AD_excitation

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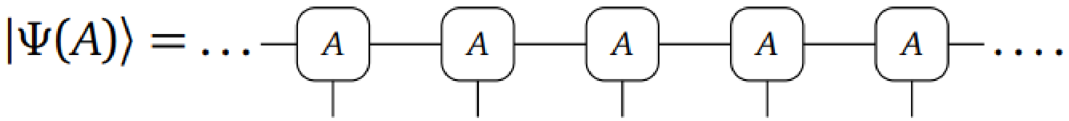
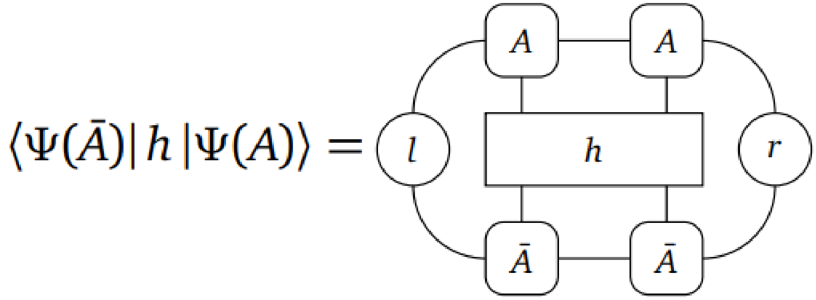
2022.11.4

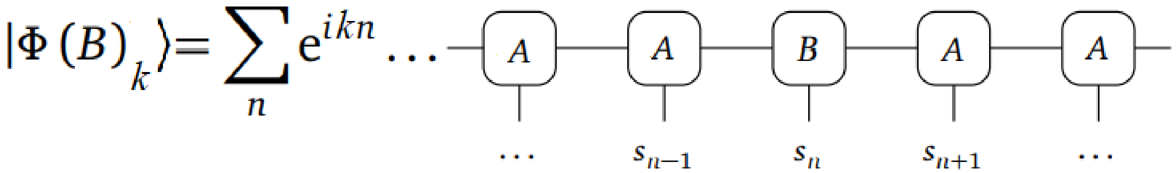
background

- Ground state





- Quasiparticle ansatz(single-mode approximation)



Steps summary and difficulties

graph summation

$\downarrow$

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

$\downarrow$ 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

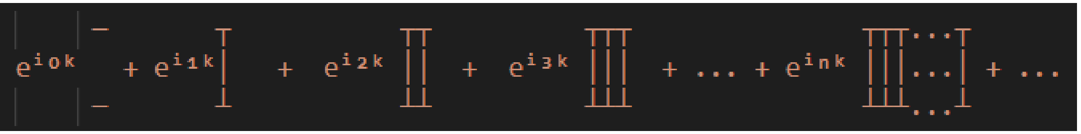
$$H_{Nbeff}(k)X = \omega X$$

Correct graph summation

- Correct series summation

$s1$ is series summation of

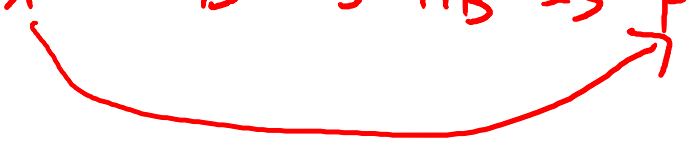
$s2$ is series summation of



They are divergent

f

$X \to B \to HB \to Hx$

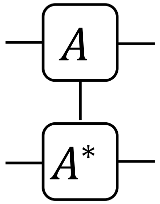


```
1. Bu, Bd* and H on the same site:

 ┌──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

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

$T =$  $\qquad T^0 = \mathbb{1}$

- 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

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Geometric Sums of Transfer Matrices(2/3)

- projectors

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

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

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

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

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).

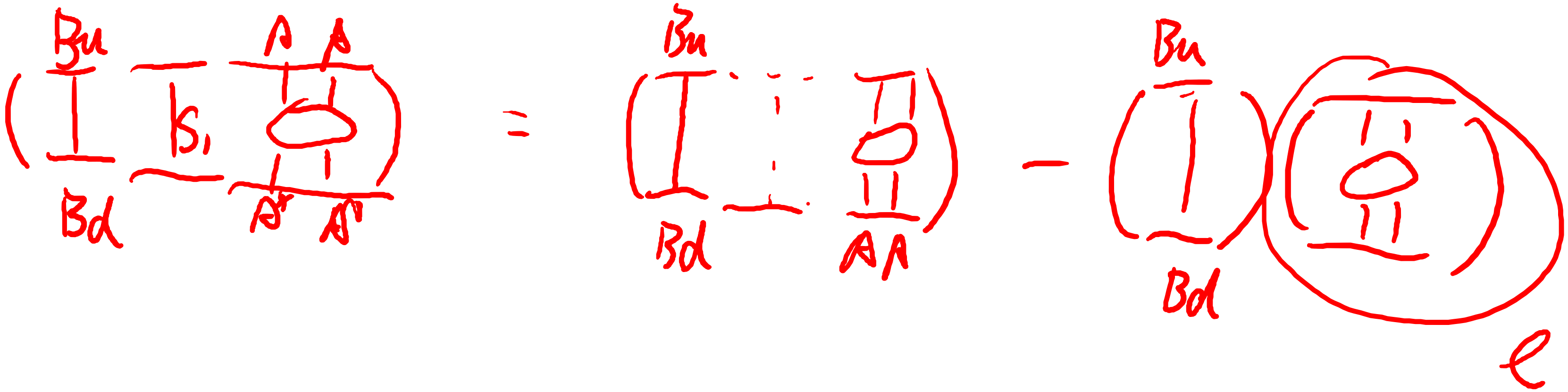
Geometric Sums of Transfer Matrices(3/3)

- Linear solve

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

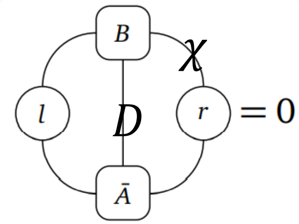
$$(\mathbb{1} - \mathcal{T})|y) = Q|x)$$

P $\quad T - P$


Bu
A A
Bd
Bu
Bd
A A
Bu
Bd
e

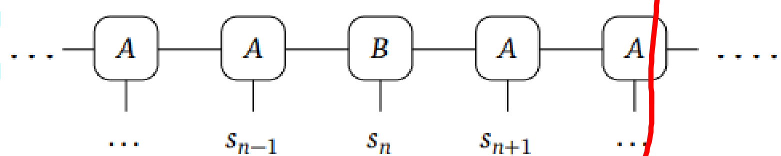
Orthogonal Parameterization of $\Phi(B)$(1/2)

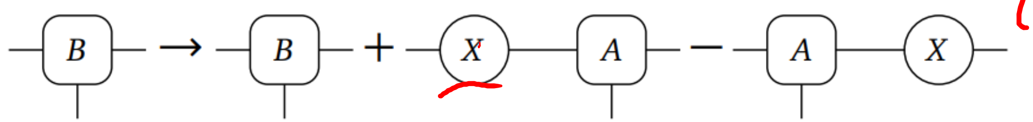
- $\Phi(B)$ is Orthogonal to $\psi(A)$



- Gauge Invariant of Tangent vector

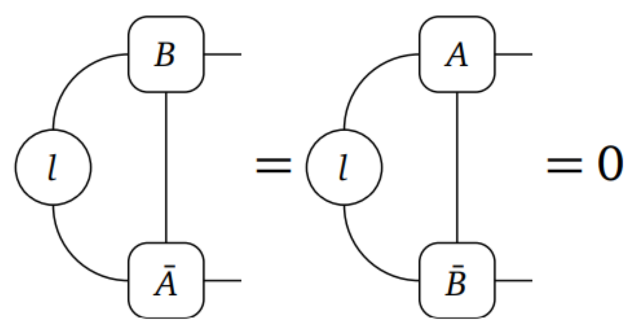
$$|\Phi(B;A)\rangle = B^i \frac{\partial}{\partial A_i} |\Psi(A)\rangle = \sum_n$$





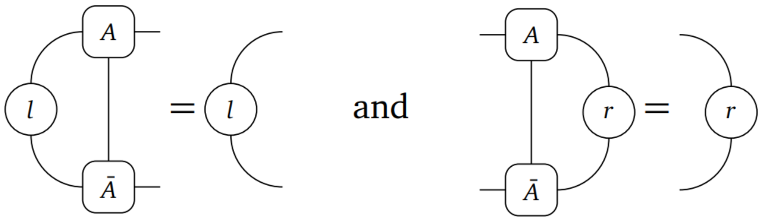
Parameters $D\chi^2 \rightarrow D\chi^2 - 1 \rightarrow D\chi^2 - \chi^2$

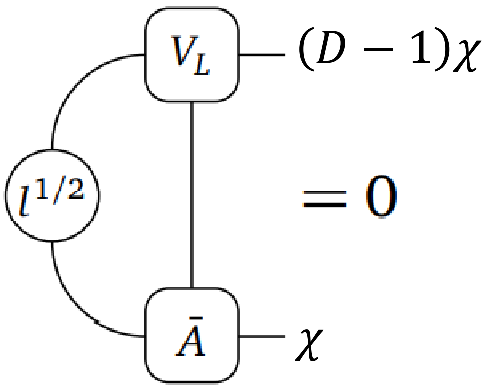
- Left gauge-fixing condition

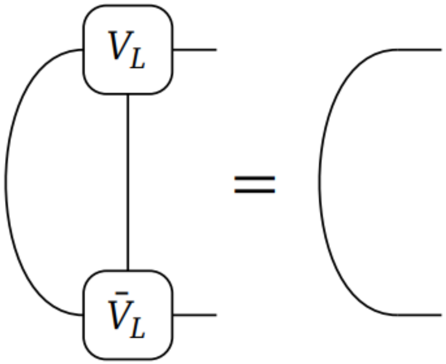


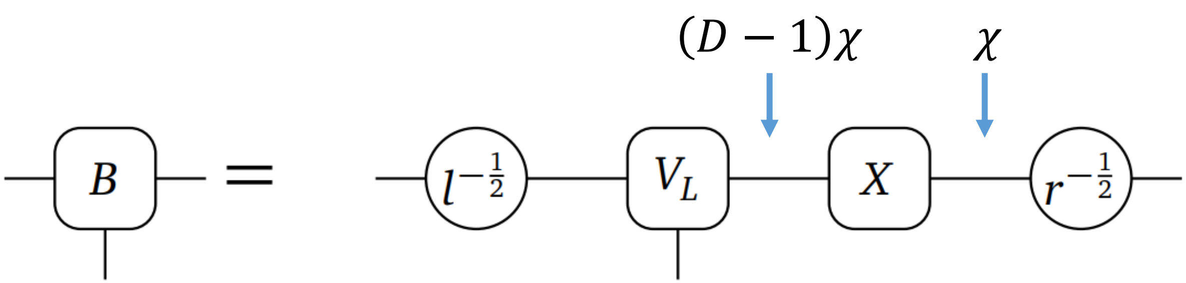
Orthogonal Parameterization of $\Phi(B)$(2/2)

- parameterization



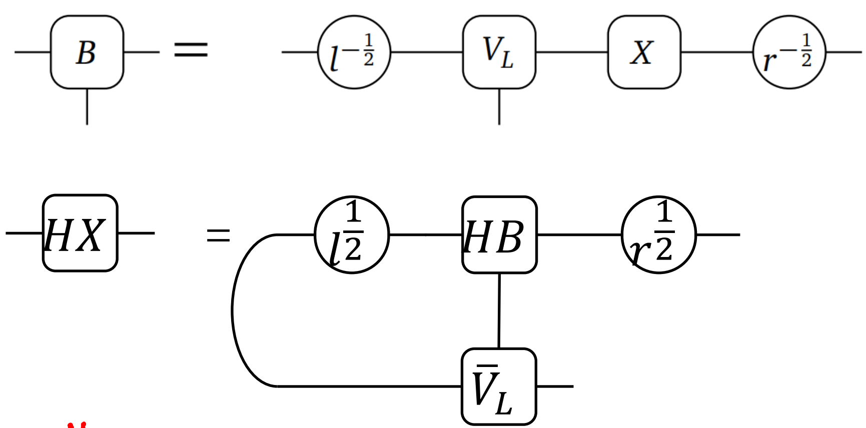




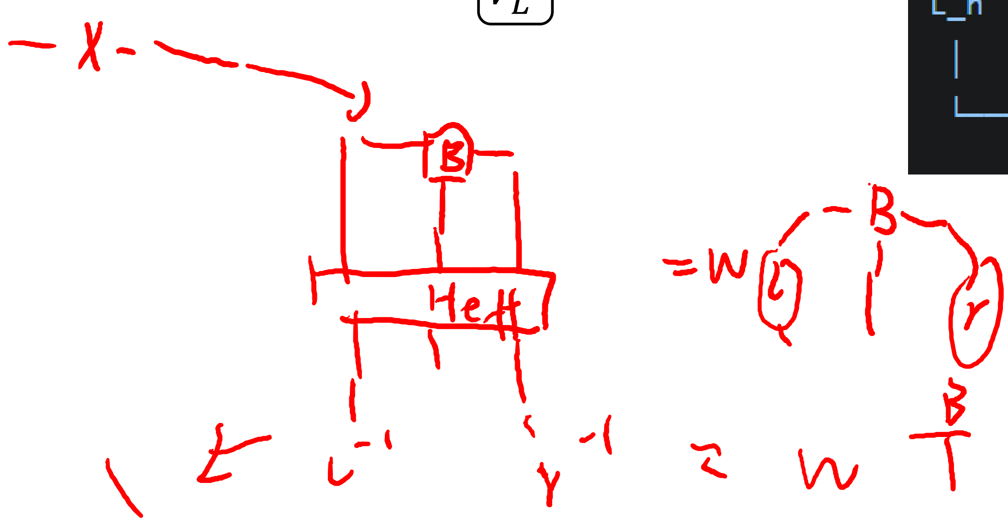


ordinary eigenvalue problem

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



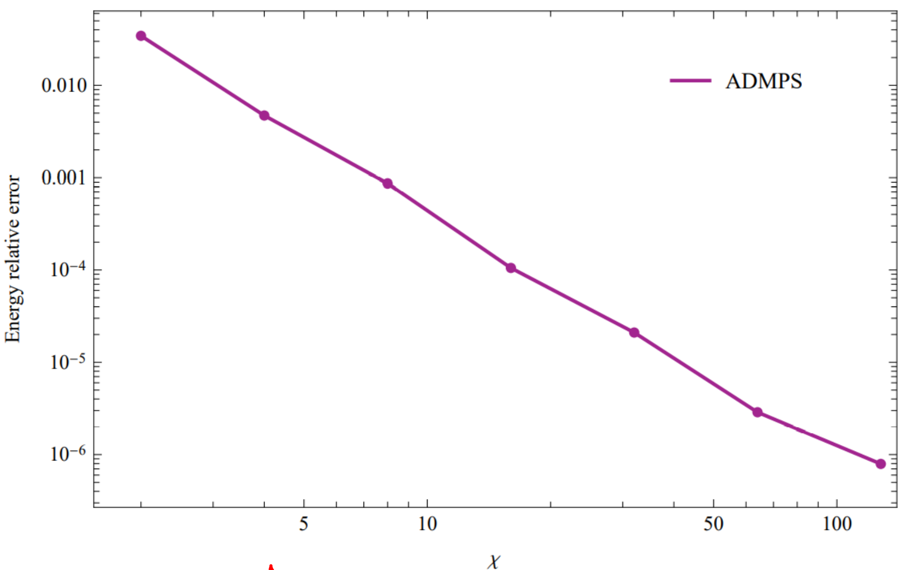

```
1. Bu, Bd* on the same site

┌───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*─┘
```

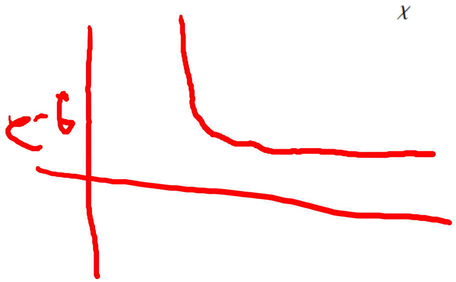


Ground state by AD

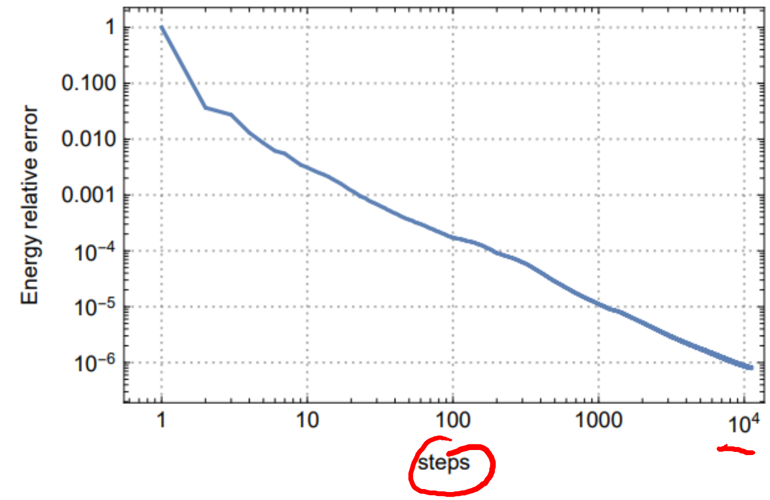
- Heisenberg $S = 1/2$

error exponentially-dependent on χ

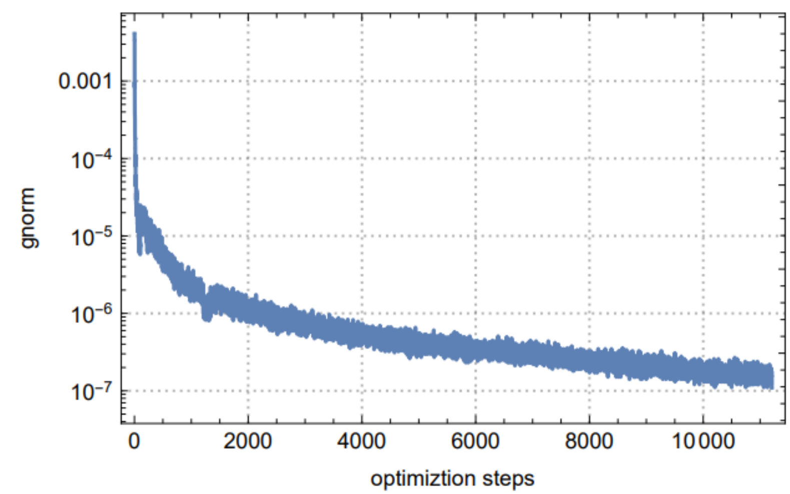




E−steps χ=128

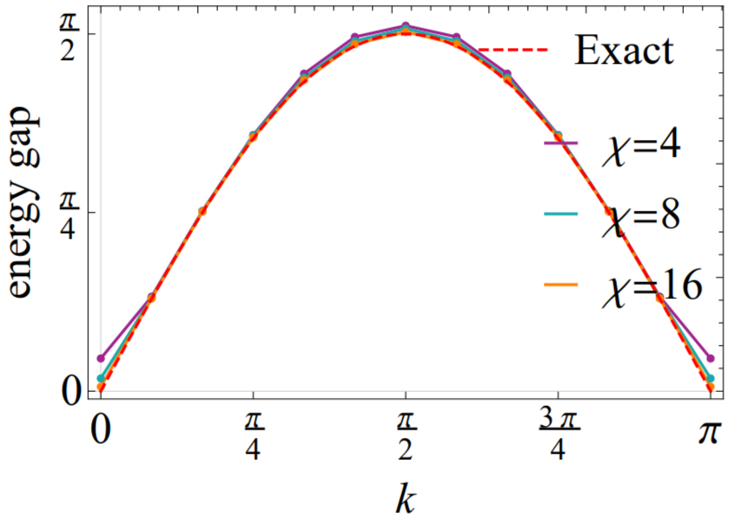


gnrom−steps χ=128

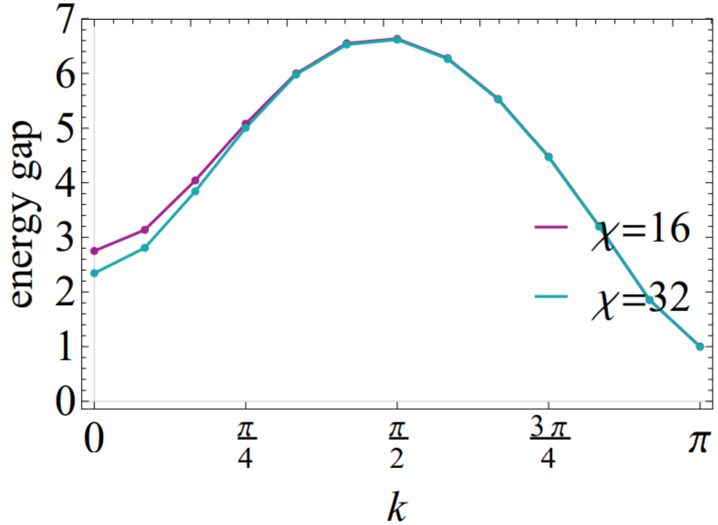


gap

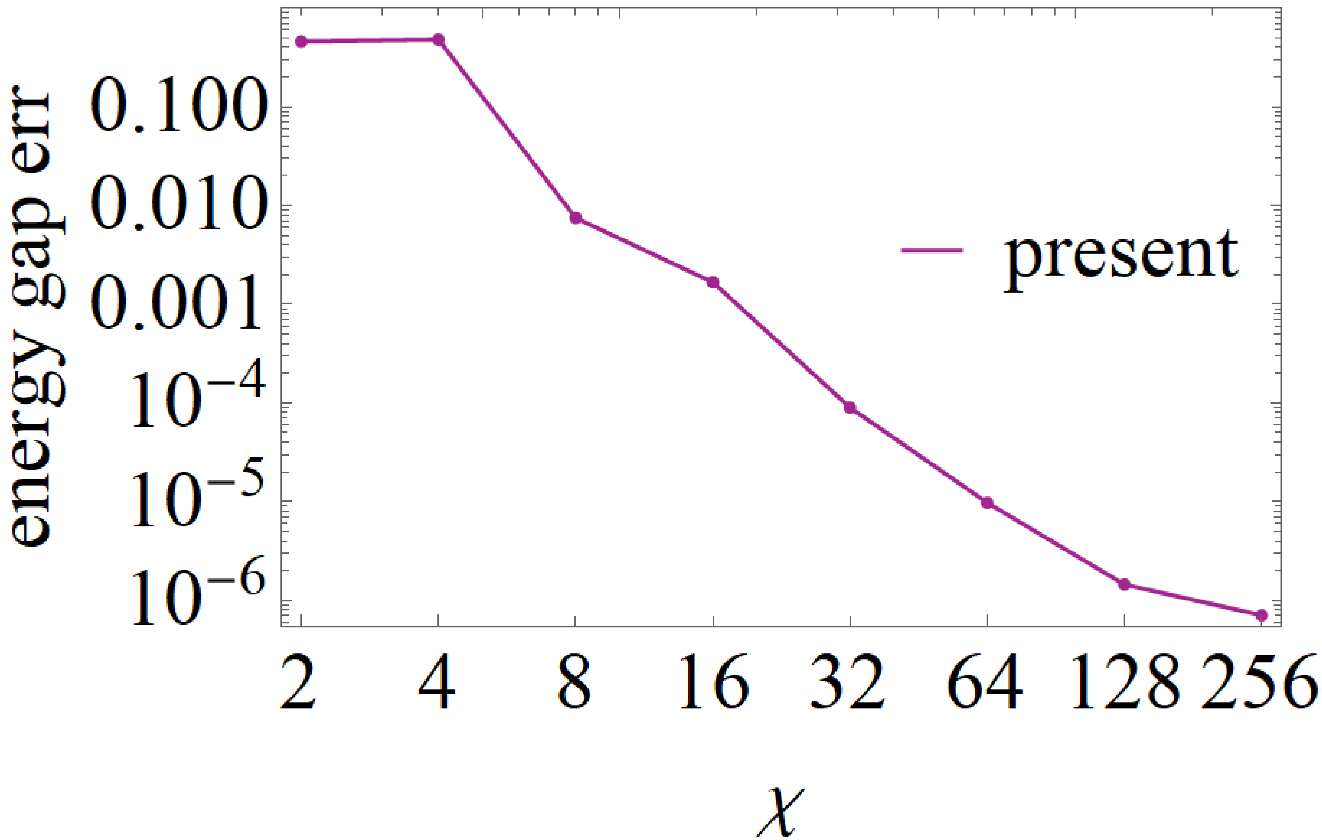
- Heisenberg $S = 1/2$



- Heisenberg $S = 1$



$k = \pi$ Haldane gap error



10-8

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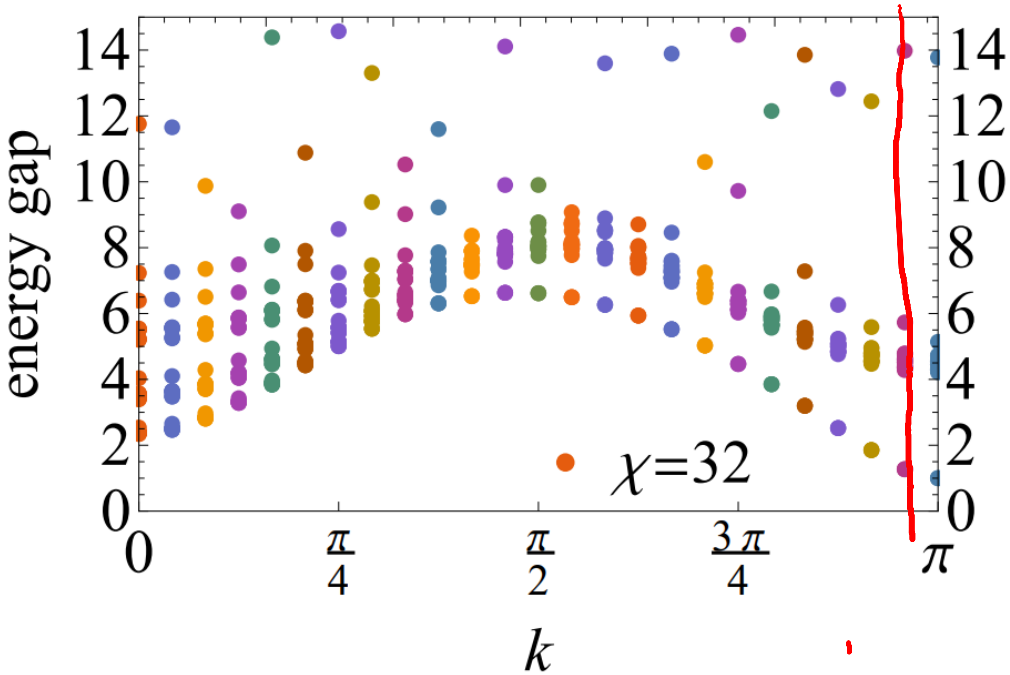
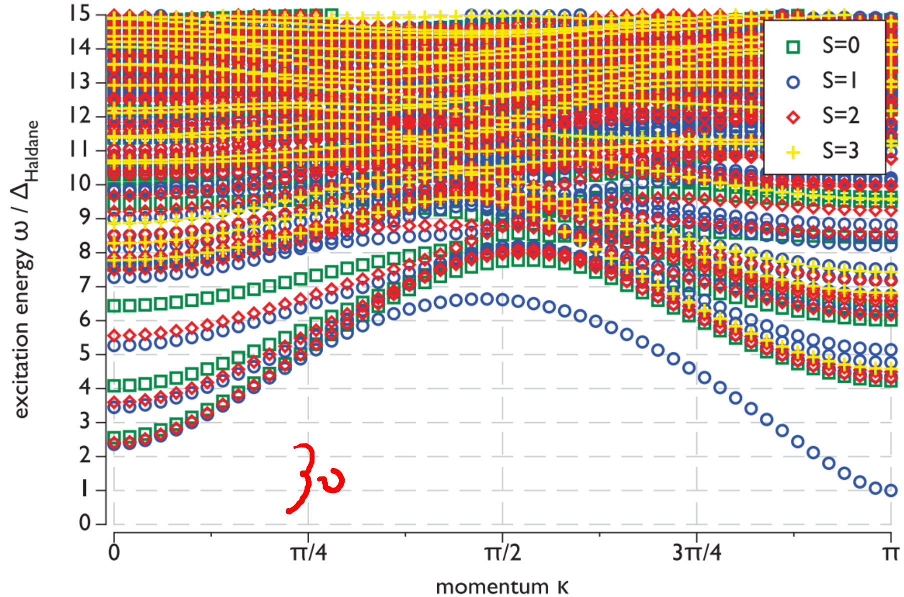
For $\chi = 256$

AD for ground state ~ 8h 10000 steps

Eigsolve for excitation state ~ 500s

Heisenberg $S = 1$ excitation spectrum

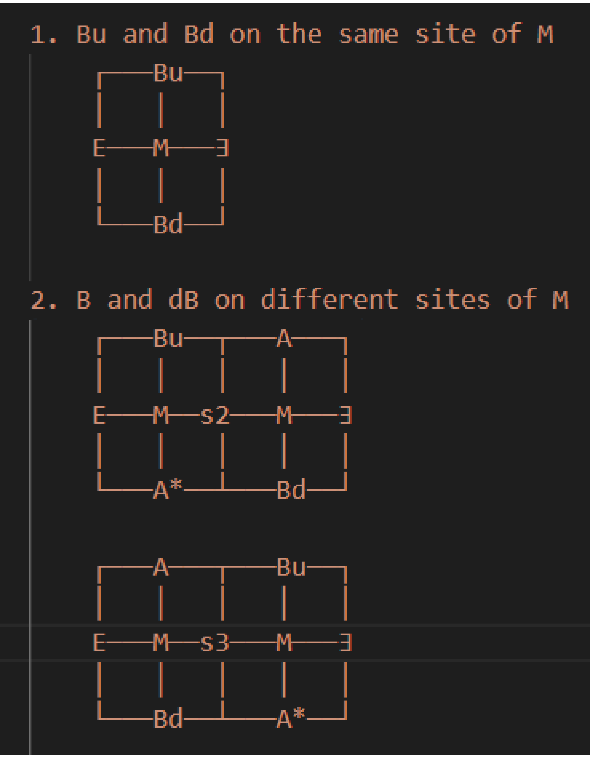




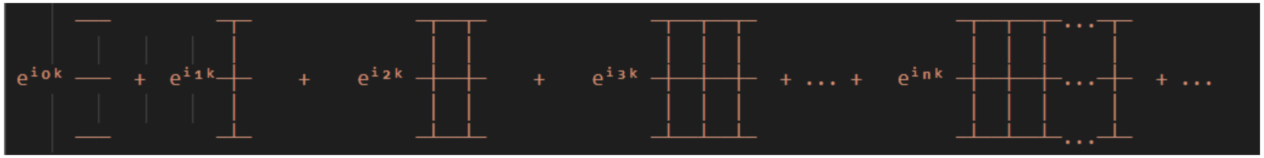
https://github.com/XingyuZhang2018/AD_Excitation/blob/main/project/result.pdf

result.pdf

MPO graph summation



s2

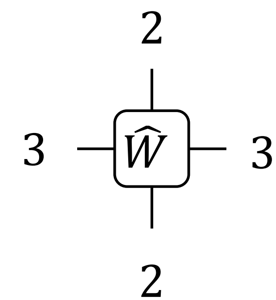


MPO

- TFIsing

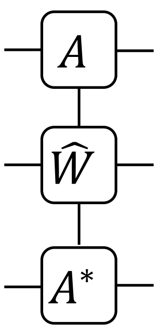
$$H_{\mathrm{TFI}} = -J \sum_j \sum_{n>0} \lambda^{n-1} X_j X_{j+n} - h \sum_j Z_j$$

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



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

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



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

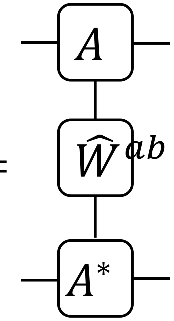
Overlap(E, Ǝ) = 0   E王Ǝ = 0

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

Fixed point equations

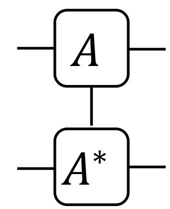
- Left and right environment EƎ

$$Ϲ_a = Ϲ_a ⌶^{aa} + Є_a \qquad Є_a = \textstyle\sum_{b>a} Ϲ_b ⌶^{ba}$$
$$Ͻ_a = ⌶^{aa} Ͻ_a + Э_a \qquad Э_a = \textstyle\sum_{b<a} ⌶^{ab} Ͻ_b$$

$⌶^{ab} =$ 

- $⌶^{aa} = 0$

$$Ϲ_a = Є_a$$
$$Ͻ_a = Э_a$$

$⌶ =$ 

- $⌶^{aa} = \lambda_a ⌶$

$$Ϲ_a = \lambda_a Ϲ_a ⌶ + Є_a \qquad Ϲ_a(1 - \lambda_a ⌶) = Є_a$$
$$Ͻ_a = \lambda_a ⌶ Ͻ_a + Э_a \qquad (1 - \lambda_a ⌶)Ͻ_a = Э_a$$

- $⌶^{aa} = ⌶$

$$Ϲ_a(1 - ⌶) = Є_a$$
$$(1 - ⌶)Ͻ_a = Э_a$$

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

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

$$Ϲ_a(1 - ⌶ - ɔc) = Є_a - Є_a ɔc$$
$$(1 - ⌶ - ɔc)Ͻ_a = Э_a - ɔcЭ_a$$
$$\text{energy} = cЭ_w = Є_1 ɔ$$

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$e - e'$

k

$w =$

e

Thank you for listening!

Q&A?