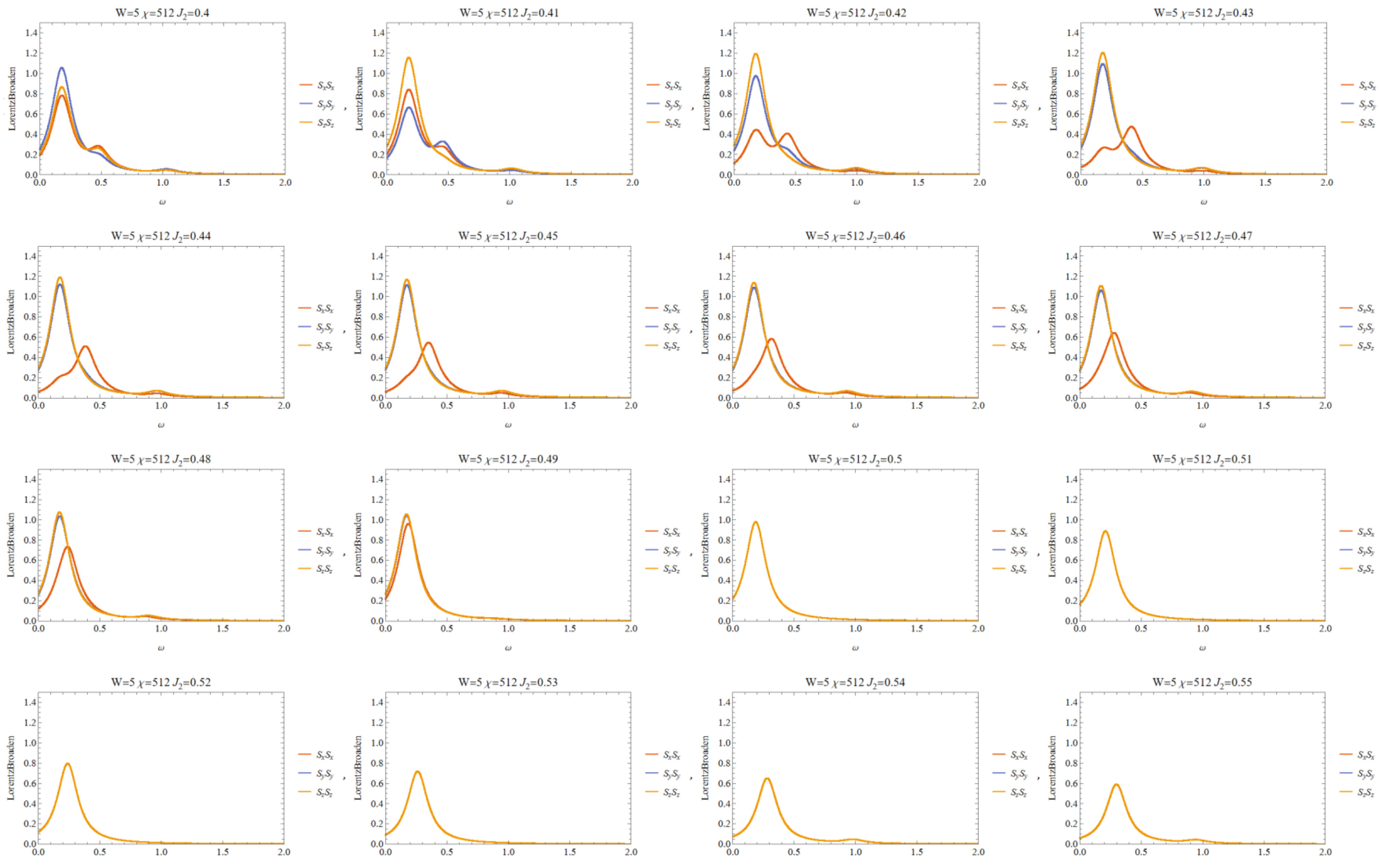
S_xS_x

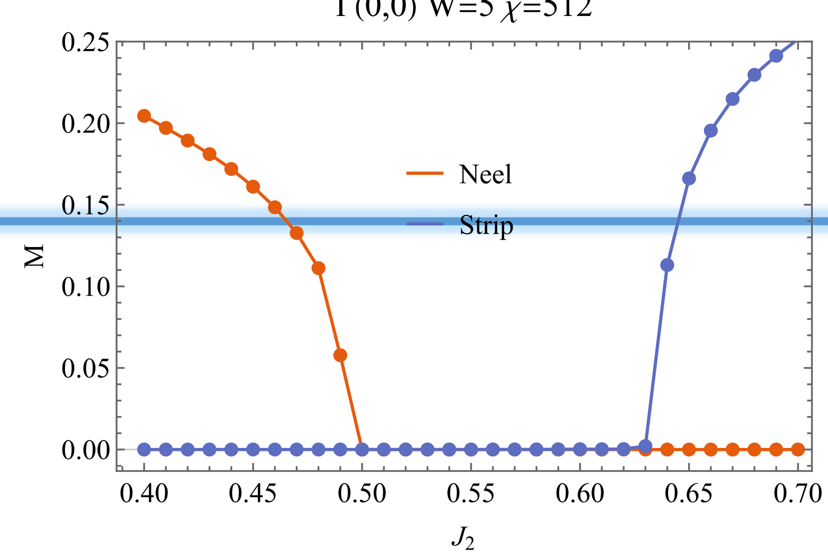
S_yS_y

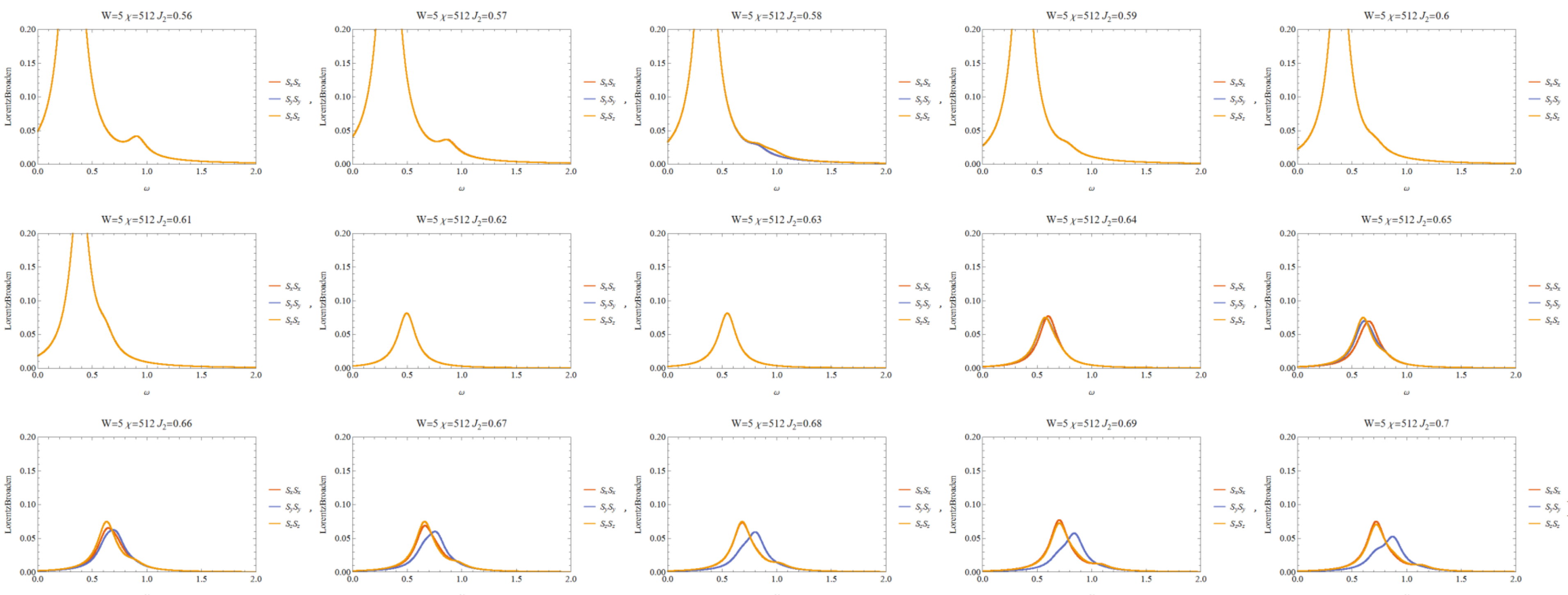
S_zS_z

$$\Delta_n = E_n - E_0$$

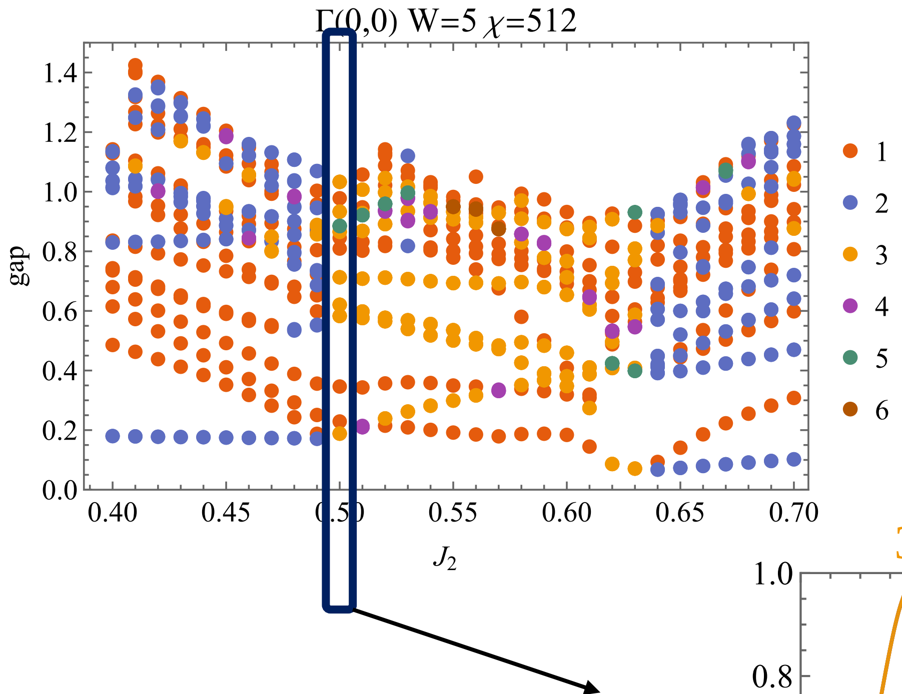
$$\sum_n \frac{\mathrm{S}(k, \Delta_\mathrm{n})\delta}{(\omega - \Delta_\mathrm{n})^2 + \delta^2} \frac{1}{\pi}$$


W=5 χ=512 J_2=0.4
W=5 χ=512 J_2=0.41
W=5 χ=512 J_2=0.42
W=5 χ=512 J_2=0.43
W=5 χ=512 J_2=0.44
W=5 χ=512 J_2=0.45
W=5 χ=512 J_2=0.46
W=5 χ=512 J_2=0.47
W=5 χ=512 J_2=0.48
W=5 χ=512 J_2=0.49
W=5 χ=512 J_2=0.5
W=5 χ=512 J_2=0.51
W=5 χ=512 J_2=0.52
W=5 χ=512 J_2=0.53
W=5 χ=512 J_2=0.54
W=5 χ=512 J_2=0.55
LorentzBroaden
ω
S_xS_x
S_yS_y
S_zS_z

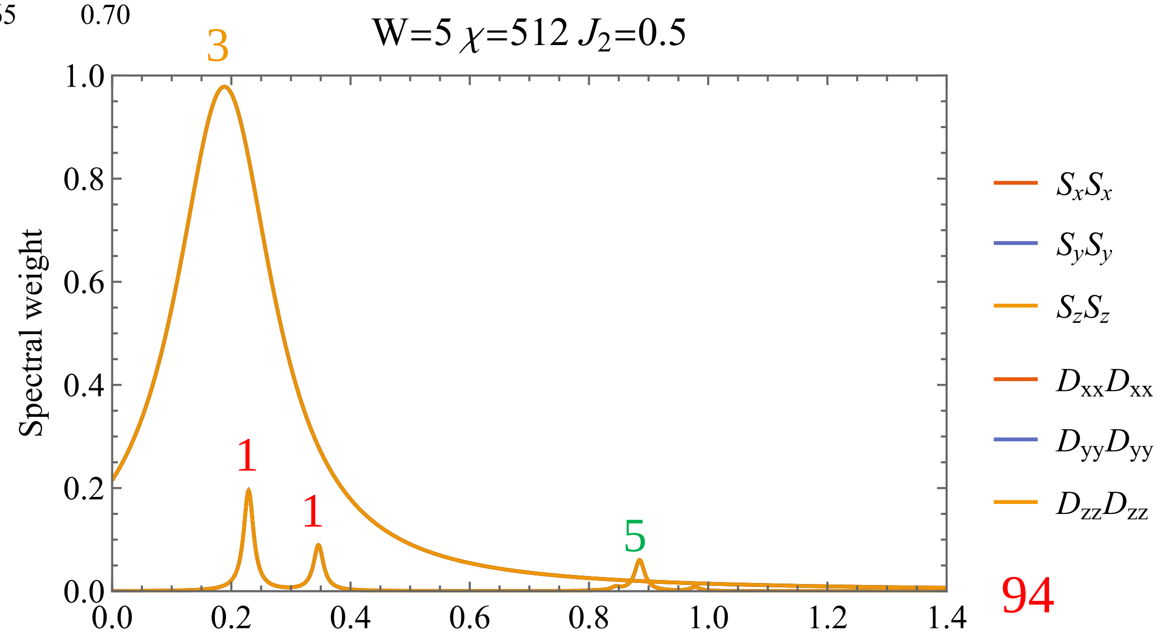

Γ(0,0) W=5 χ=512
0.25
0.20
0.15
0.10
0.05
0.00
M
Neel
Strip
0.40 0.45 0.50 0.55 0.60 0.65 0.70
J2

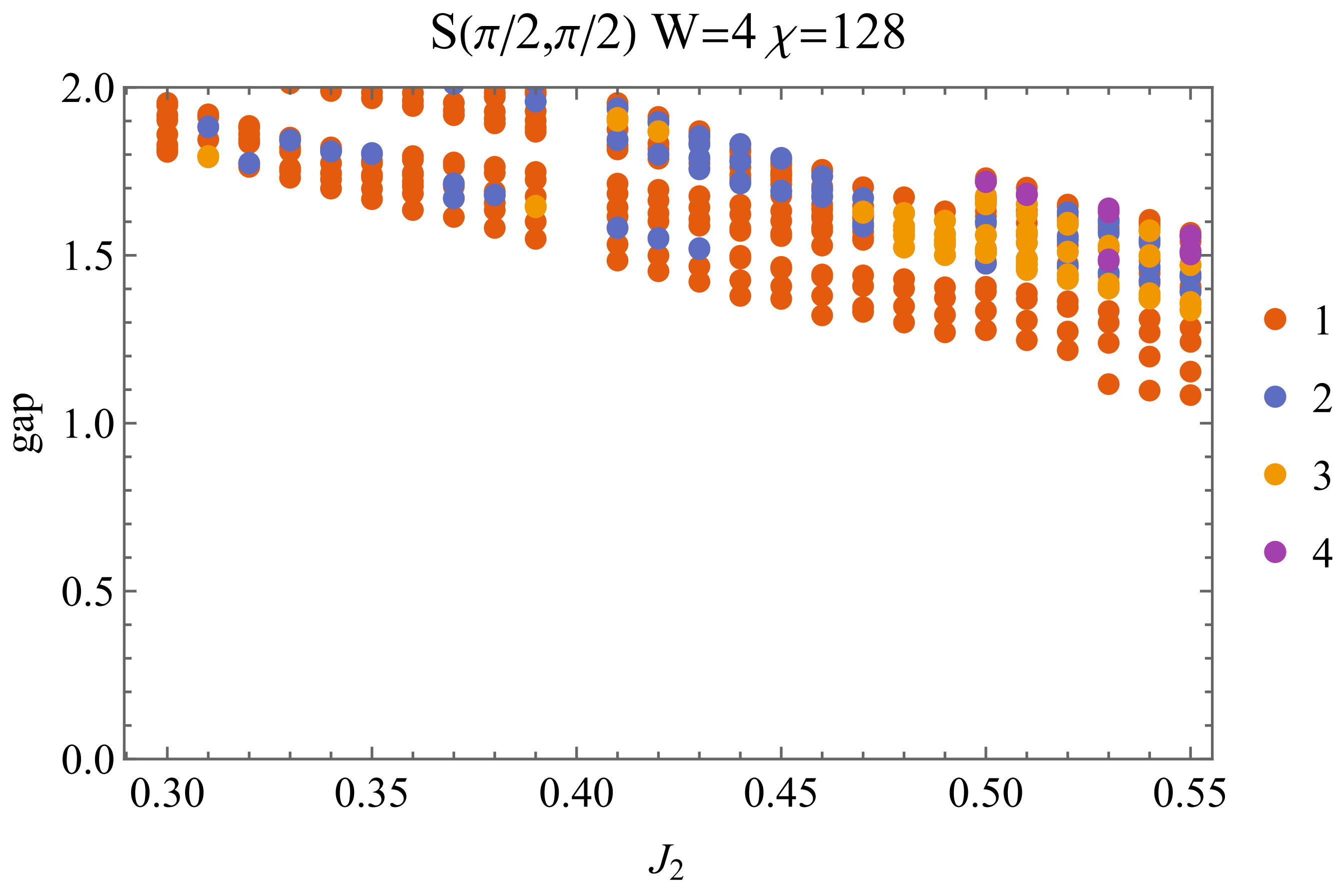

W=5 χ=512 J2=0.56
W=5 χ=512 J2=0.57
W=5 χ=512 J2=0.58
W=5 χ=512 J2=0.59
W=5 χ=512 J2=0.6
W=5 χ=512 J2=0.61
W=5 χ=512 J2=0.62
W=5 χ=512 J2=0.63
W=5 χ=512 J2=0.64
W=5 χ=512 J2=0.65
W=5 χ=512 J2=0.66
W=5 χ=512 J2=0.67
W=5 χ=512 J2=0.68
W=5 χ=512 J2=0.69
W=5 χ=512 J2=0.7
LorentzBroaden
ω
SxSx
SySy
SzSz

Dimer spectral weight at 0.5



gap	degeneracy
0.188307	3
0.228967	1
0.346287	1
0.885025	5





S(π/2,π/2) W=4 χ=128
2.0
1.5
1.0
0.5
0.0
gap
0.30
0.35
0.40
0.45
0.50
0.55
J2
1
2
3
4

- non-zero mag
  - IDMRG DMRG
  - 1-row 2-row
- 5 degeneracy SO5