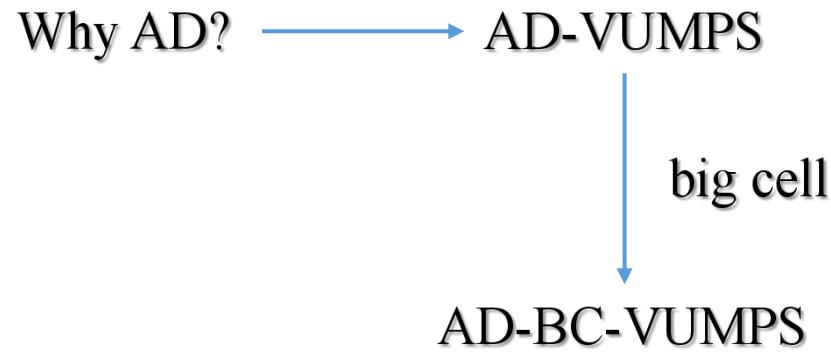


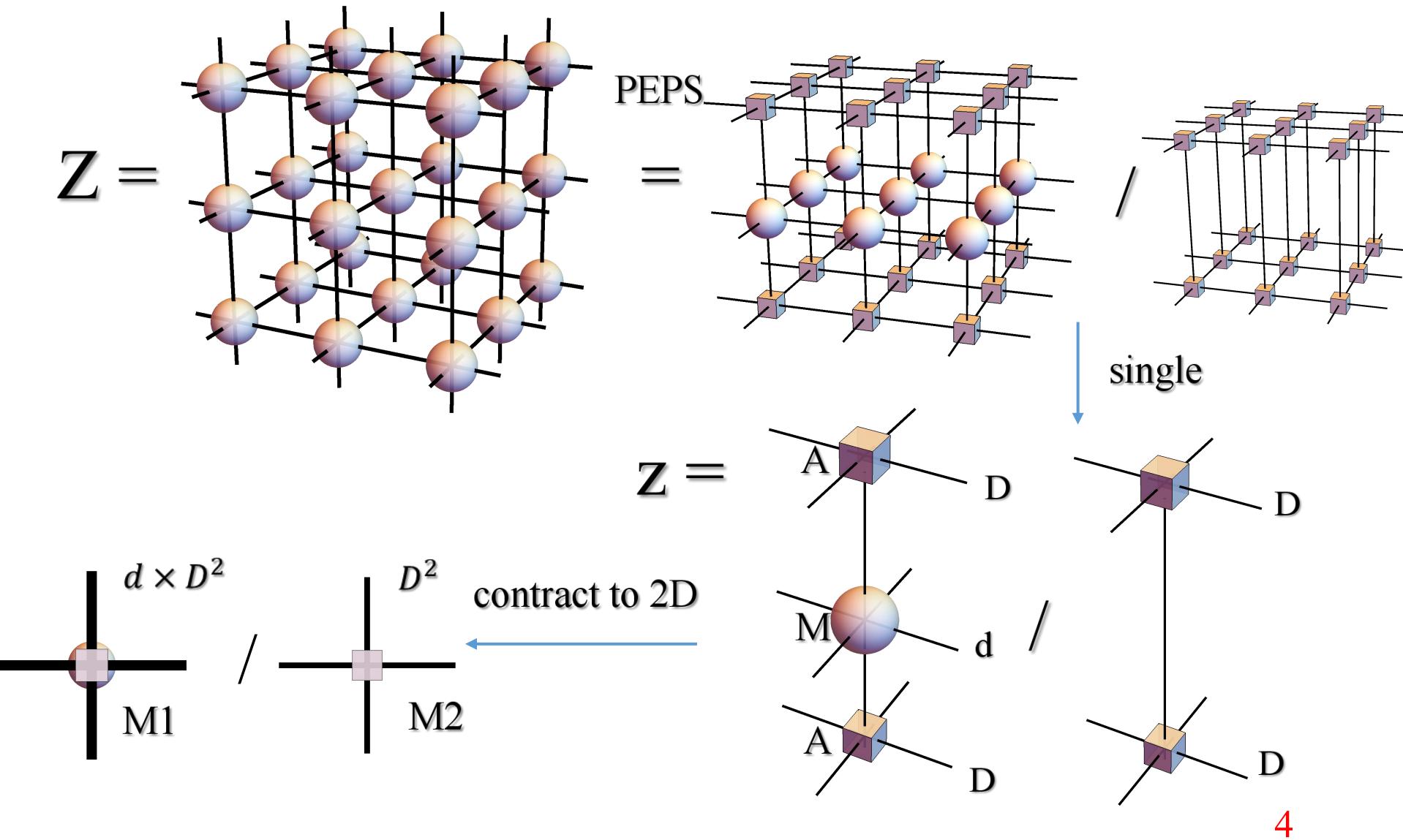
# AD-BC-VUMPS

# Contents

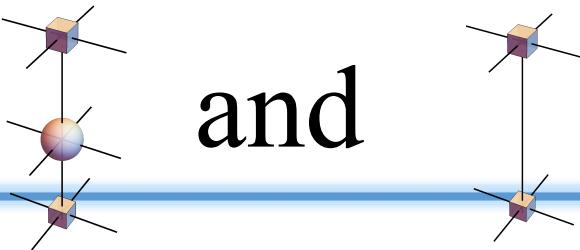


# Why AD?

# 3Dising contract

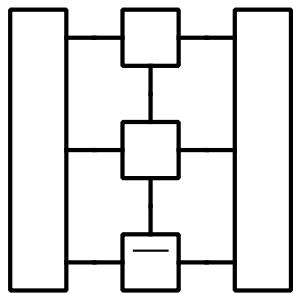


# Gradient to and

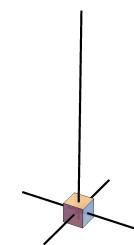
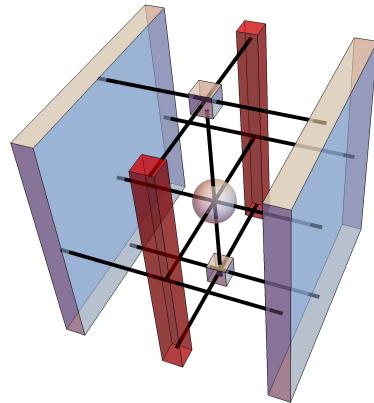
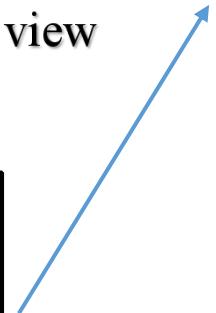


$$\frac{\partial}{\partial A} (\text{ )} = 2$$

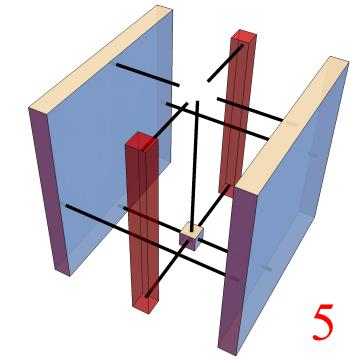
Two diagrams illustrating a gradient field. The left diagram shows a sphere with a color gradient from blue at the bottom to orange at the top, with a grid of lines radiating from its center. The right diagram shows a similar setup but with a different gradient or a different configuration of lines. Between them is the mathematical expression  $\frac{\partial}{\partial A} (\text{ )} = 2$ .



3D view



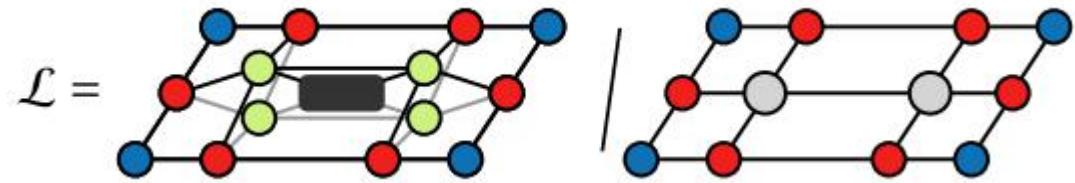
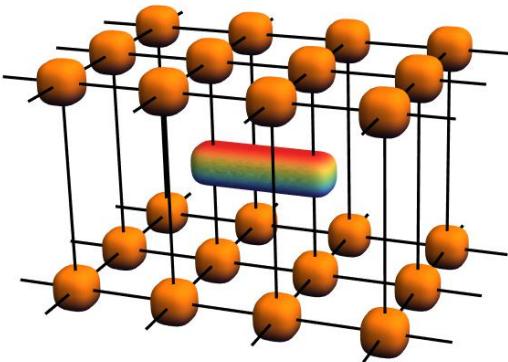
add envir



# Quantum case

- 2D Energy

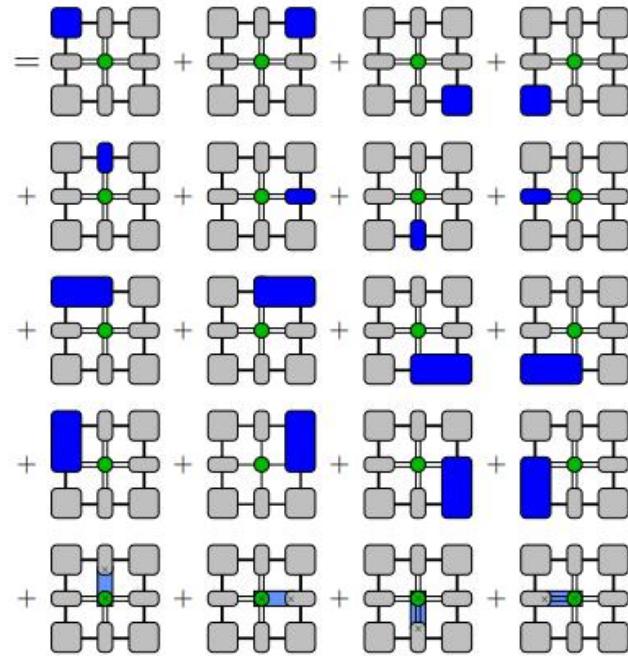
$$\min_A E(A) = \min_A \frac{\langle \Psi(A) | \hat{H} | \Psi(A) \rangle}{\langle \Psi(A) | \Psi(A) \rangle}$$



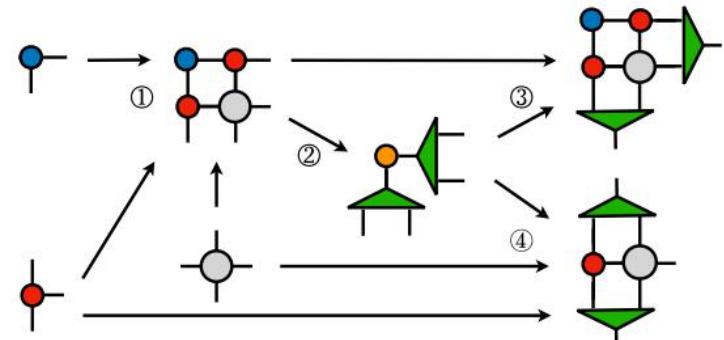
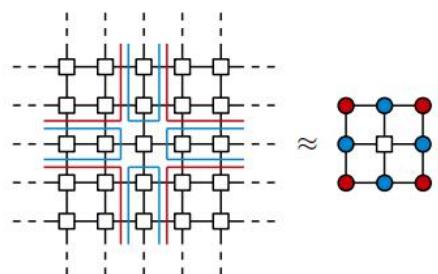
$$T_{uldr} = l \begin{array}{c} u \\ \text{---} \\ d \end{array} r = \begin{array}{c} \text{---} \\ u \\ \text{---} \\ d \end{array}$$

# CTMRG

$$\langle \Psi | \hat{H} | \Psi \rangle =$$



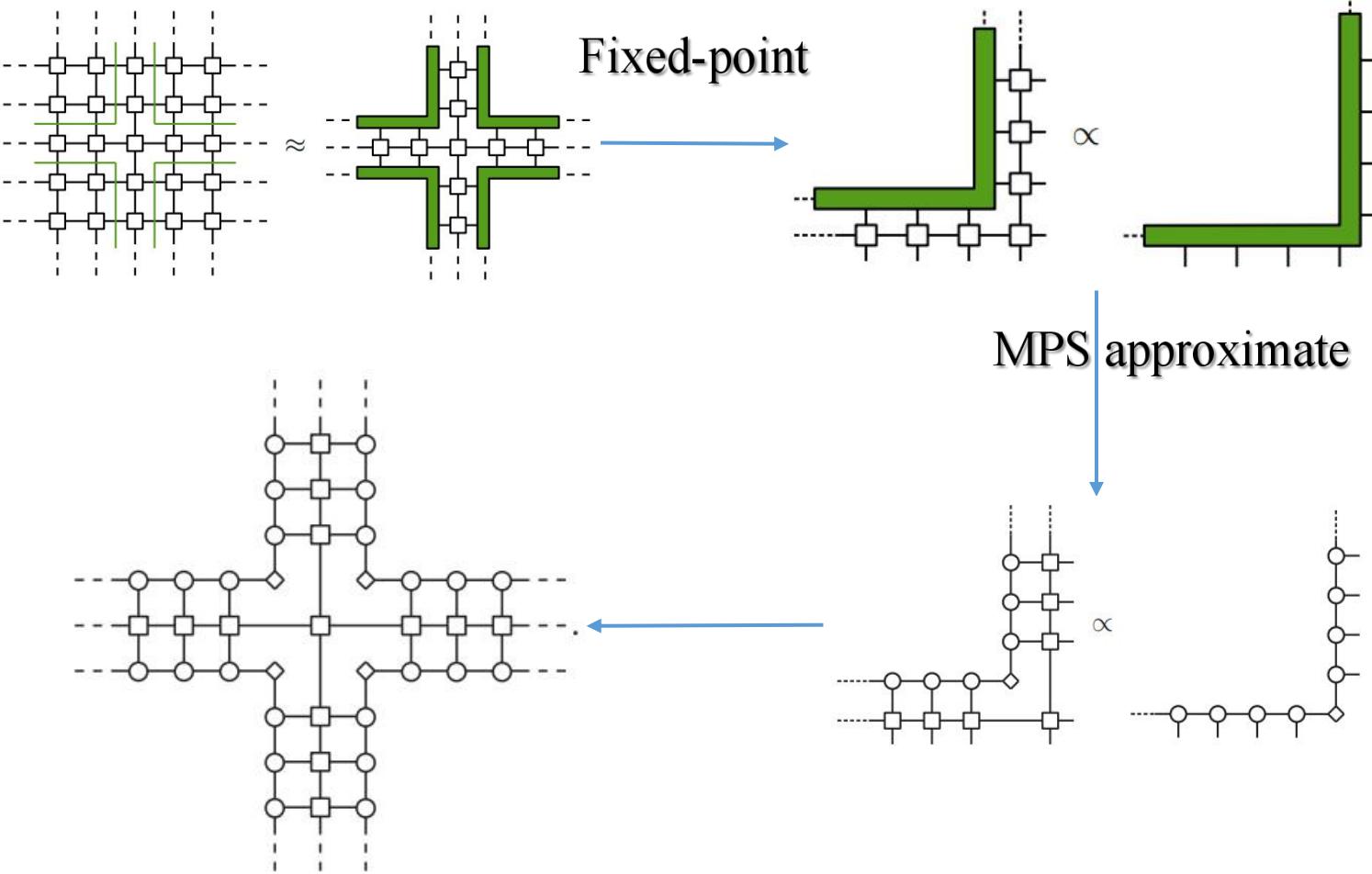
$$\begin{aligned} \tilde{C}_1 &= \text{[Blue Box]} = \text{[Box with 2x2 grid]} + \text{[Box with 2x2 grid]} + \text{[Box with 2x2 grid]} + \dots \\ \tilde{T}_4 &= \text{[Blue Box]} = \text{[Box with 2x2 grid]} + \text{[Box with 2x2 grid]} + \text{[Box with 2x2 grid]} + \dots \\ \tilde{C}_{v1} &= \text{[Blue Box]} = \text{[Box with 2x2 grid]} + \text{[Box with 2x2 grid]} + \text{[Box with 2x2 grid]} + \dots \end{aligned}$$



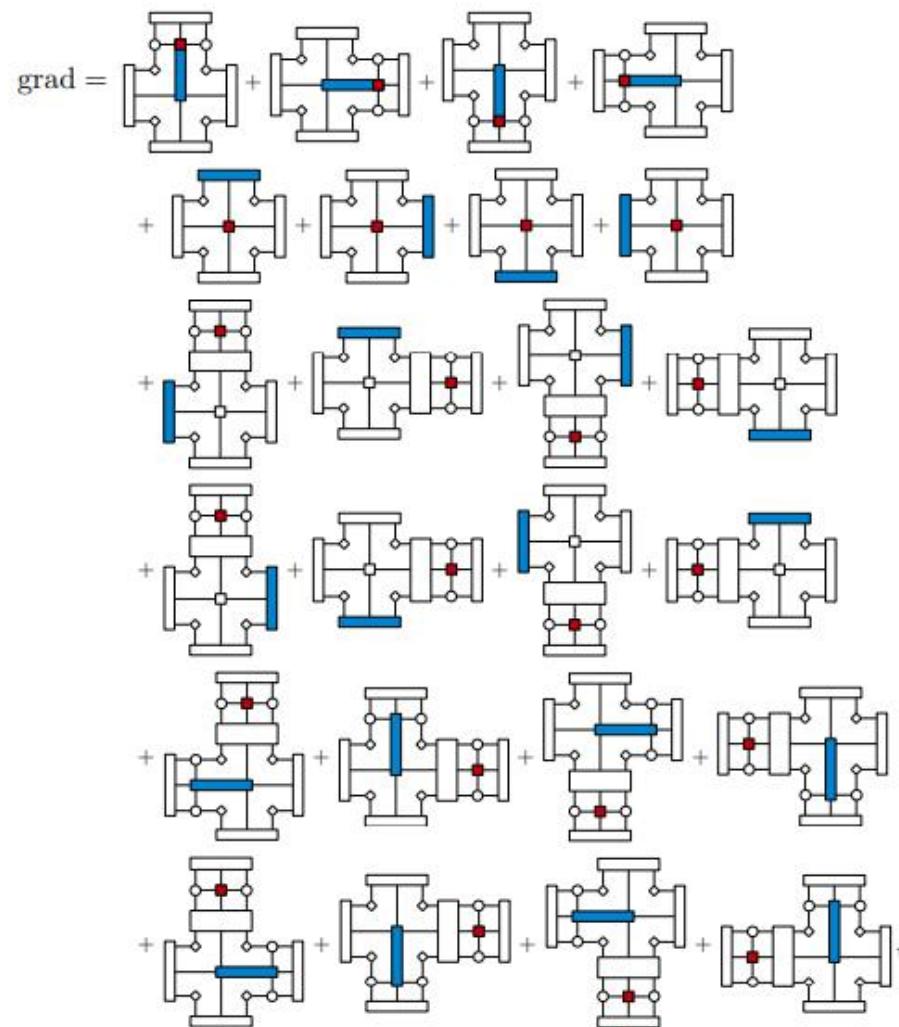
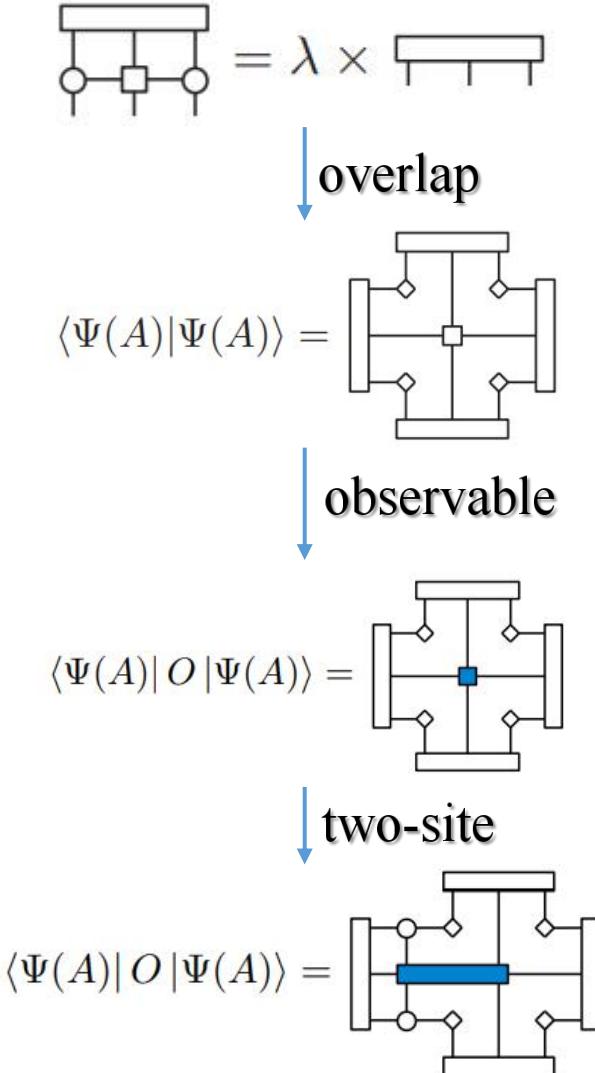
- Experimental optimization method

- (1) Compute  $E(1)$  (corresponding to the previous energy with the old tensor  $A' = A$ ) and  $E(0.5)$  (corresponding to the energy with  $A' = \tilde{A}$ ).
- (2) If  $E(0.5) < E(1)$ , take  $A' = \tilde{A}$  as the solution and exit.
- (3) Define an initial step size  $\Delta_0$  (e.g.,  $\Delta_0 = 0.1$ ) and a tiny step size  $h$  (e.g.,  $h = 10^{-4}$ ).
- (4) If  $E(1 + h) < E(1)$ , set  $\Delta = \Delta_0$ , else  $\Delta = -\Delta_0$ .
- (5) For  $iter = 1$  to  $maxiter$ 
  - (a) If  $E(1 + \Delta) < E(1)$ , accept solution [44] with  $\lambda = 1 + \Delta$  and exit.
  - (b) Else  $\Delta = \Delta/2$ .

# Channel environments

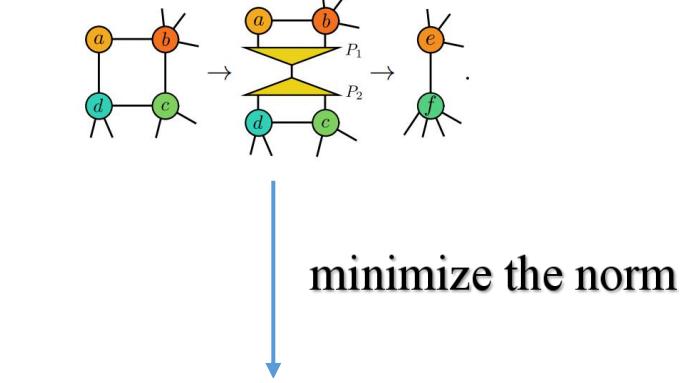


# Gradient

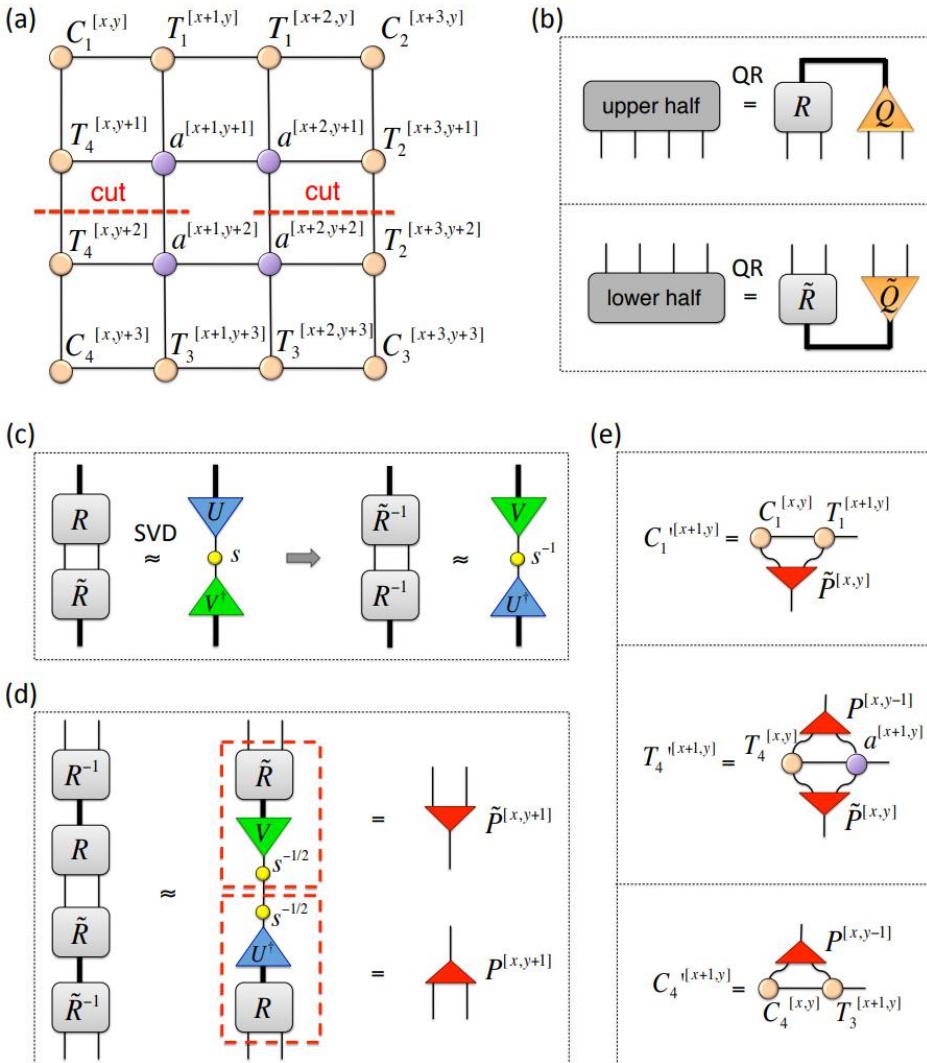


# Big Cell CTMRG

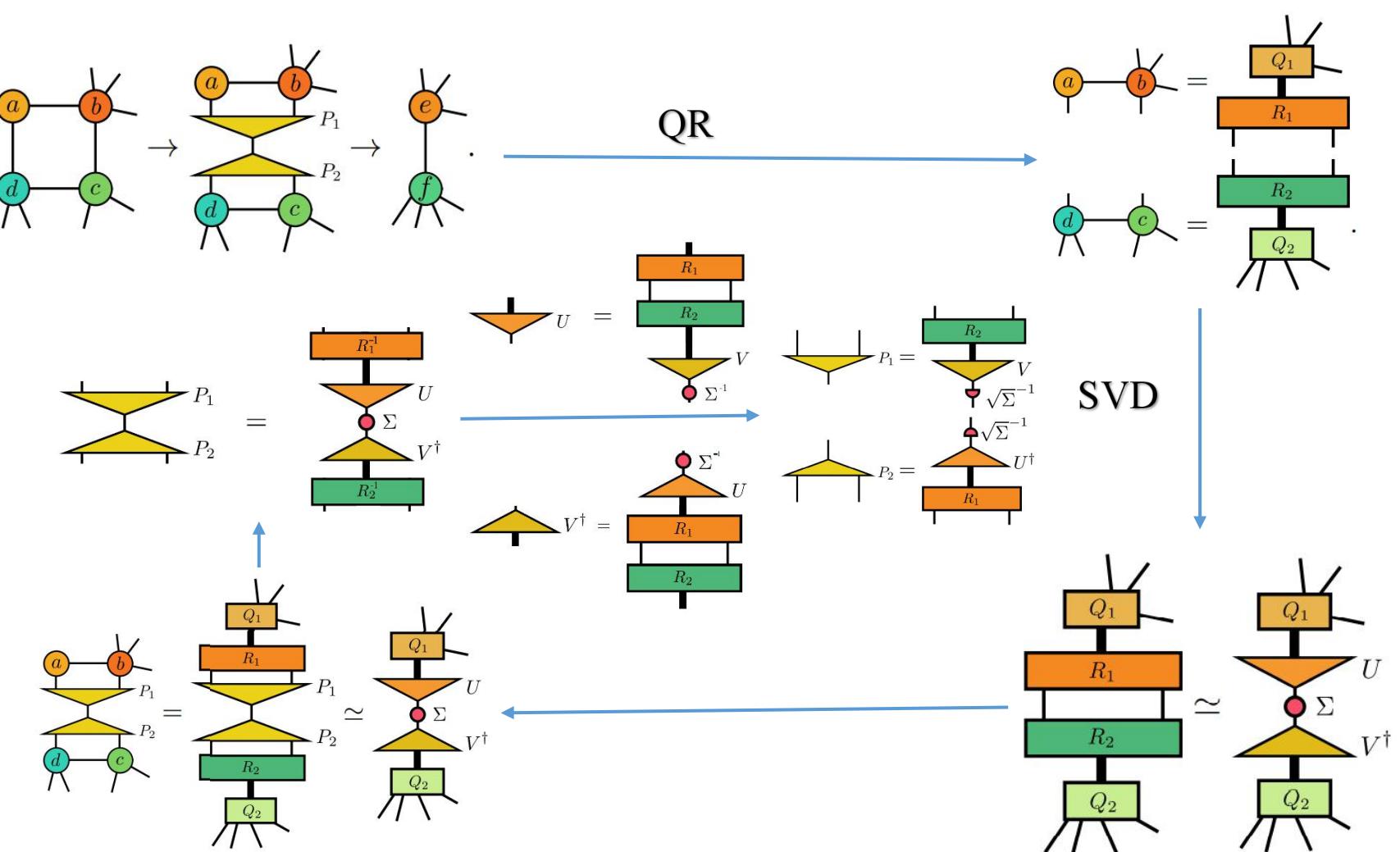
- General case



$$\mathcal{C} = \left| \begin{array}{c} \text{Initial Cluster} \\ - \\ \text{Transformed State} \end{array} \right|^2$$



# Get $P_1$ and $P_2$



# AD-VUMPS

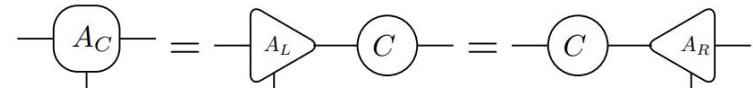
# VUMPS-algorithm

# Initial orthonormal form MPS

$M = \text{classical2Disingmpo}(\beta; J = 1.0, h = 0.)$

$AL, C = \text{leftorth}(A)$

$AR = \text{rightorth}(AL, C)$

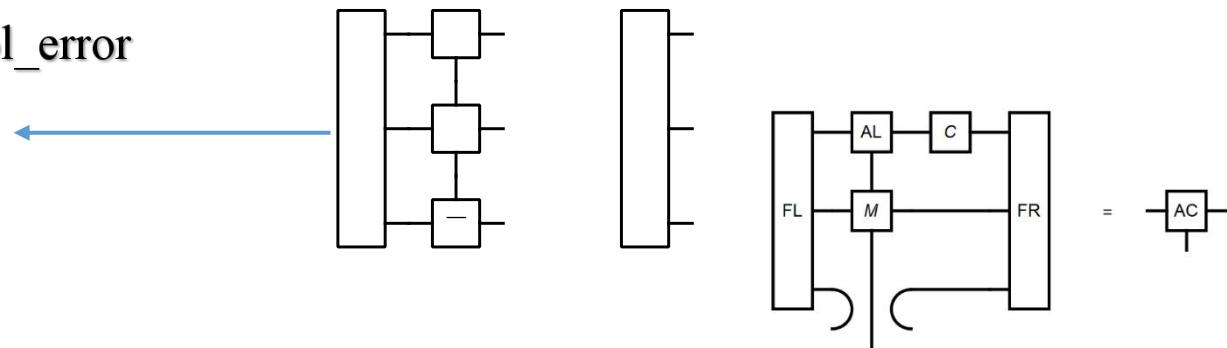


while  $\text{error}(AC, FL, FR, M) > \text{tol\_error}$

# Get environment

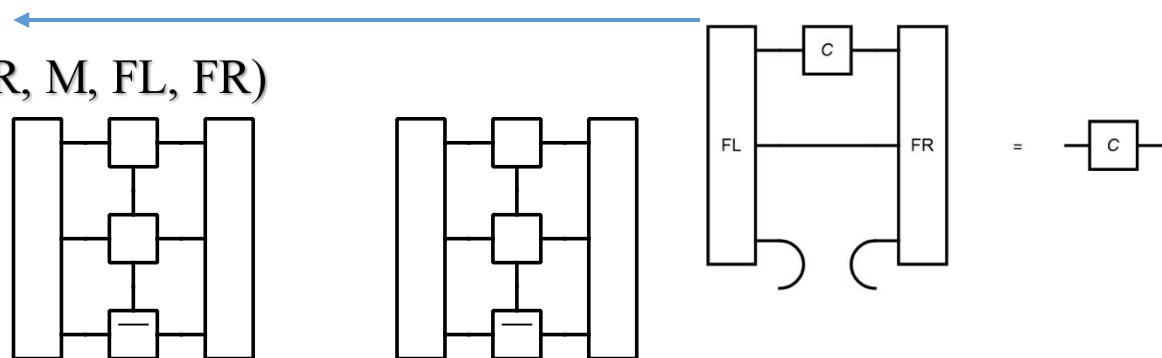
$FL = \text{leftenv}(AL, M)$

$FR = \text{rightenv}(AR, M)$



# Get orthonormal form

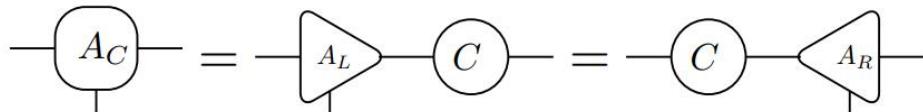
$AC, C = \text{vumpsstep}(AL, C, AR, M, FL, FR)$



# calculate observable

$Obs = \text{obser}(O, AC, M, FL, FR)$

# QR to avoid inverse



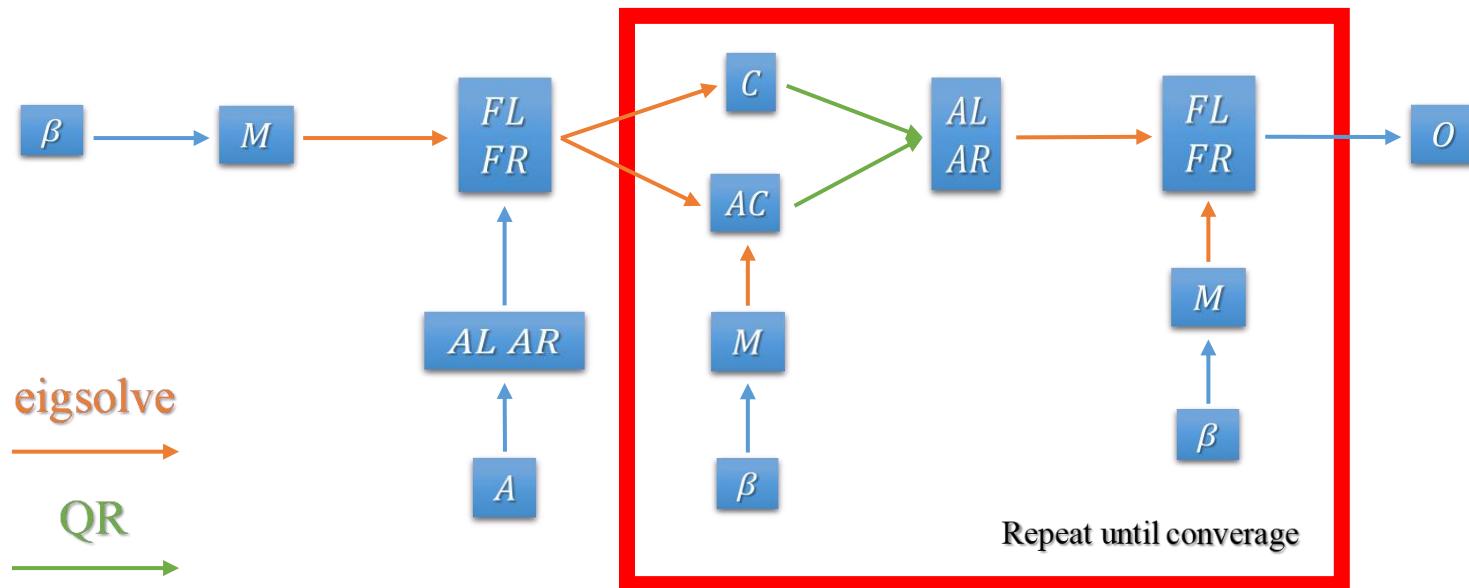
$$A_C = Q_{A_C} \cdot R_{A_C}$$
$$C = Q_C \cdot R_C$$

$$\begin{aligned} A_L &= A_C \cdot C^{-1} \\ &= Q_{A_C} \cdot R_{A_C} \cdot R_C^{-1} \cdot Q_C^{-1} \\ &= Q_{A_C} \cdot R_{A_C} \cdot R_C^{-1} \cdot Q_C^T \\ &\approx Q_{A_C} \cdot Q_C^T \end{aligned}$$

$$\text{Error} = R_{A_C} - R_C$$

$$A_L^T \cdot A_L = Q_C \cdot Q_{A_C}^T \cdot Q_{A_C} \cdot Q_C^T = 1 \quad \text{inverse and orthogonality at the same time}$$

# Computation Graphs



# Adjoint of eigsolve

- $\mathbf{l}^T A = \lambda \mathbf{l}^T, \quad A \mathbf{r} = \lambda \mathbf{r}, \quad \mathbf{l}^T \mathbf{r} = 1,$

$$\begin{aligned} (A - \lambda I) \xi_l &= (1 - \mathbf{r} \mathbf{l}^T) \bar{\mathbf{l}}, & \mathbf{l}^T \xi_l &= 0 \\ (A^T - \lambda I) \xi_r &= (1 - \mathbf{l} \mathbf{r}^T) \bar{\mathbf{r}}, & \mathbf{r}^T \xi_r &= 0 \end{aligned} \longrightarrow \bar{A} = \bar{\lambda} \mathbf{l} \mathbf{r}^T - \mathbf{l} \xi_l^T - \xi_r \mathbf{r}^T$$

gauge invariant

$$\mathbf{l}^T \bar{\mathbf{l}} = \mathbf{r}^T \bar{\mathbf{r}} = 0$$

$$(A - \lambda I) \xi_l = \bar{\mathbf{l}}, \quad \mathbf{l}^T \xi_l = 0$$

$$(A^T - \lambda I) \xi_r = \bar{\mathbf{r}}, \quad \mathbf{r}^T \xi_r = 0$$

Only  $\mathbf{l}$

$$(A - \lambda I) \xi_l = \bar{\mathbf{l}}, \quad \mathbf{l}^T \xi_l = 0$$

$$(A^T - \lambda I) \xi_r = 0, \quad \mathbf{r}^T \xi_r = 0$$

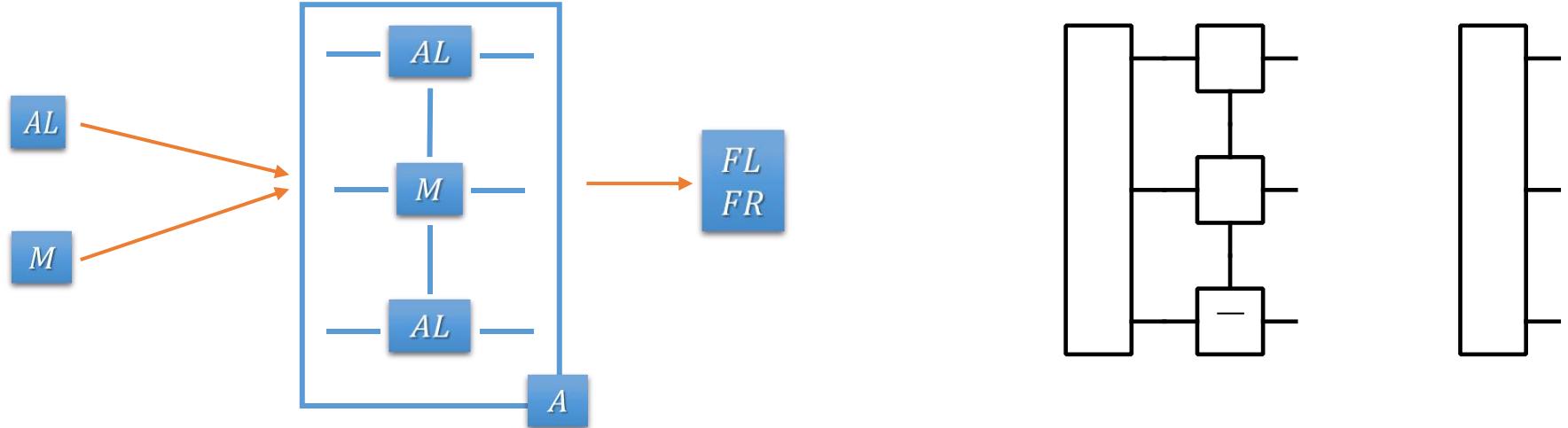
Only  $\mathbf{r}$

$$(A - \lambda I) \xi_l = 0, \quad \mathbf{l}^T \xi_l = 0$$

$$(A^T - \lambda I) \xi_r = \bar{\mathbf{r}}, \quad \mathbf{r}^T \xi_r = 0$$

$$\boxed{\bar{A} = -\xi_r \mathbf{r}^T}$$

# Adjoint of VUMPS environment



$$(A - \lambda I)\xi_l = \bar{l}, \quad l^T \xi_l = 0$$

$$\bar{A} = -l \xi_l^T$$

$$\overline{AL} = \bar{A} \cdot \frac{\partial A}{\partial AL}$$

$$\overline{M} = \bar{A} \cdot \frac{\partial A}{\partial M}$$

$$dM = - \begin{bmatrix} & AL \\ FL & \cdots & \cdots & \xi_l \\ & AL \end{bmatrix}$$

$$dAL = - \begin{bmatrix} & | \\ FL & \cdots & M & \cdots & | \\ & AL \end{bmatrix} \xi_l - \begin{bmatrix} & AL \\ FL & \cdots & M & \cdots & | \\ & AL \end{bmatrix} \xi_l$$

# Adjoint of QR

- $A = QR$

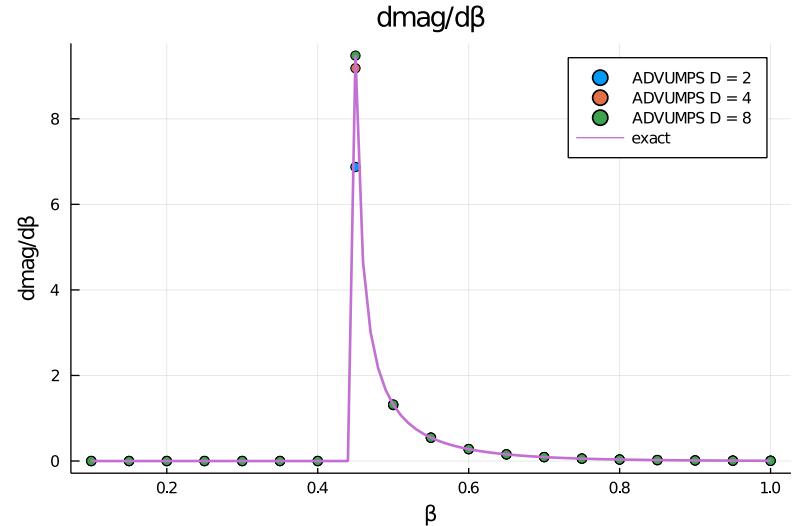
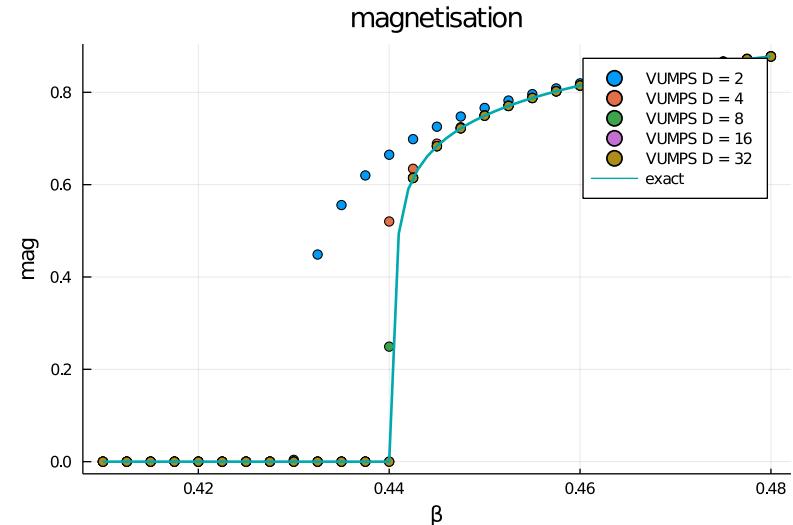
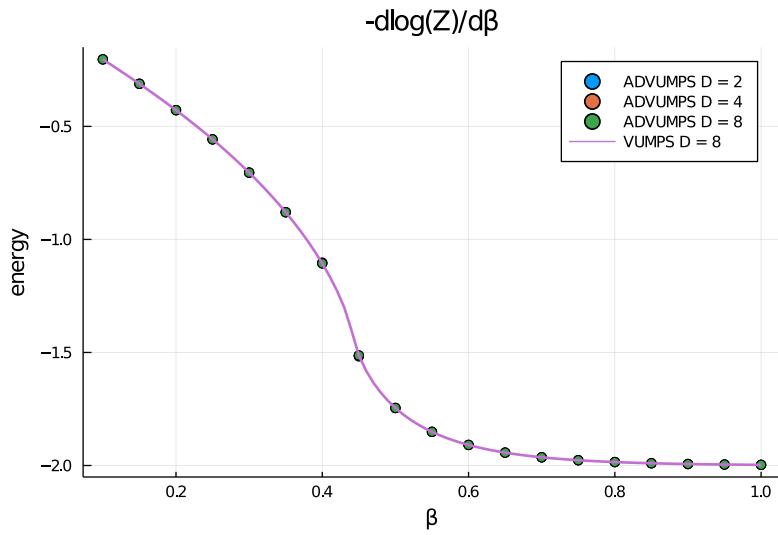
$$\bar{A} = [\bar{Q} + Q \text{copyltu}(M)] R^{-T}$$

$$M = R \bar{R}^T - \bar{Q}^T Q$$

$$[\text{copyltu}(M)]_{ij} = M_{\max(i,j), \min(i,j)}$$

- Trick: add  $\delta = 10^{-6}$  to R's diagonal element for the stability of inverse

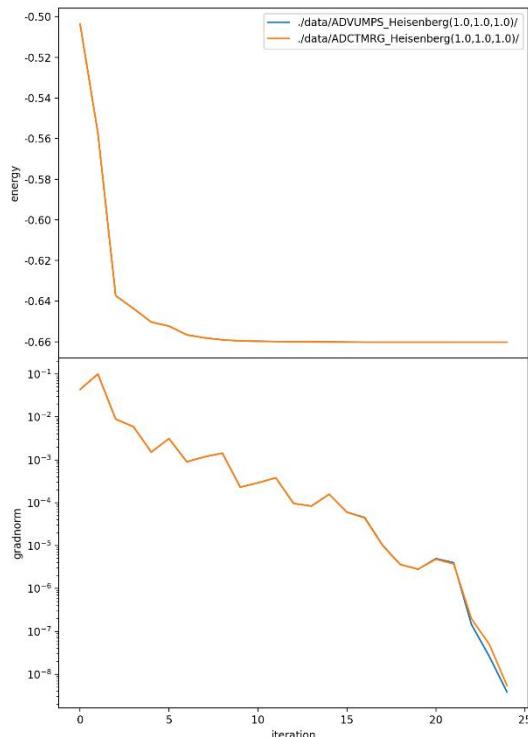
# 2D Classical Ising Model



# Finding the Ground State of infinite 2D Heisenberg model

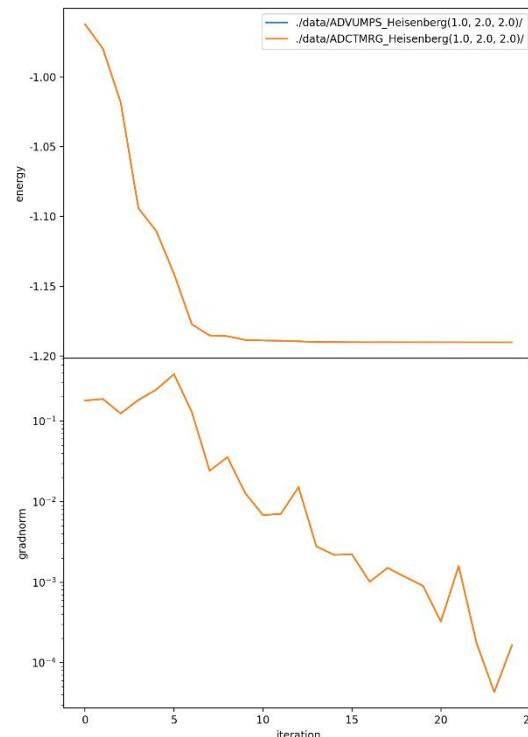
ADVUMPS vs ADCTMRG  $D = 2 \chi = 20 \delta = 10^{-12}$

33.76s vs 15.62s



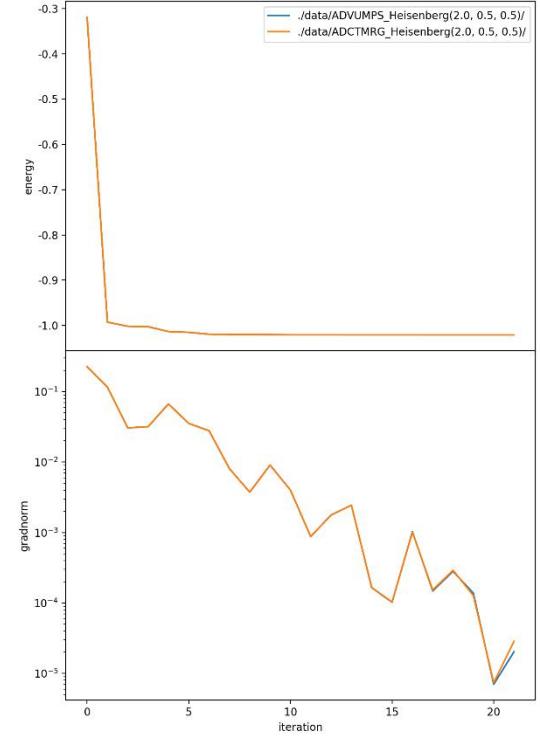
Difference  $\sim 1e-14$

29.11s vs 15.58s



Difference  $\sim 1e-9$

16.61s vs 4.94s



Difference  $\sim 1e-9$

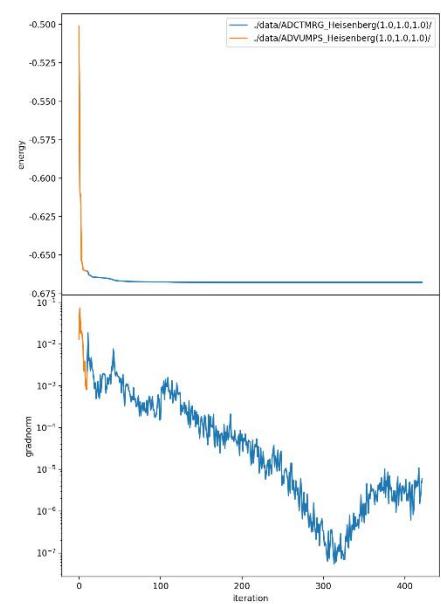
Time				Allocations			
Tot / % measured:	8.66s / 100%			7.54GiB / 100%			
Section	ncalls	time	%tot	avg	alloc	%tot	avg
backward	61	6.22s	72.1%	102ms	6.11GiB	81.0%	103MiB
forward	61	2.41s	27.9%	39.5ms	1.43GiB	19.0%	24.0MiB

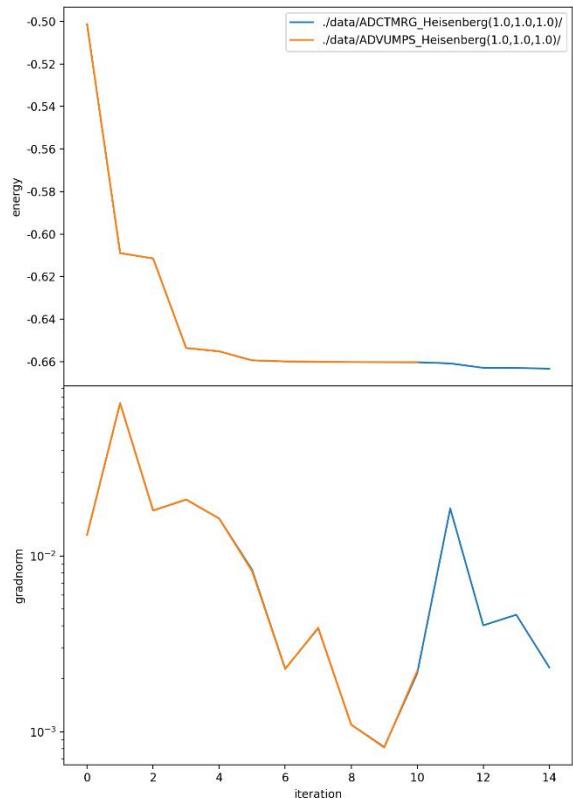
Time				Allocations			
Tot / % measured:	30.2s / 100%			26.2GiB / 100%			
Section	ncalls	time	%tot	avg	alloc	%tot	avg
backward	62	22.8s	75.8%	368ms	20.1GiB	76.6%	332MiB
forward	62	7.30s	24.2%	118ms	6.13GiB	23.4%	101MiB

# Problem of D=3

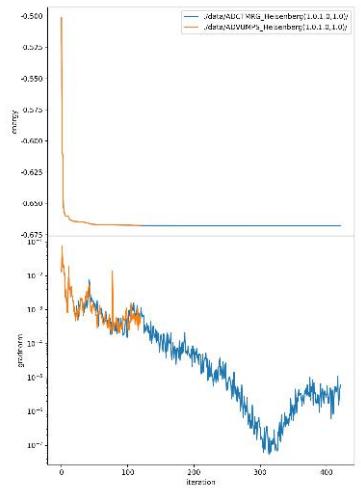
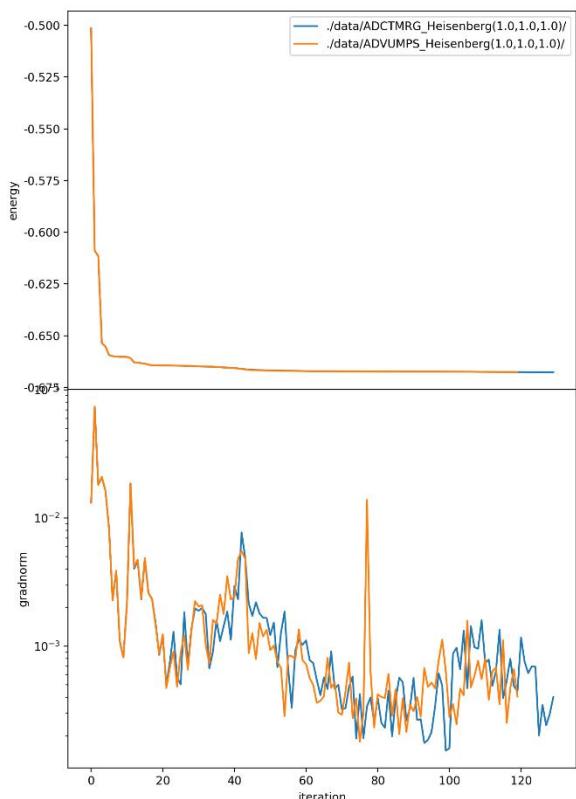
- QR isn't stable for  $R^{-1}$



tol=1e-10



tol=1e-20



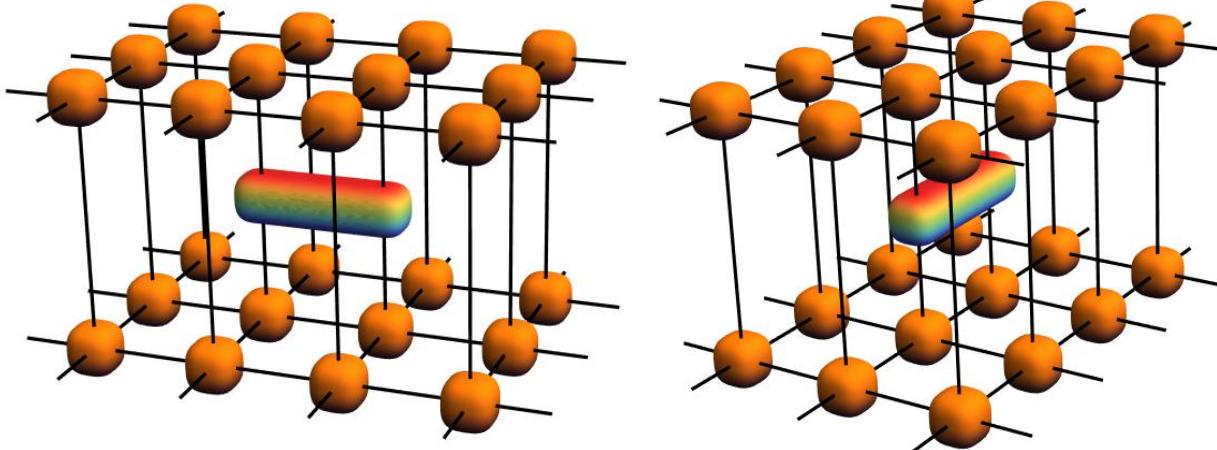
# Problem of iPEPS symmetry

- When only require up and down symmetry, Heisenberg(1,1,1)

$$E_0 = -0.85 < -0.66$$

$$T_{uldr} = \begin{array}{c} l \text{---} \textcircled{u} \text{---} r \\ | \qquad \qquad | \\ d \text{---} \textcircled{d} \text{---} \end{array} = \begin{array}{c} \textcolor{green}{\textcircled{u}} \\ \textcolor{green}{\textcircled{d}} \end{array}$$

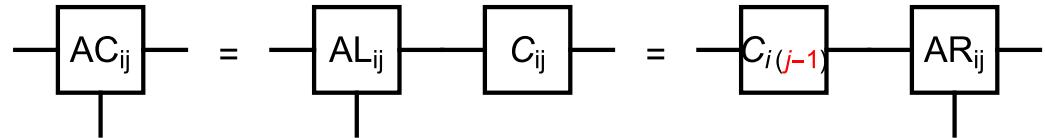
- Vertical and horizontal bond energy should be optimized at the same time



---

# AD-BC-VUMPS

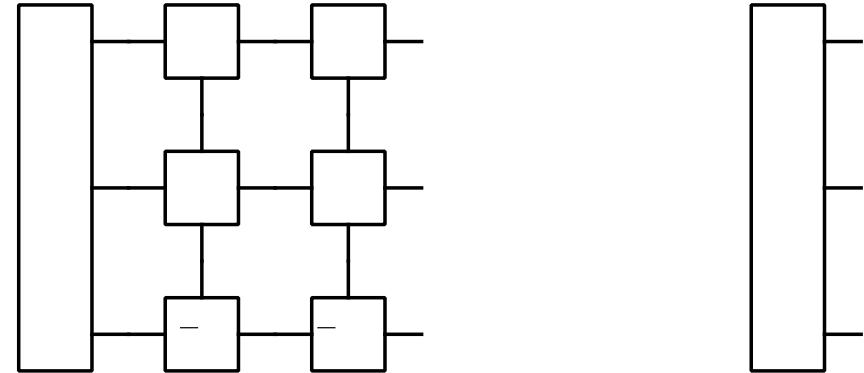
# BCVUMPS-algorithm



while  $\text{error}(AC, FL, FR, M) > \text{tol\_error}$

# Get environment

$AL[i, j] = \text{leftenv}(AL[:, :], M[:, :])$   
 $AR[i, j] = \text{rightenv}(AR[:, :], M[:, :])$

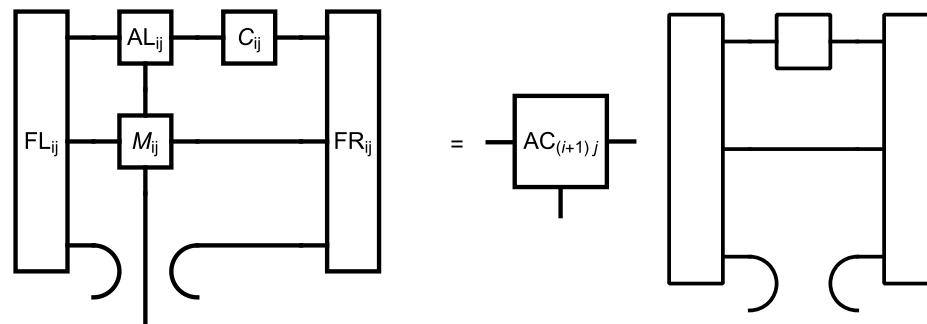


# Get orthonormal form

$AC[i, j], C[i, j] = \text{vumpsstep}(AL[:, j], C[:, j], AR[:, j], M[:, j], FL[:, j], FR[:, j])$

# calculate observable

$Obs = \text{obser}(O, AC, M, FL, FR)$



# AD for array of array

```
# example to solve differential of array of array
# use `[]` list then reshape
A = Array{Array,2}(undef, 2, 2)
for j = 1:2,i = 1:2
    A[i,j] = rand(2,2)
end
function foo2(x)
    # B[i,j] = A[i,j].*x  # mistake
    B = reshape([A[i].*x for i=1:4],2,2)
    return sum(sum(B))
end
@test Zygote.gradient(foo2, 1)[1] ≈ num_grad(foo2, 1)
```

# Be careful of index and replaced function!

$$dM_{ij} = \begin{bmatrix} A_{ij} & \cdots & A_{iJ} & \cdots \\ L_{ij} - M_{ij} & \cdots & \cdots & R_{ij} \\ A_{i+1j} & \cdots & A_{i+1J} & \cdots \end{bmatrix}$$

$$dA_{ij} = \begin{bmatrix} A_{ij} & \cdots & \cdots & \cdots \\ L_{ij} - M_{ij} & \cdots & dM_{ij} & \cdots & R_{ij} \\ A_{i+1j} & \cdots & A_{i+1J} & \cdots \end{bmatrix}$$

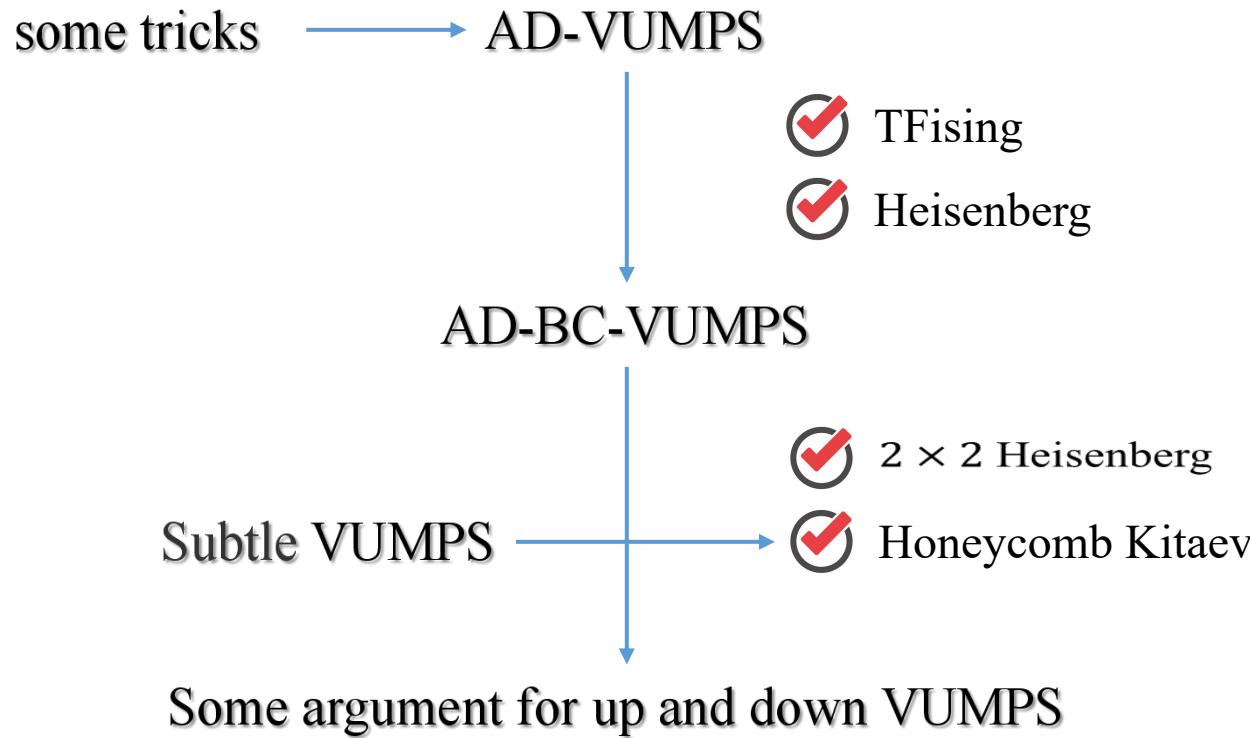
$$A_{i+1j} = \begin{bmatrix} A_{ij} & \cdots & A_{iJ} & \cdots & \cdots \\ L_{ij} - M_{ij} & \cdots & dM_{ij} & \cdots & R_{ij} \\ A_{i+1j} & \cdots & \cdots & \cdots \end{bmatrix}$$

$$dFLI_{j+1} = \begin{bmatrix} C_{ij} \\ FL_{ij+1} & FR_{ij} \\ \vdots & \vdots \\ \cdots & \cdots \\ Cd_{ij} \end{bmatrix}$$

$$dFRI_j = \begin{bmatrix} C_{ij} \\ FL_{ij+1} & FR_{ij} \\ \vdots & \vdots \\ \cdots & \cdots \\ Cd_{ij} \end{bmatrix}$$

# AD-BC-VUMPS

# Contents



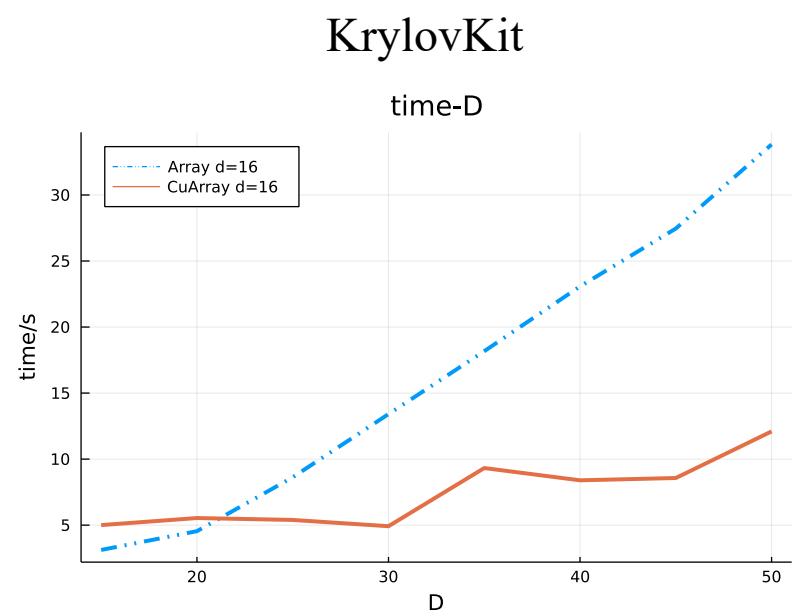
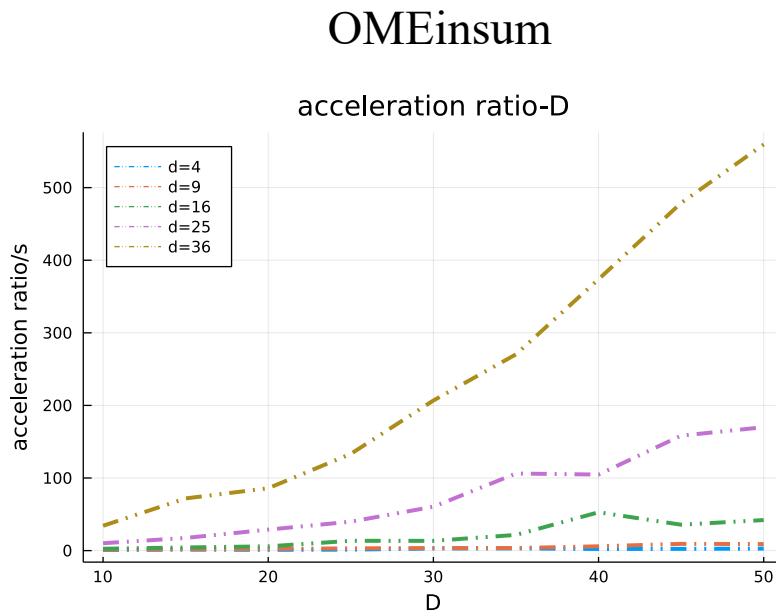
# some Tricks

# some tricks to accelerate

- Save vumps environment
- Optimize the contract order
- Set maxiter = 1 for linsolve but **eigsolve not**
- GPU

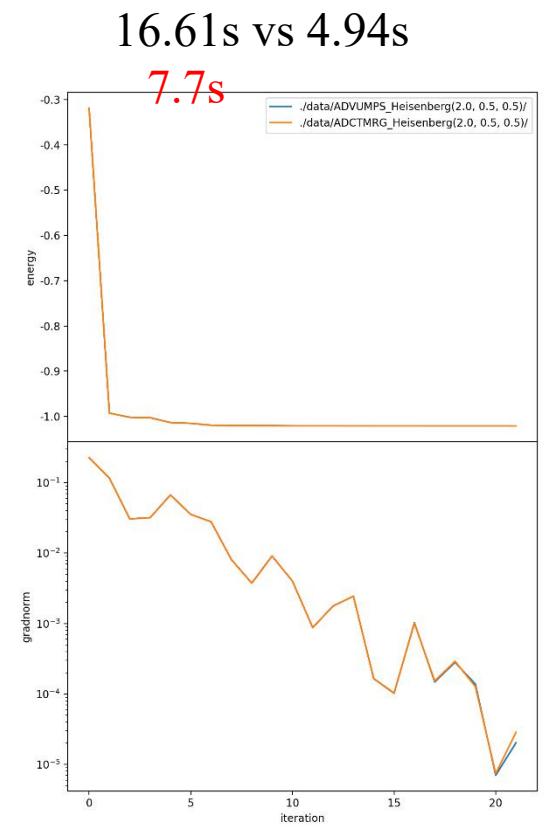
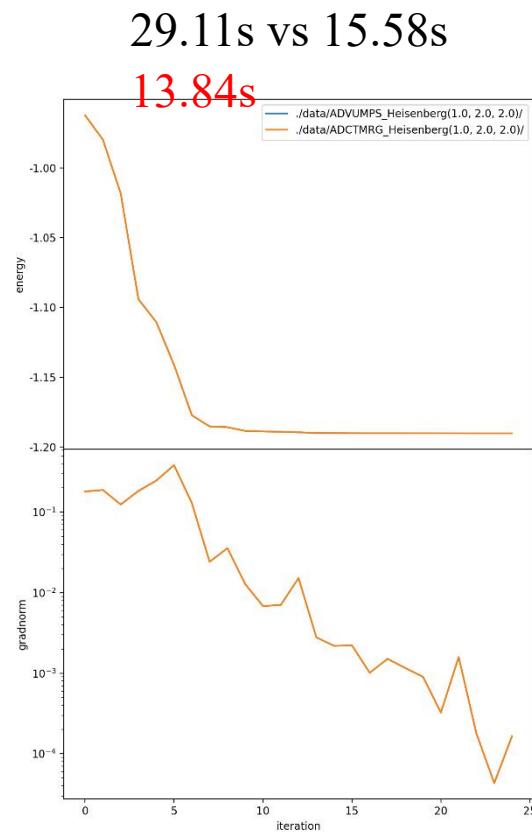
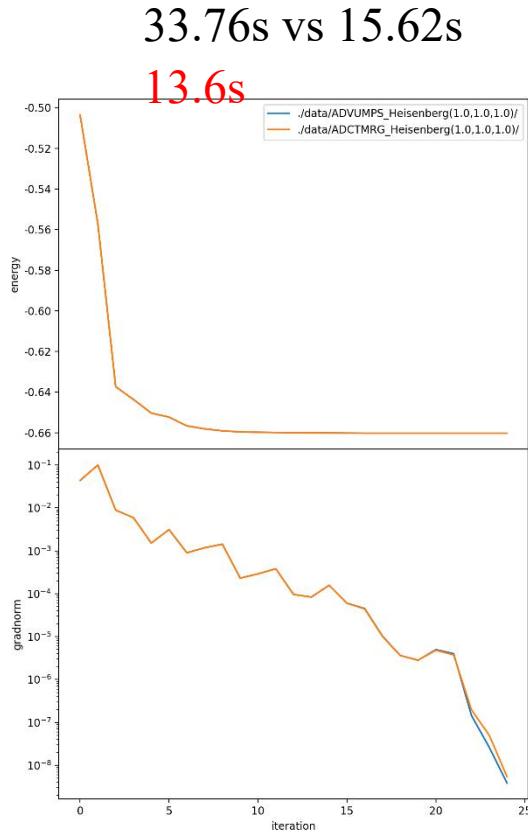
For Julia OMEinsum

`optimize_greedy(; method=MinSpaceDiff())`



# Finding the Ground State of infinite 2D Heisenberg model

ADVUMPS vs ADCTMRG  $D = 2 \chi = 20 \delta = 10^{-12}$



Difference  $\sim 1e-14$

Backward  
forward

9.91s	72.3%
3.79s	27.7%

Difference  $\sim 1e-9$

10.7s	77.1%
3.19s	22.9%

Difference  $\sim 1e-9$

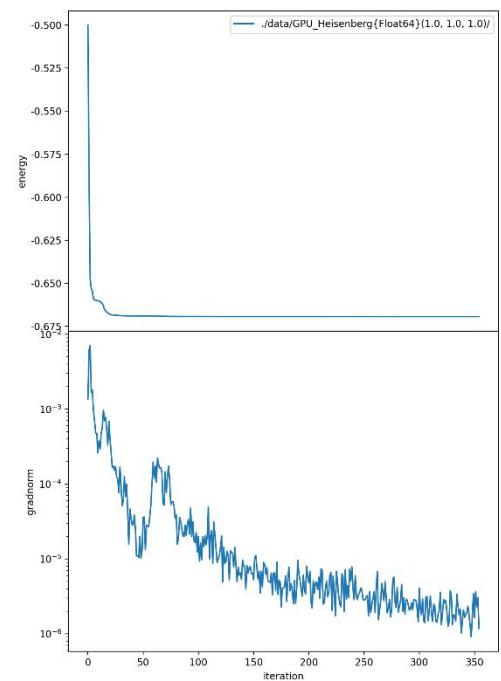
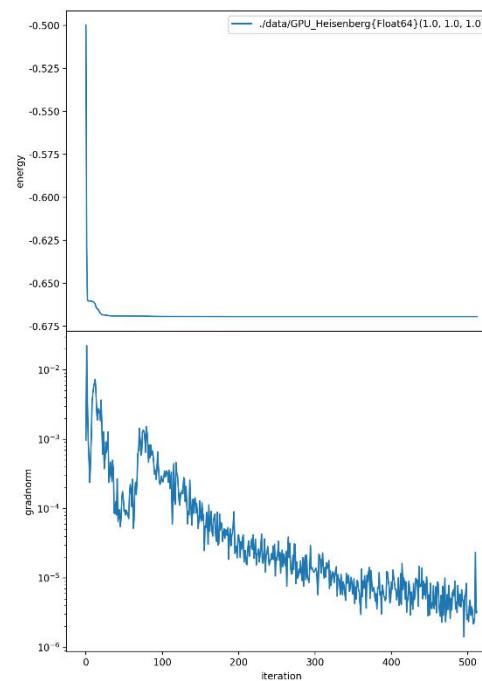
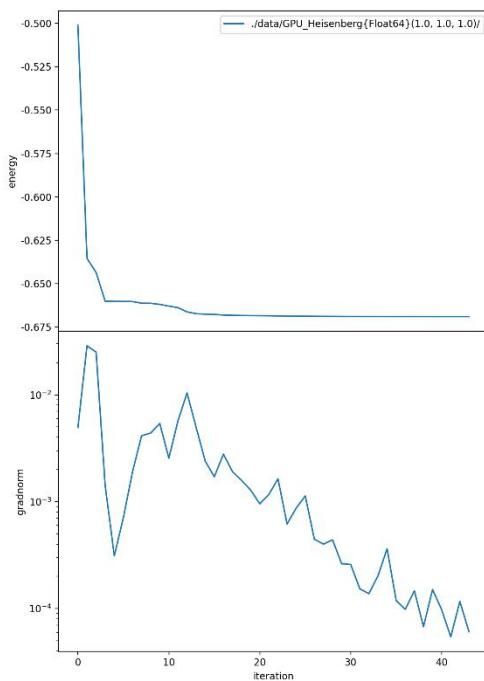
6.14s	76.9%
1.84s	23.1%

# Heisenberg model $D = 4,5,6$

one RTX2060-6G

$D$	$\chi$	iteration	time	E	error
4	30	44	22.7 min	-0.6689534	$7.3 \times 10^{-4}$
5	30	513	6.6h	-0.6693341	$1.6 \times 10^{-4}$
6	30	355	16.1h	-0.6693380	$1.56 \times 10^{-4}$

MC: -0.6694421



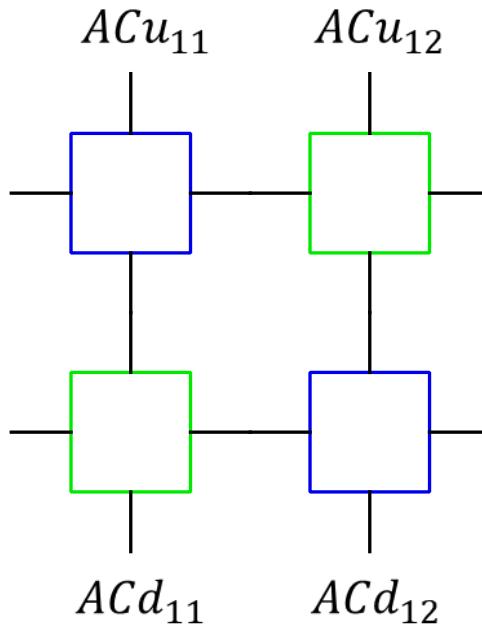
# **2×2 AD-BC-VUMPS**

# symmetry environment

$$\bullet H = \sum_{ij} S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+)$$

$$S_j \leftarrow \sigma_x S_j \sigma'_x$$

$$\bullet H = - \sum_{ij} S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^+ + S_i^- S_j^-)$$



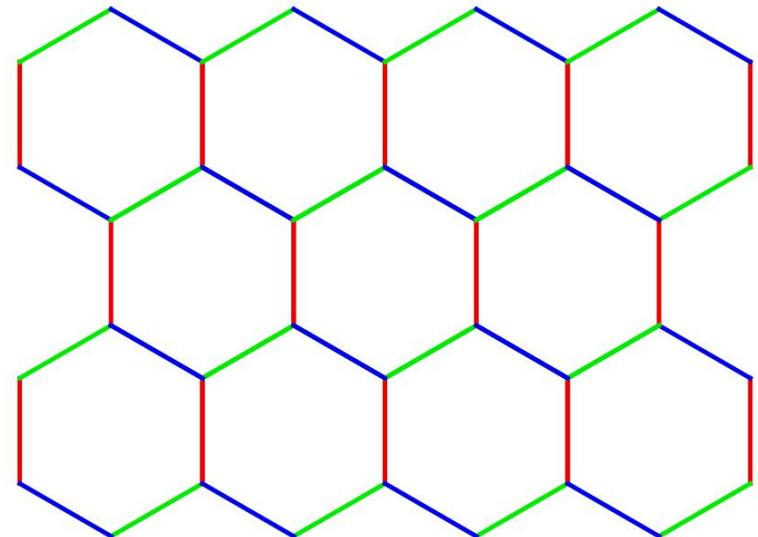
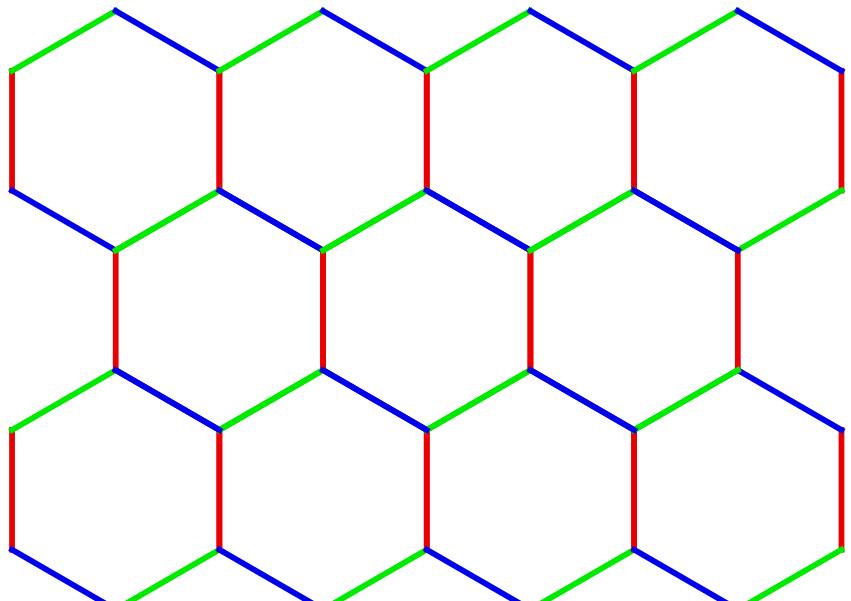
Up-and-down-symmetry assumption

$$ACd_{11} = ACu_{12}$$

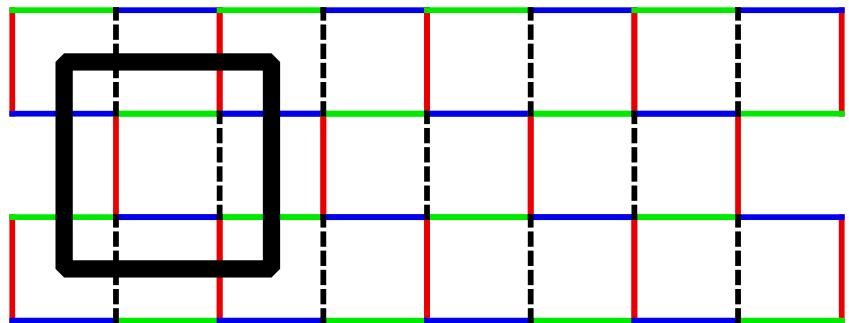
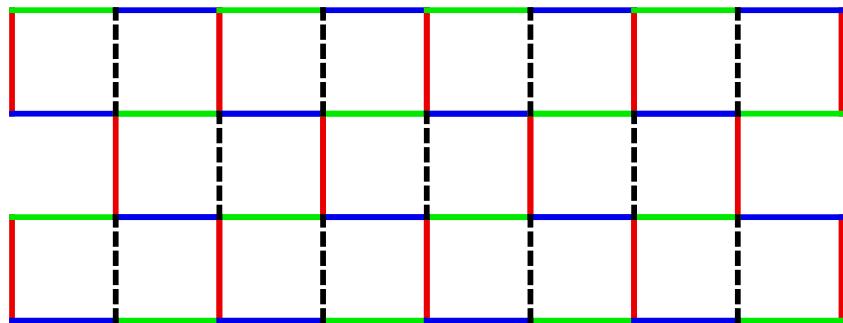
$$ACd_{12} = ACu_{11}$$

D	$\chi$	iteration	time	E
2	20	25	122.9s	-0.6602265
4	32	134	5.5h	-0.6689648
4	32	86	2.5h	-0.6689539
4	30	513	22.7 min	-0.6689534

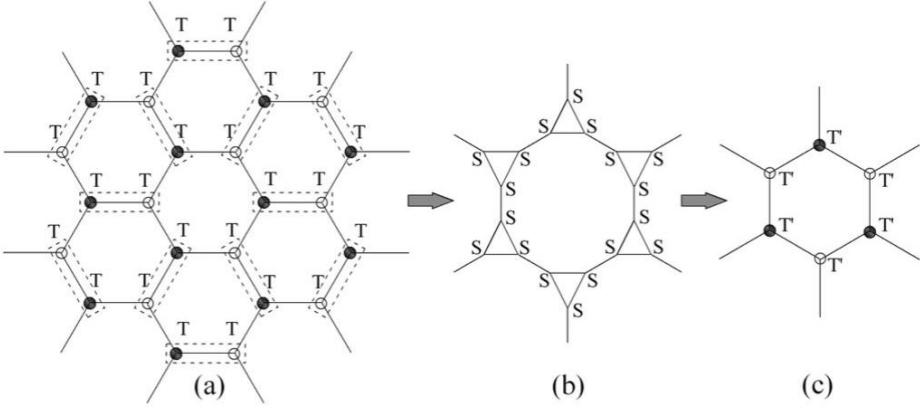
# Honeycomb lattice to square



$2 \times 2$  AB iPEPS assumption



# Honeycomb Heisenberg



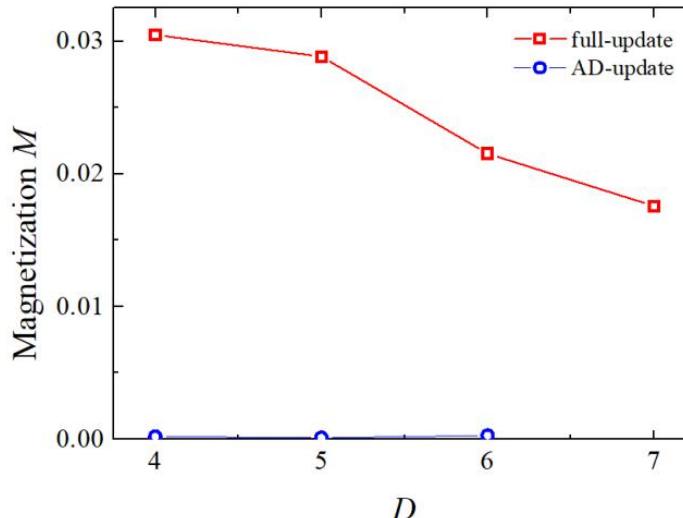
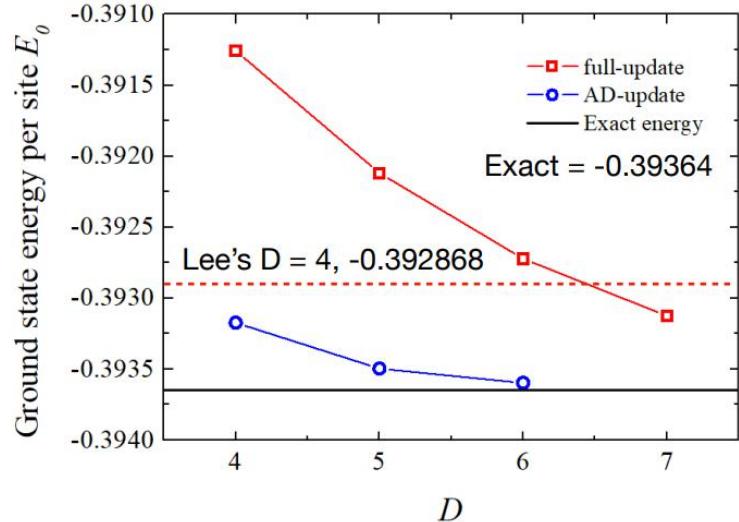
$D$	$\chi$	$E$	$M$
2	20	-0.5400	0.243
3	20	-0.5430	0.222
4	20	-0.5440	0.200

$D$	$E$	$M$
3	-0.5365	0.249
4	-0.5456	0.228
5	-0.5488	0.220
6	-0.5513	0.206
7	-0.5490	0.216
8	-0.5506	0.212

Method	$E$	$M$
Spin wave [12]	-0.5489	0.24
Series expansion [13]	-0.5443	0.27
Monte Carlo [14]	$-0.5450 \pm 0.001$	$0.22 \pm 0.03$
Ours $D = 8$	-0.5506	$0.21 \pm 0.01$

# Honeycomb Kitaev

Iregui, et. al., PRB 90, 195102 (2014)



CTMRG +  
imaginary-time  
evolution  
vs.  
TEBD + AD

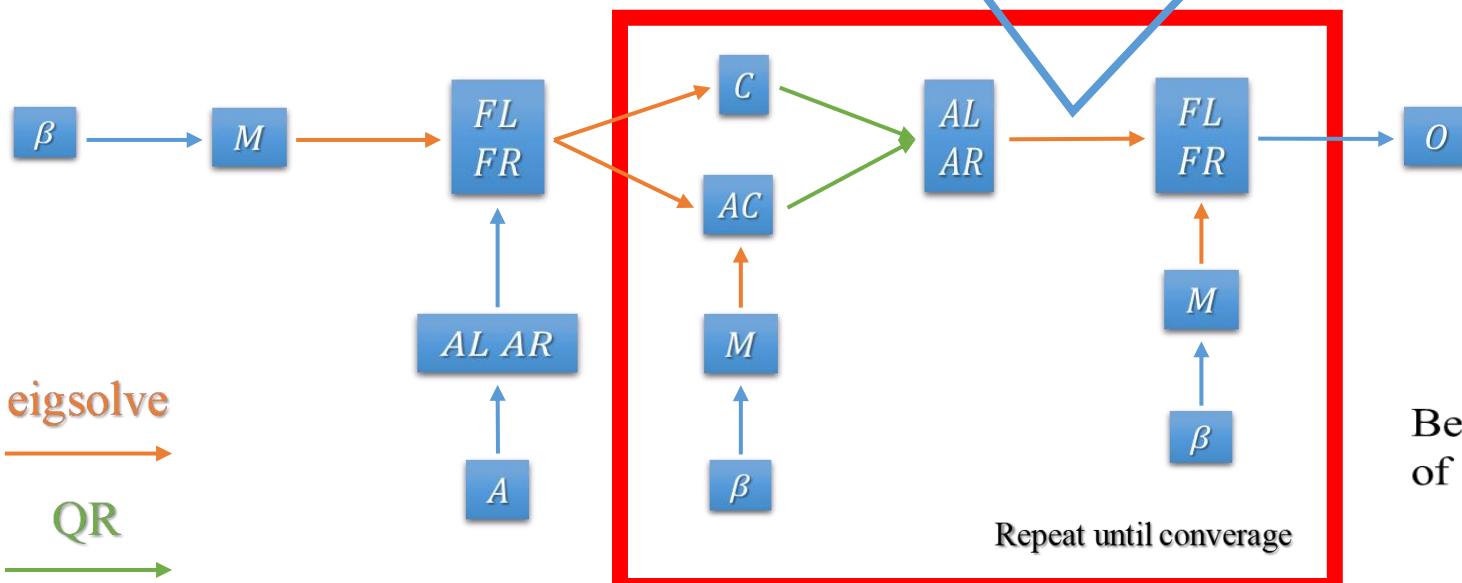
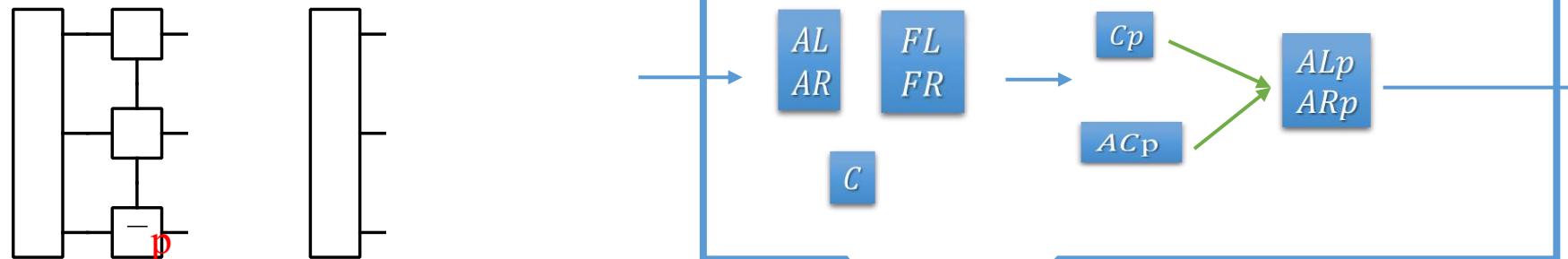
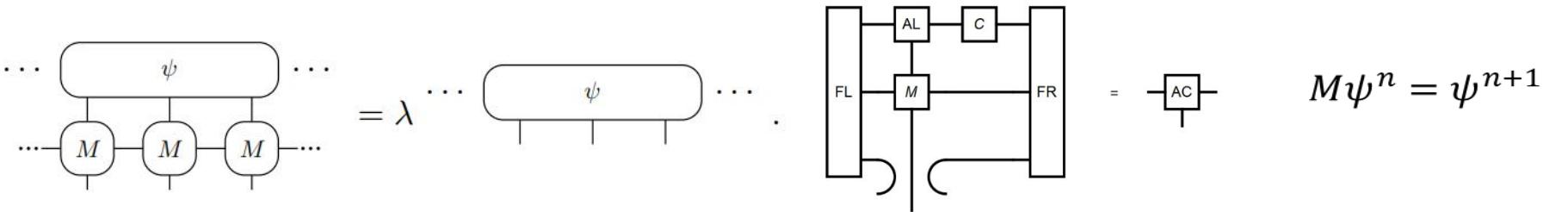
$D$	$\chi$	$E_n$	$M$
3	50	-0.3795995949421732	0.27211012905099785
4	80	-0.3931735662139908	0.0001872923118720
5	100	-0.3934970101949562	0.0000972301264798
6	100	-0.3935976940110233	0.0002659684803263

Theoretical value: -0.3936 0

$D$	$\chi$	$E$	$M$
2	20	-0.3759726	
4	20	-0.3914..	0.02..

VUMPS doesn't converge for error  $\approx 0.1$

# Computation Graphs



eigsolve

QR

Better convergence  
of  $10^{-3}$

# result

D	chi	En	M
3	50	-0.3795995949421732	0.27211012905099785
4	80	-0.3931735662139908	0.0001872923118720
5	100	-0.3934970101949562	0.0000972301264798
6	100	-0.3935976940110233	0.0002659684803263

D	$\chi$	E	M
4	20	-0.3933225282386825	0.0005
4	30	-0.39343584624314554	0.002

VUMPS up error  $\approx 1e-6$   
 down error  $\approx 1e-6$

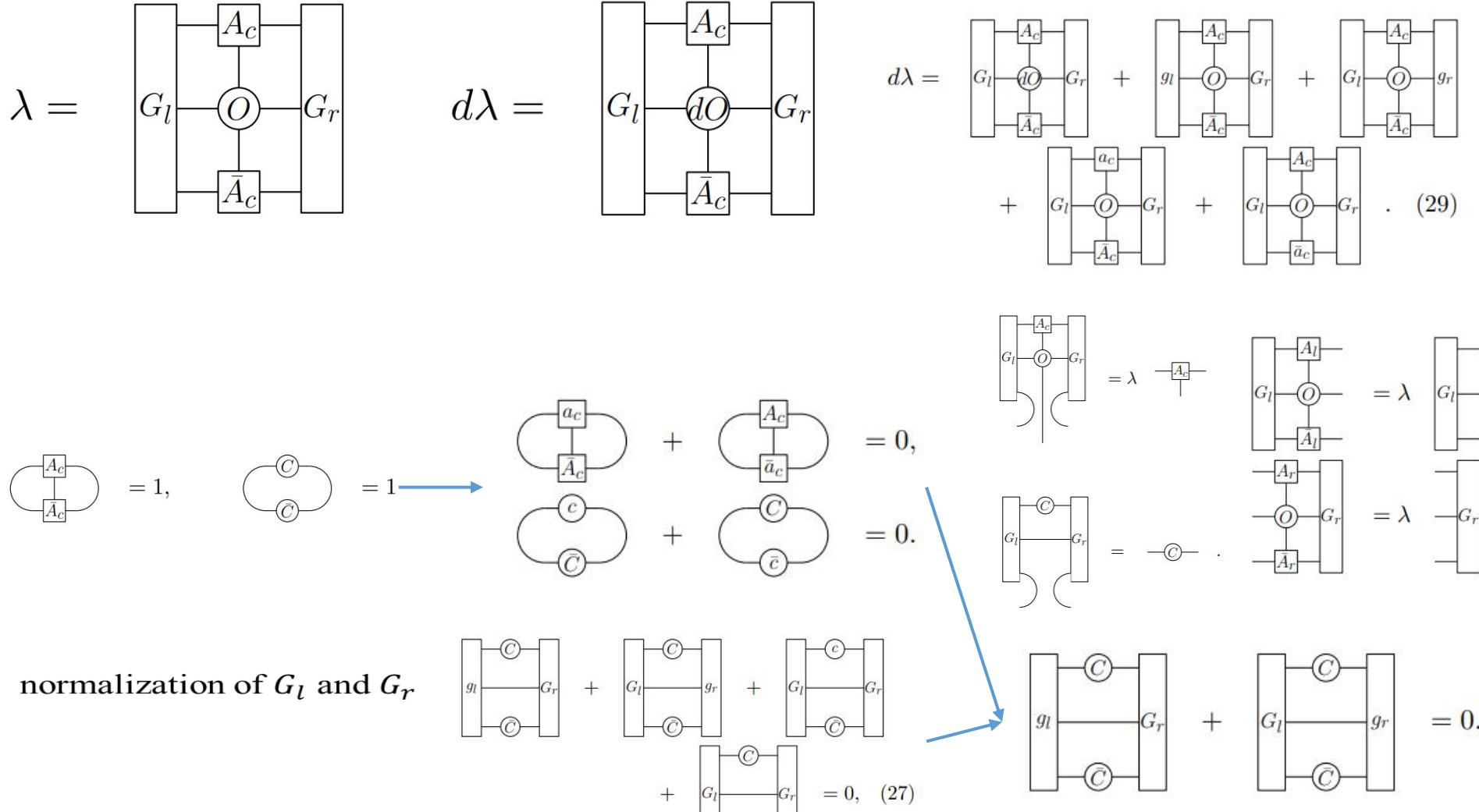
VUMPS up error  $\approx 1e-7$   
 down error  $\approx 1e-2$

$$E = -0.3933 \sim -0.3929$$

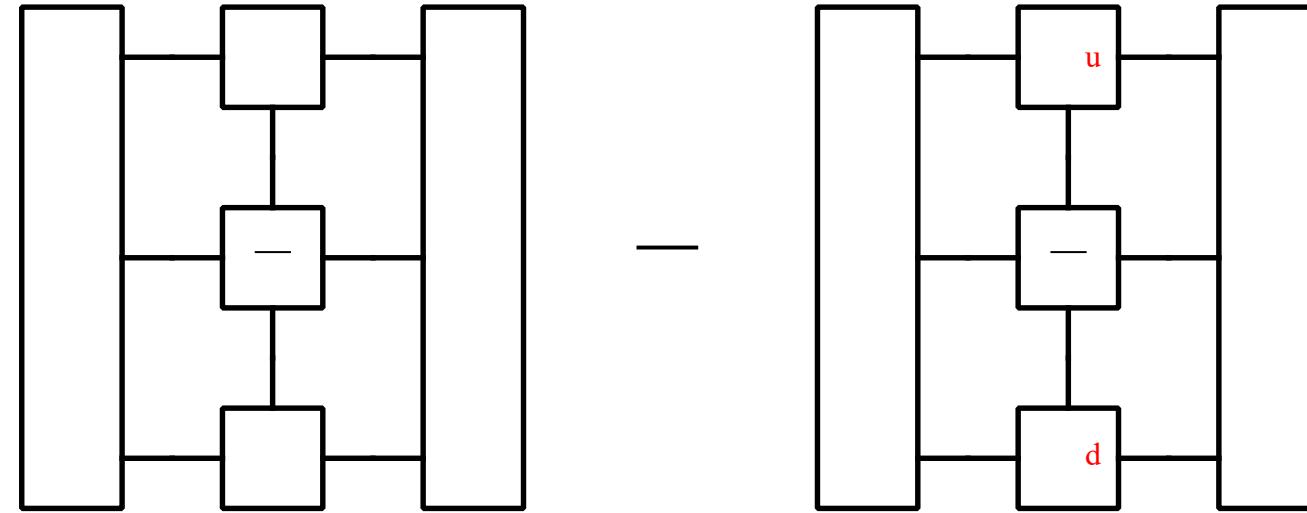
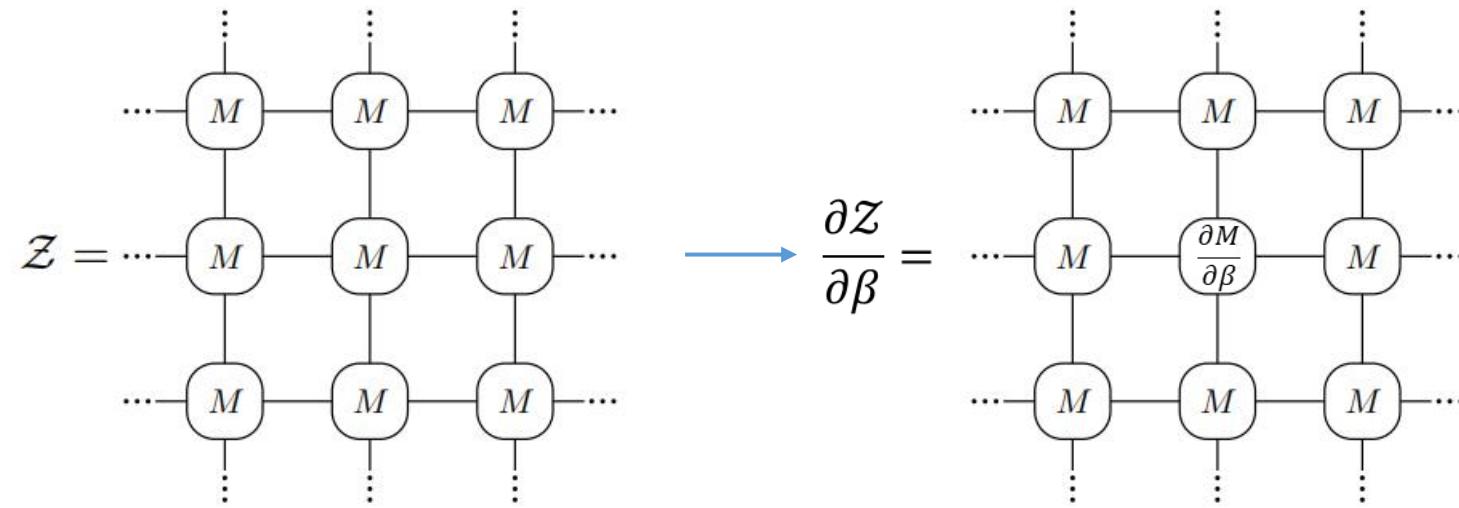
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# Some arguments for up and down VUMPS

# Differential for observable

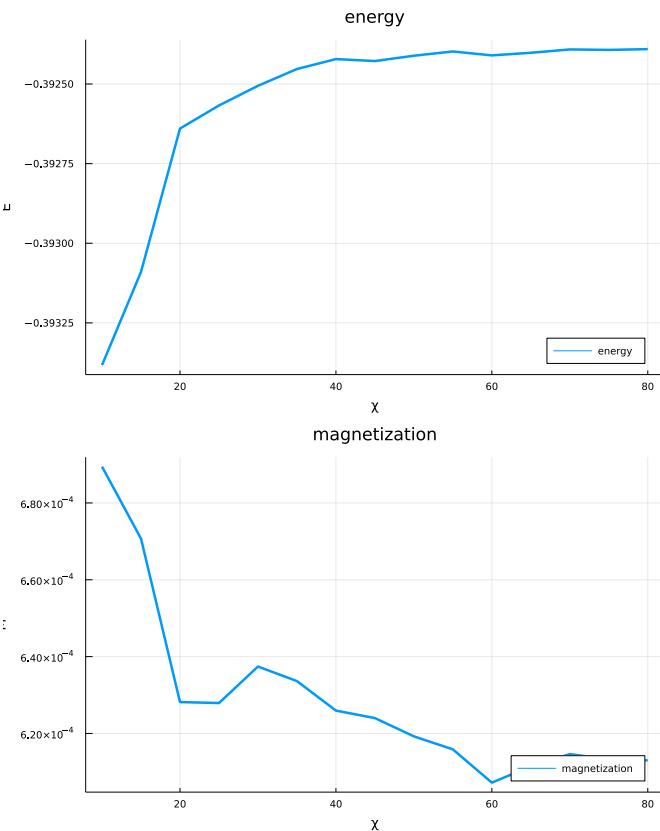


# Contradictory result for up and down

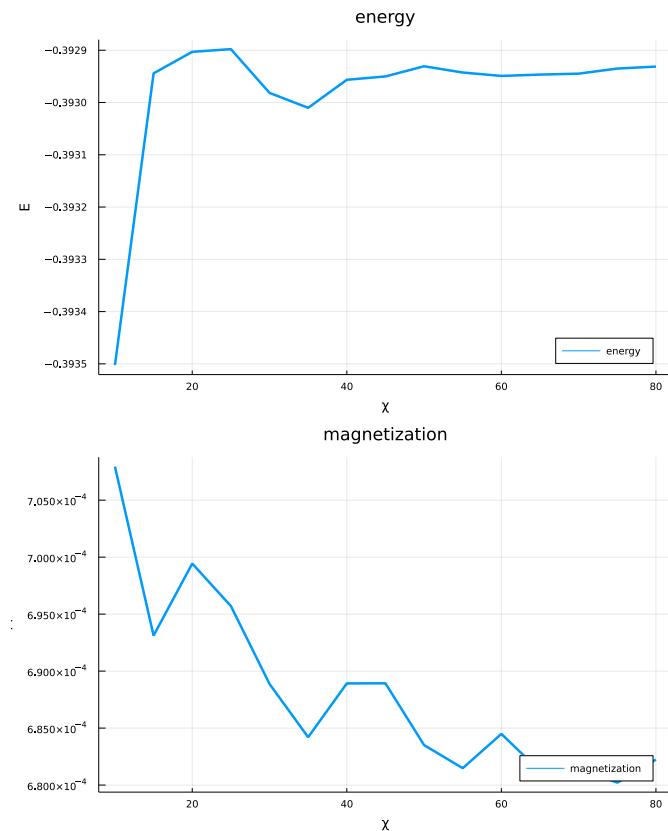


# $E - \chi$

$D = 4 \chi = 20$



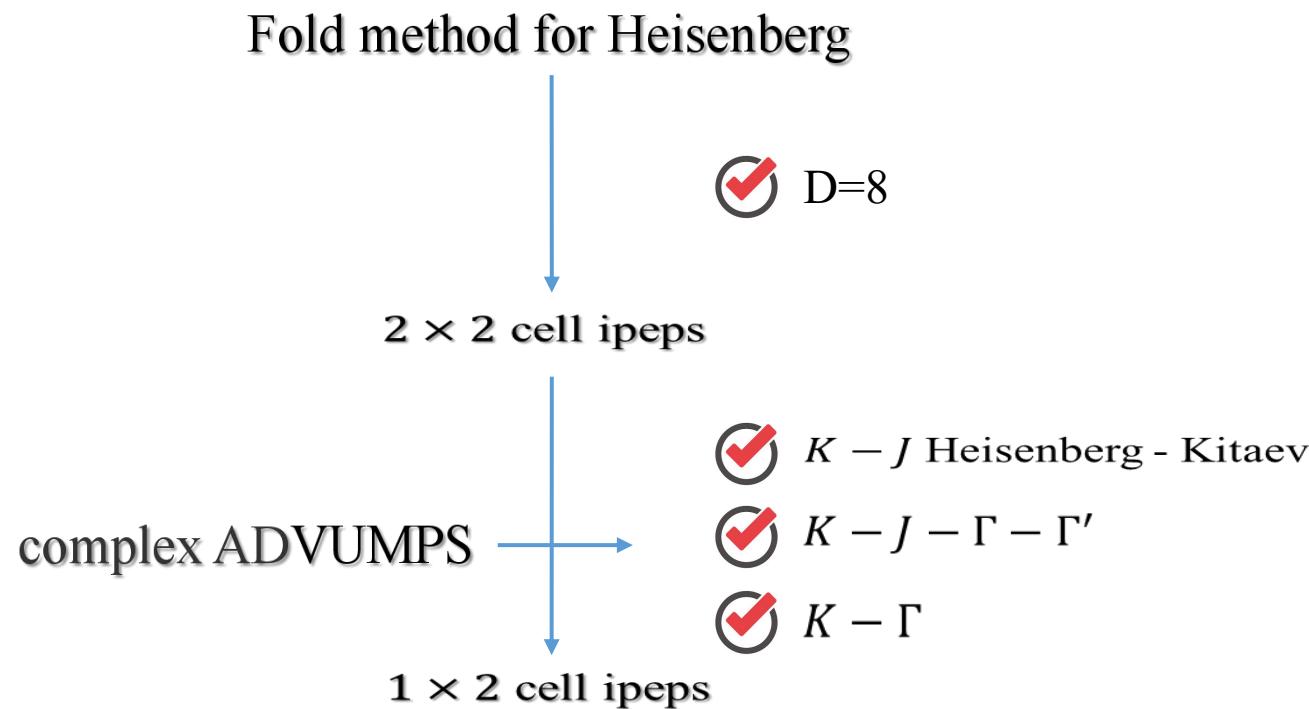
$D = 4 \chi = 80$



# Optimize $\langle \phi | H | \psi \rangle / \langle \phi | \psi \rangle$

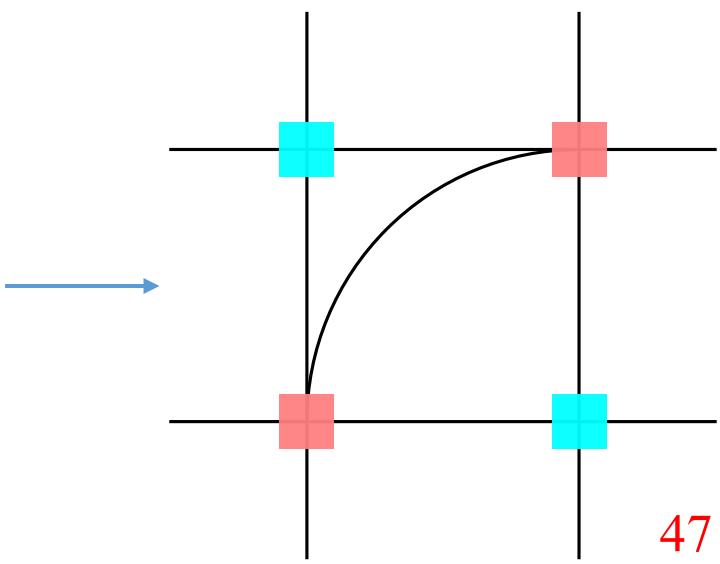
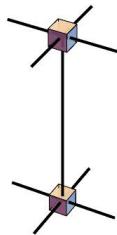
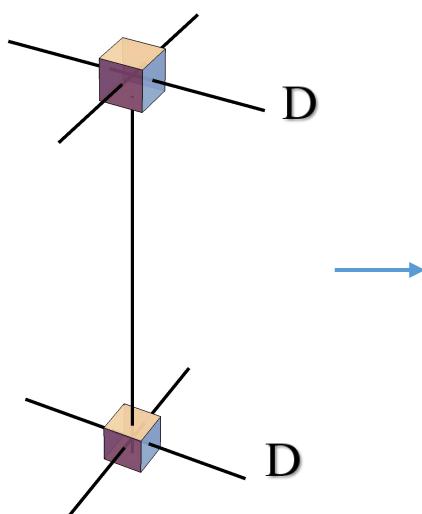
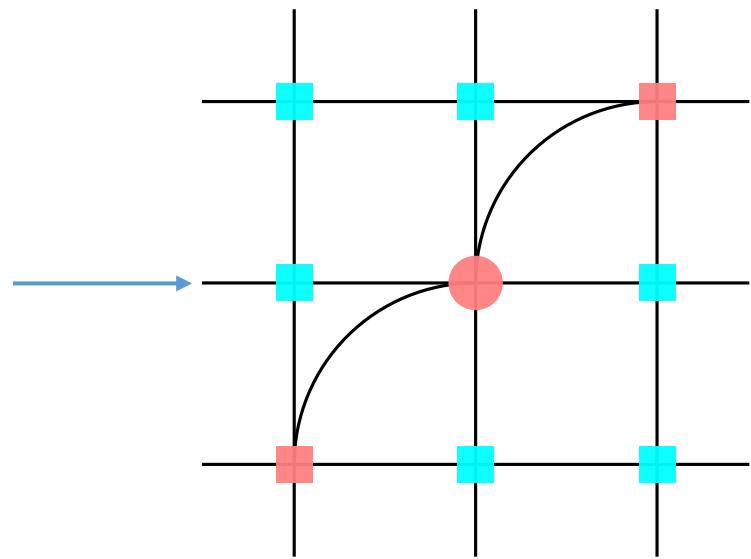
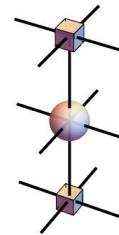
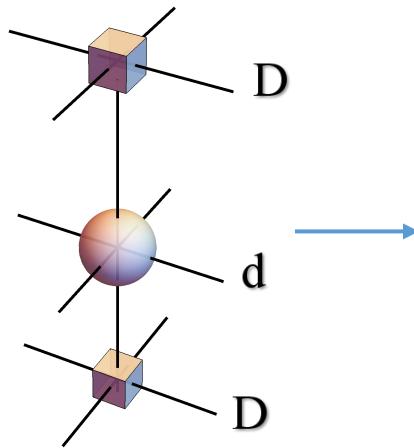
Question: how to find  $\phi$  is in a nonorthogonal space of  $\psi$ ?

# Contents



# Fold method for Heisenberg

# Fold method



# Some details

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- Just one side
- FL and FR is simple to get
- $\text{norm}(\rho - \rho') = 0$

# Result

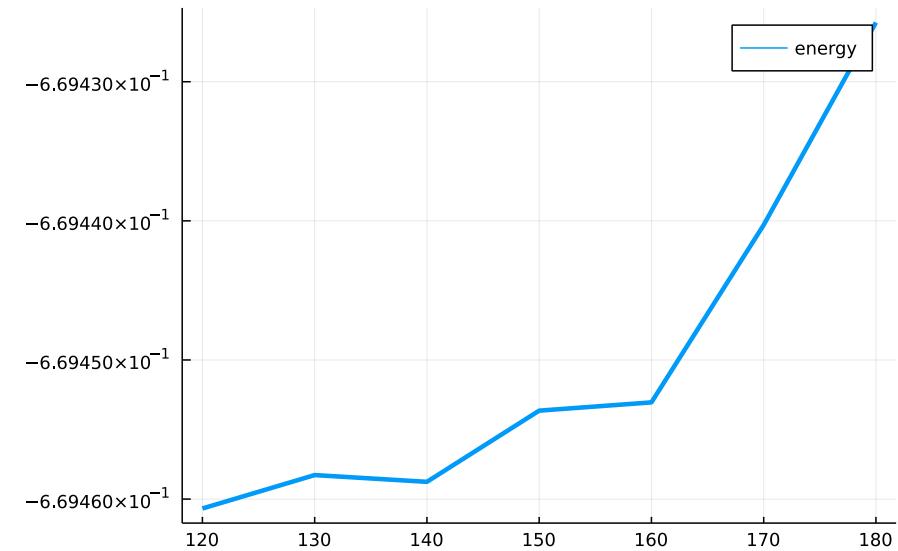
	E	$D = 8$	time	steps	E
$D = 6 \chi = 144$	-0.6694555693910015	$\chi = 64$	1.5h	92	-0.66939453601441
$D = 7 \chi = 160$	-0.6694572428974581	$\chi = 128$	1.9h	75	-0.66940379584180
Liao2019-PRX	-0.6694245109061838	$\chi = 160$	3.7h	108	-0.66945318815880
MC	-0.6694421	$\chi = 192$	10.5h	39	-0.66944042736926

Iteration=50

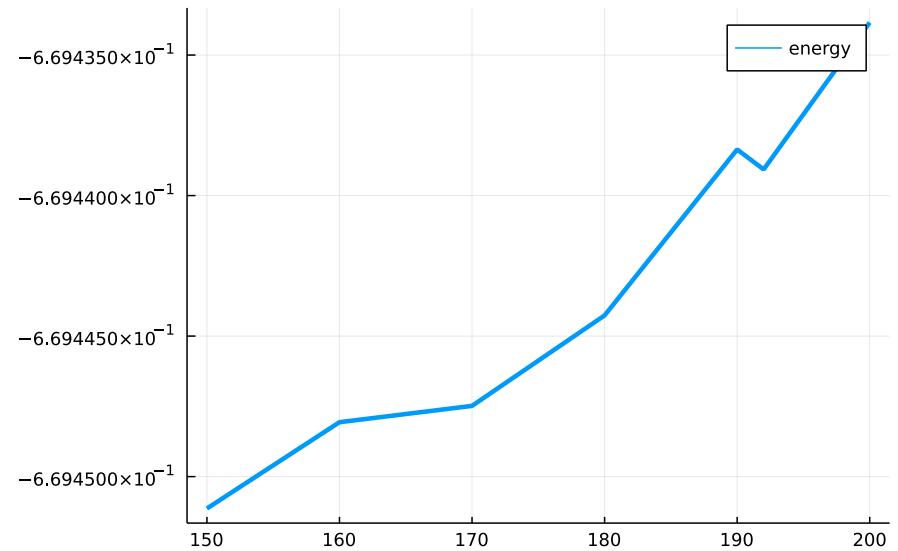
-0.6694257436261145

-0.669433842168528

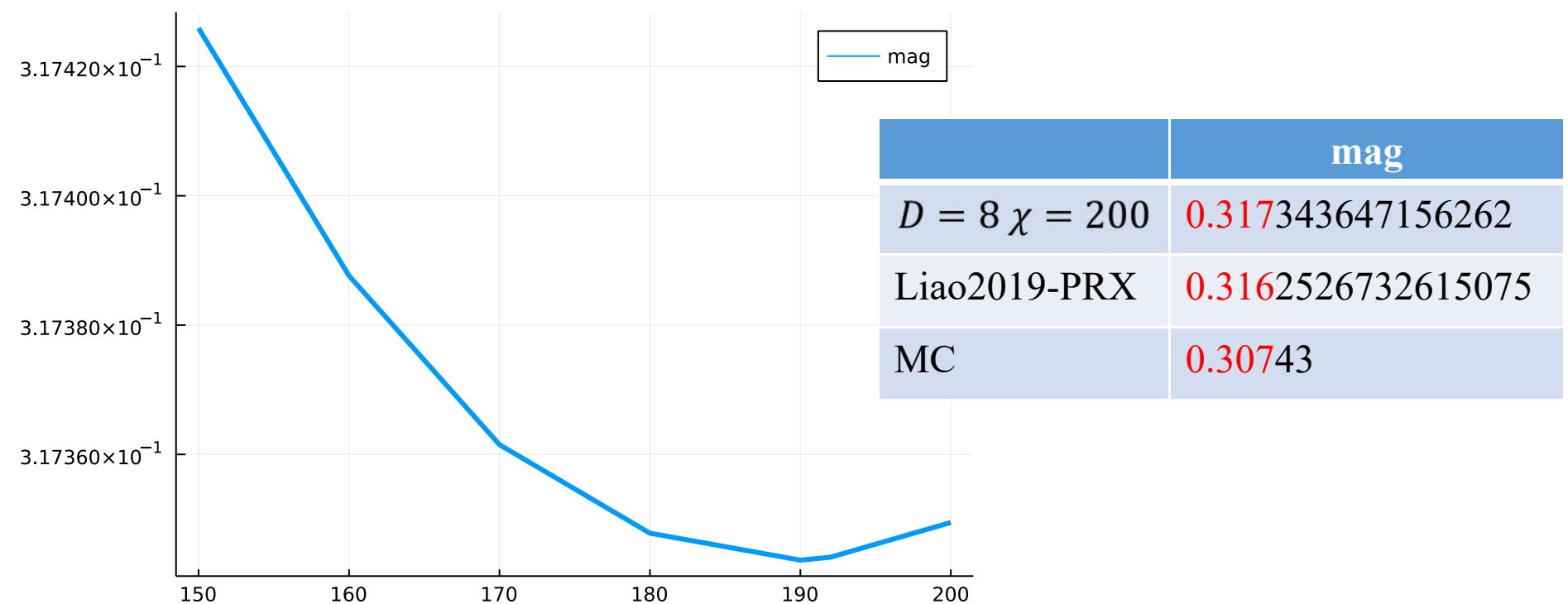
energy



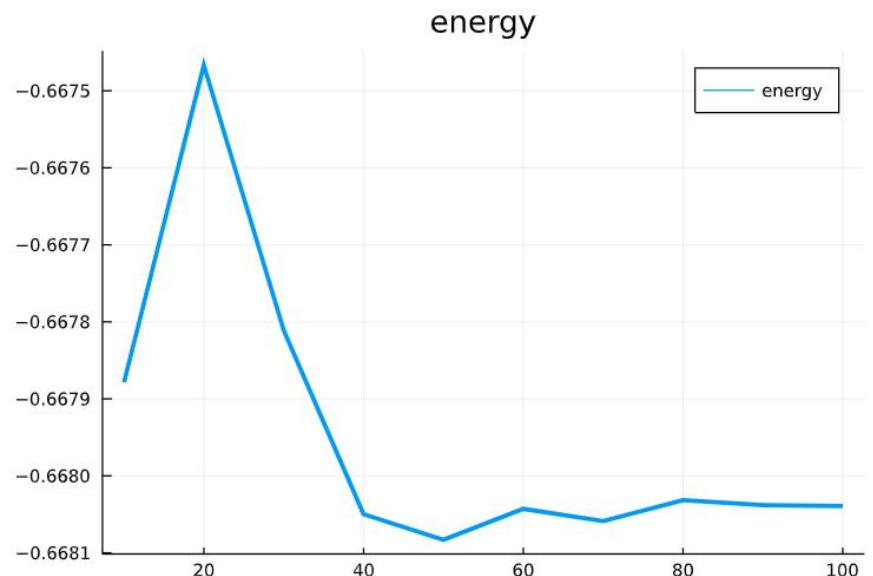
energy



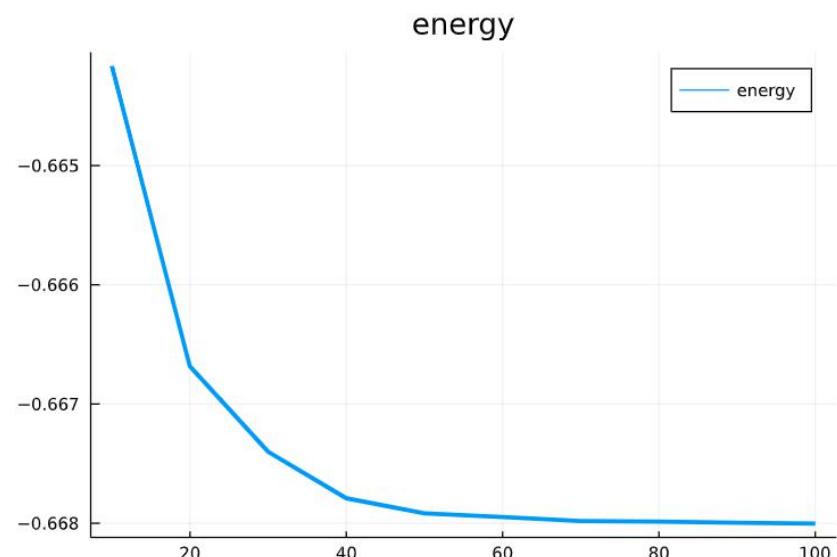
mag



# Different FL FR $D = 3$ $\chi = 50$



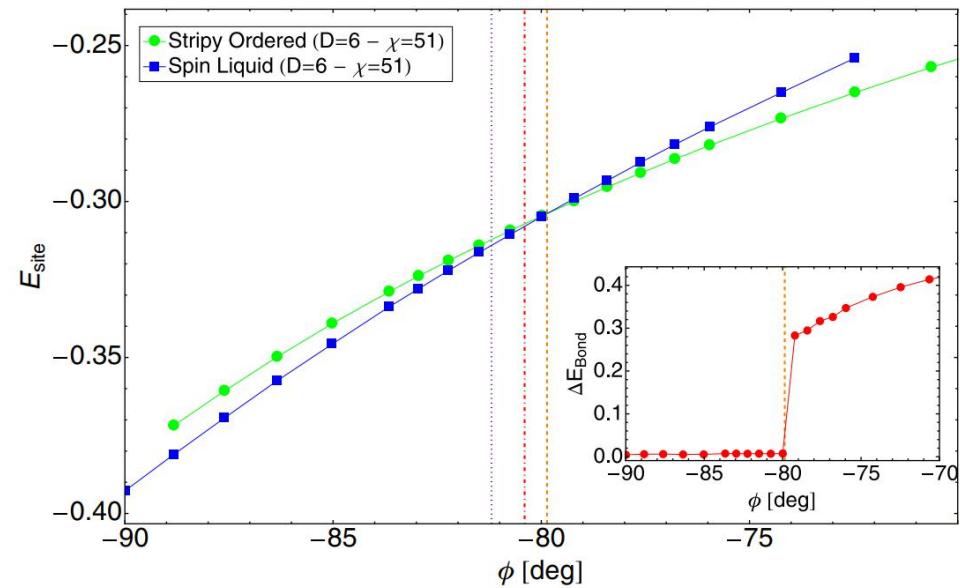
$33 \rightarrow 4$



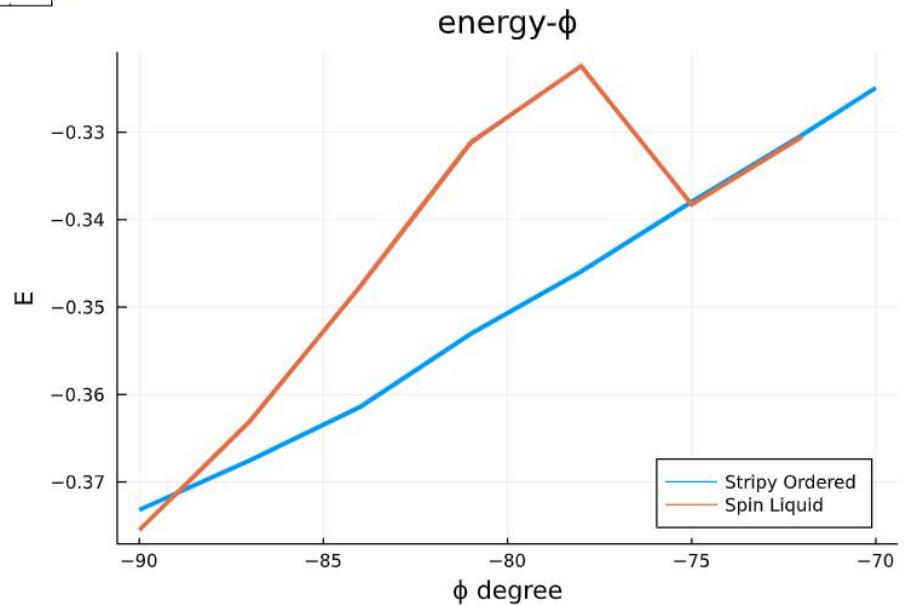
Direct 4

# Kitaev-Heisenberg

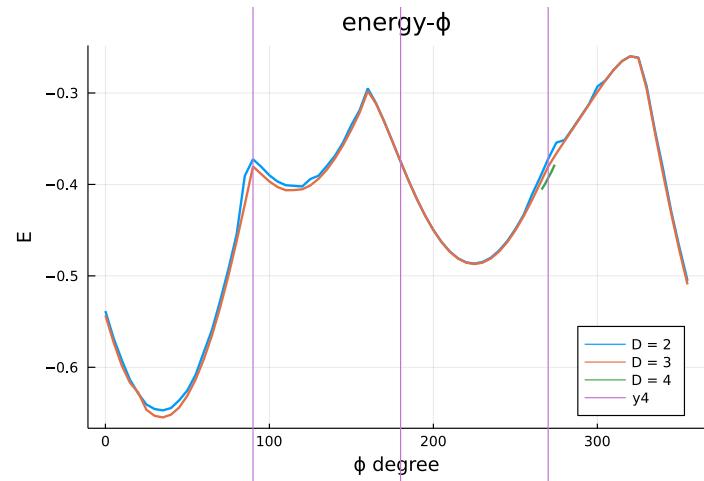
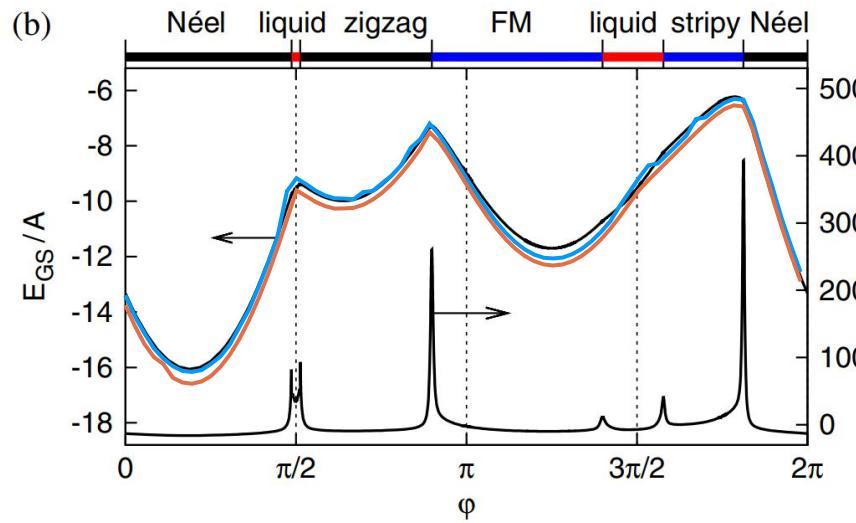
# energy



$D=2$



# energy and magnetization



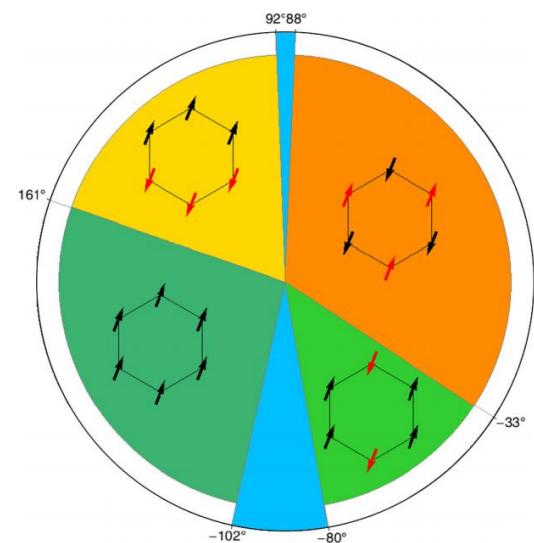
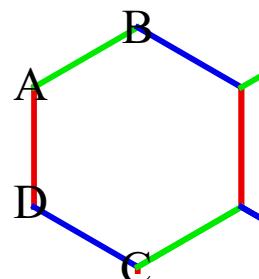
$$O_{\text{mag}} = \sqrt{\frac{1}{4}(\langle \vec{\sigma}_A \rangle^2 + \langle \vec{\sigma}_B \rangle^2 + \langle \vec{\sigma}_C \rangle^2 + \langle \vec{\sigma}_D \rangle^2)},$$

$$O_{\text{ferro}} = \sqrt{\frac{1}{4}(\langle \vec{\sigma}_A \rangle + \langle \vec{\sigma}_B \rangle + \langle \vec{\sigma}_C \rangle + \langle \vec{\sigma}_D \rangle)^2},$$

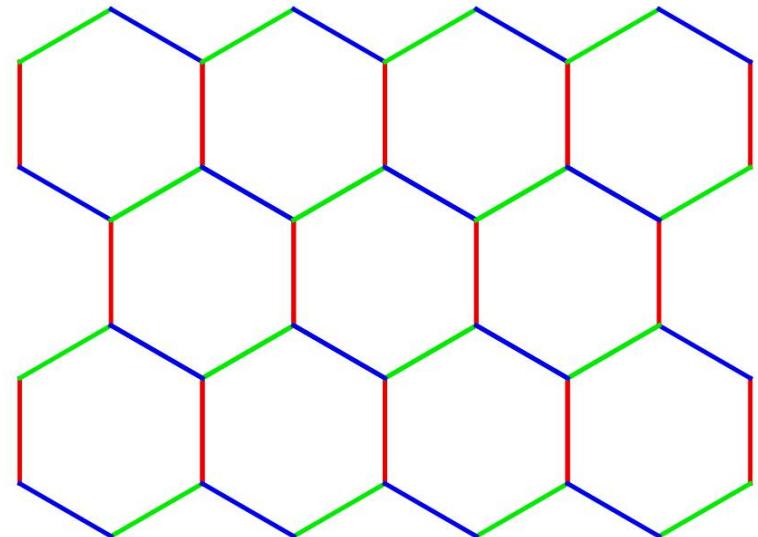
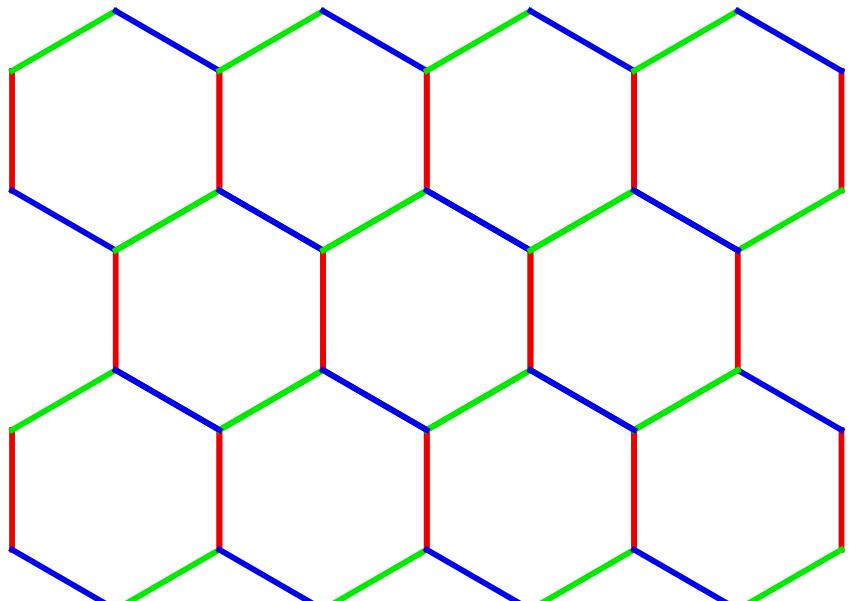
$$O_{\text{stripy}} = \sqrt{\frac{1}{4}(\langle \vec{\sigma}_A \rangle - \langle \vec{\sigma}_B \rangle - \langle \vec{\sigma}_C \rangle + \langle \vec{\sigma}_D \rangle)^2},$$

$$O_{\text{zigzag}} = \sqrt{\frac{1}{4}(\langle \vec{\sigma}_A \rangle + \langle \vec{\sigma}_B \rangle - \langle \vec{\sigma}_C \rangle - \langle \vec{\sigma}_D \rangle)^2},$$

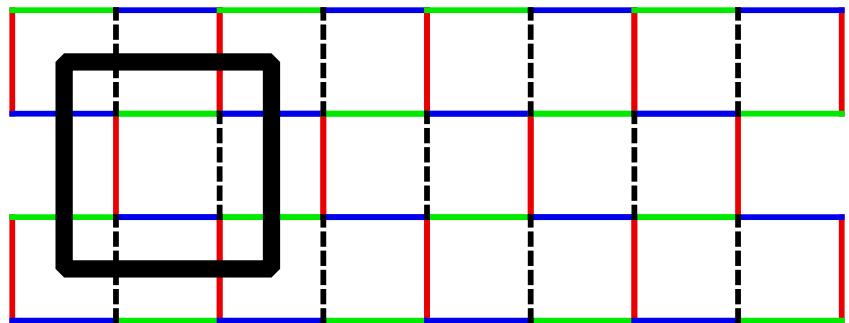
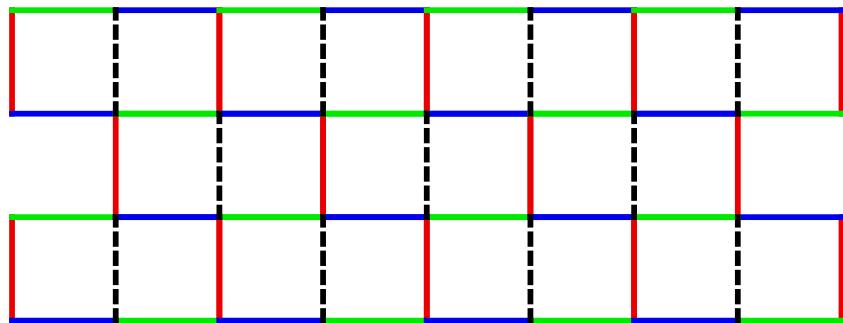
$$O_{\text{N\'eel}} = \sqrt{\frac{1}{4}(\langle \vec{\sigma}_A \rangle - \langle \vec{\sigma}_B \rangle + \langle \vec{\sigma}_C \rangle - \langle \vec{\sigma}_D \rangle)^2},$$



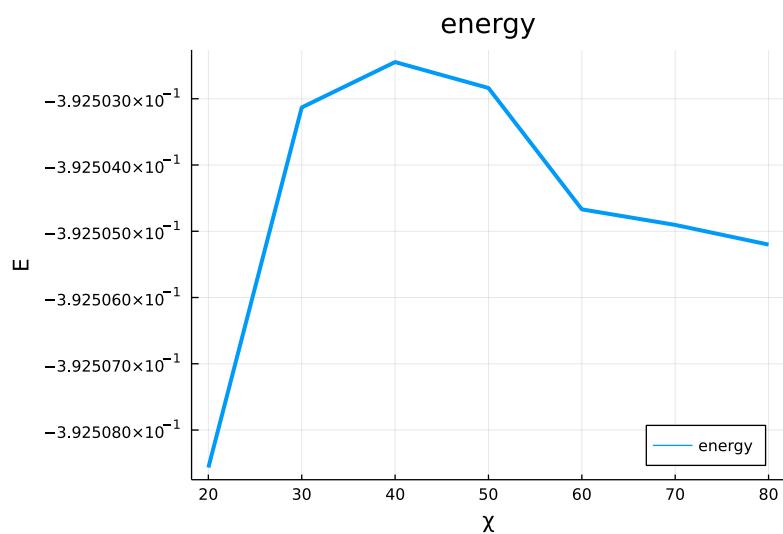
# Honeycomb lattice to square



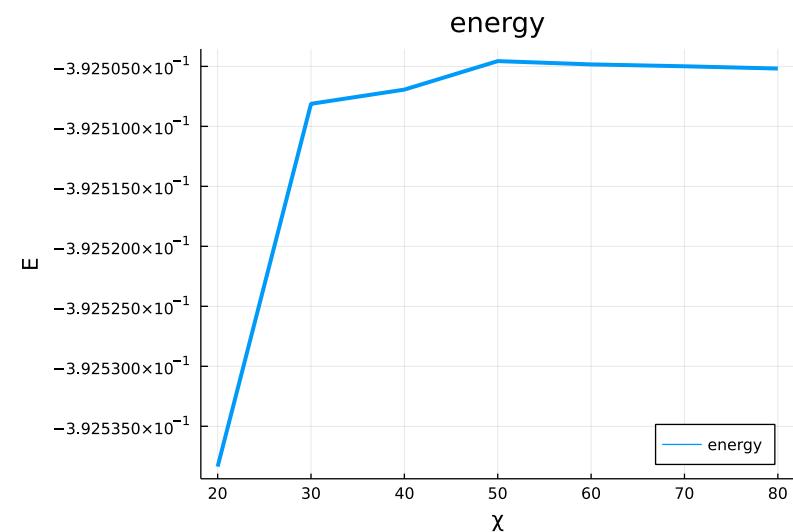
$2 \times 2$  ABCD iPEPS assumption



$$D = 4 \chi = 50$$

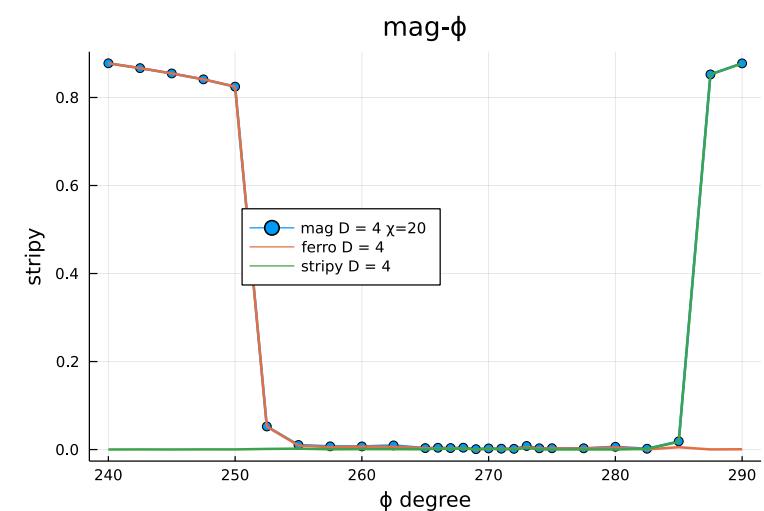
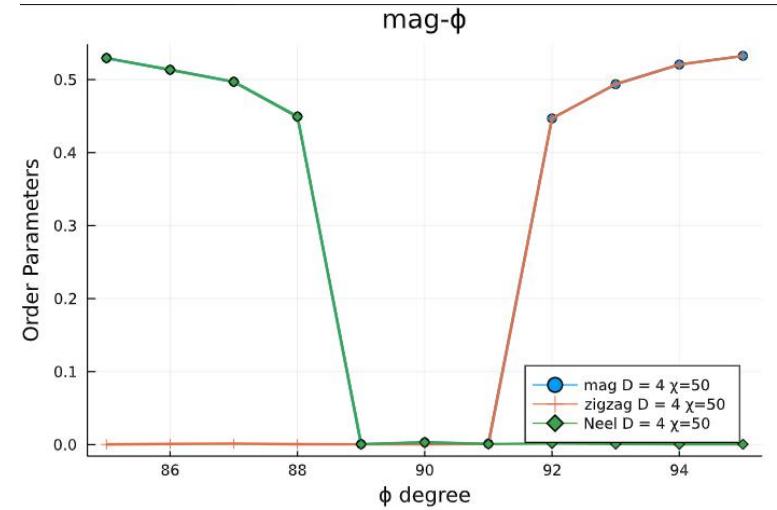
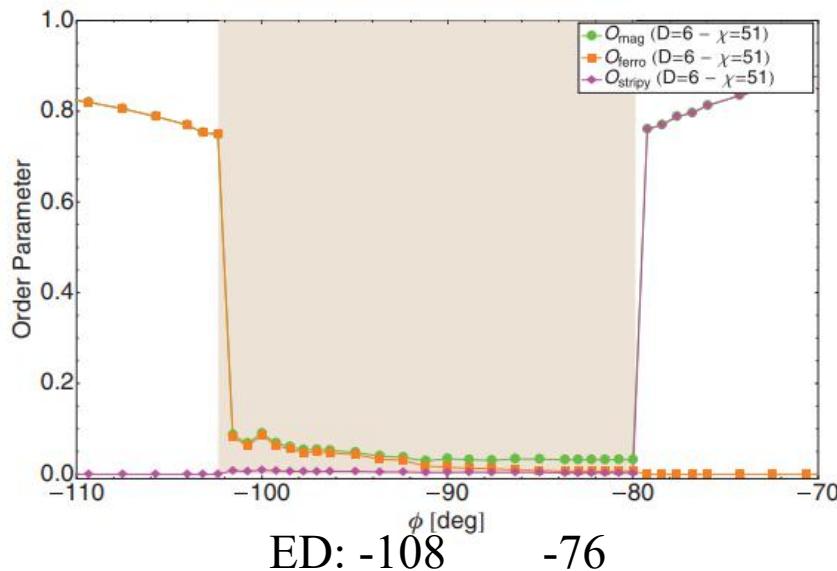
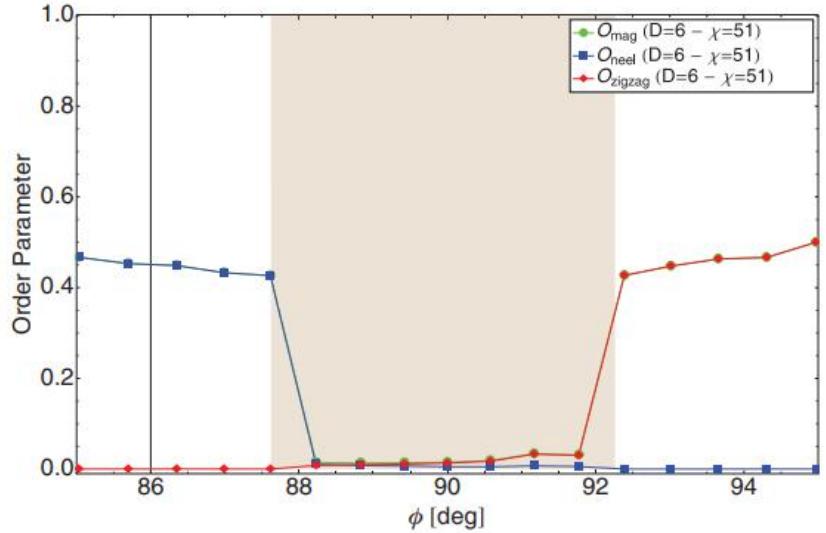


$33 \rightarrow 4$



Direct 4

# phase transition



# Complex AD for $K - J - \Gamma - \Gamma'$

# Adjoint of QR

- $A = QR \quad \bar{A} = [\bar{Q} + Q \text{ Symmetric}(M)]R^{-T}$   
 $M = R\bar{R}^T - \bar{Q}^T Q$   
↓  
 $\bar{A} = [\bar{Q} + Q \text{ Hermitian}(M)]R^{-T} \quad M = R\bar{R}' - \bar{Q}' Q$
- Trick: add  $\delta = 10^{-12}$  to R's diagonal element for the stability of inverse

# Adjoint of eigsolve $T \rightarrow '$

- $\mathbf{l}^T A = \lambda \mathbf{l}^T, \quad A \mathbf{r} = \lambda \mathbf{r}, \quad \mathbf{l}^T \mathbf{r} = 1,$

$$(A - \lambda I) \xi_l = (1 - \mathbf{r} \mathbf{l}^T) \bar{\mathbf{l}}, \quad \mathbf{l}^T \xi_l = 0$$

$$(A^T - \lambda I) \xi_r = (1 - \mathbf{l} \mathbf{r}^T) \bar{\mathbf{r}}, \quad \mathbf{r}^T \xi_r = 0 \longrightarrow \bar{A} = \bar{\lambda} \mathbf{l} \mathbf{r}^T - \mathbf{l} \xi_l^T - \xi_r \mathbf{r}^T$$

gauge invariant

$$\mathbf{l}^T \bar{\mathbf{l}} = \mathbf{r}^T \bar{\mathbf{r}} = 0$$

$$(A - \lambda I) \xi_l = \bar{\mathbf{l}}, \quad \mathbf{l}^T \xi_l = 0$$

$$(A^T - \lambda I) \xi_r = \bar{\mathbf{r}}, \quad \mathbf{r}^T \xi_r = 0$$

Only  $\mathbf{l}$

$$(A - \lambda I) \xi_l = \bar{\mathbf{l}}, \quad \mathbf{l}^T \xi_l = 0$$

$$(A^T - \lambda I) \xi_r = 0, \quad \mathbf{r}^T \xi_r = 0$$

Only  $\mathbf{r}$

$$(A - \lambda I) \xi_l = 0, \quad \mathbf{l}^T \xi_l = 0$$

$$(A^T - \lambda I) \xi_r = \bar{\mathbf{r}}, \quad \mathbf{r}^T \xi_r = 0$$

$$\boxed{\bar{A} = - \xi_r \mathbf{r}^T}$$

# Some discuss

- real-valued function is holomorphic function only when function is constant
- Gradient not derivative
  - $\nabla_z f(z) = 2 \frac{\partial f}{\partial z^*} = \frac{\partial f}{\partial x} + i \frac{\partial f}{\partial y}$
- Vumps is more stable for complex numbers

# $K - J - \Gamma - \Gamma'$

$$H = \sum_{\langle i,j \rangle_\gamma} [K S_i^\gamma S_j^\gamma + J \mathbf{S}_i \cdot \mathbf{S}_j + \Gamma (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) + \Gamma' (S_i^\gamma S_j^\alpha + S_i^\gamma S_j^\beta + S_i^\alpha S_j^\gamma + S_i^\beta S_j^\gamma)],$$

$$K = -1 \quad J = -0.1 \quad \Gamma = 0.3 \quad \Gamma' = -0.02 \\ D=5 \quad \chi=50 \quad E = -0.57654 \text{(unit cell)}$$

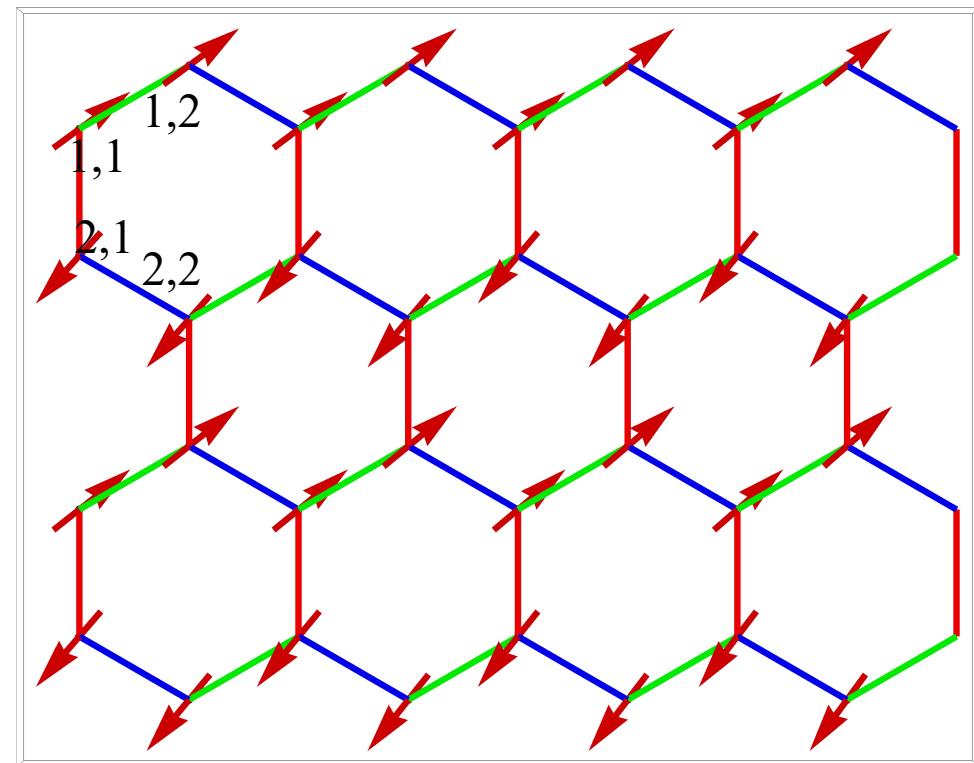
$$\mathbf{M} = [M_x, M_y, M_z]$$

$$\mathbf{M}[1,1] = [0.19091, 0.15684, -0.058433]$$

$$\mathbf{M}[2,1] = [-0.15873, -0.19096, 0.056480]$$

$$\mathbf{M}[1,2] = [0.191301, 0.15756, -0.056088]$$

$$\mathbf{M}[2,2] = [-0.15744, -0.19122, 0.057578]$$



# Field( $h_x, h_y, h_z$ )

Field = [-0.1, -0.1, 0.0]

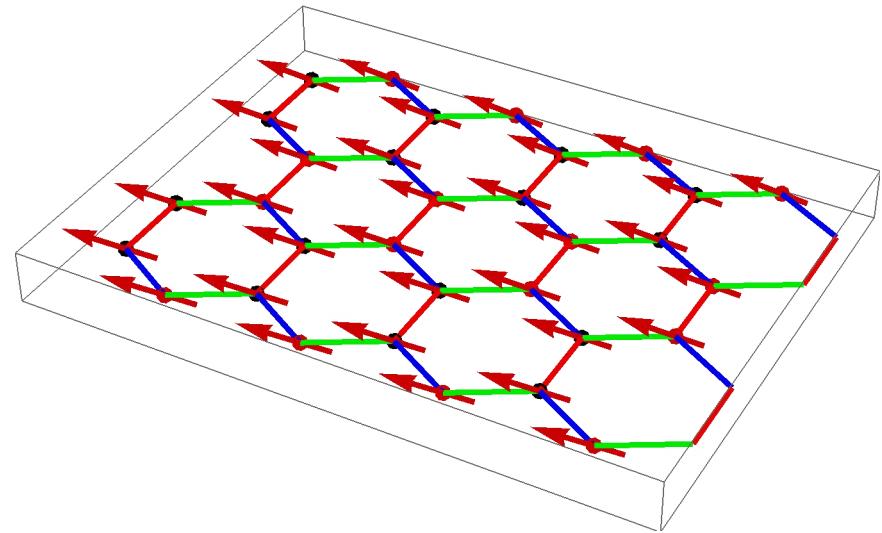
E = -0.717195

M[1,1] = [-0.24242, -0.24161, 0.2105]

M[2,1] = [-0.24139, -0.24225, 0.21112]

M[1,2] = [-0.24199, -0.2417, 0.21105]

M[2,2] = [-0.24179, -0.24223, 0.21081]



Field = [-0.1, -0.1, -0.1]

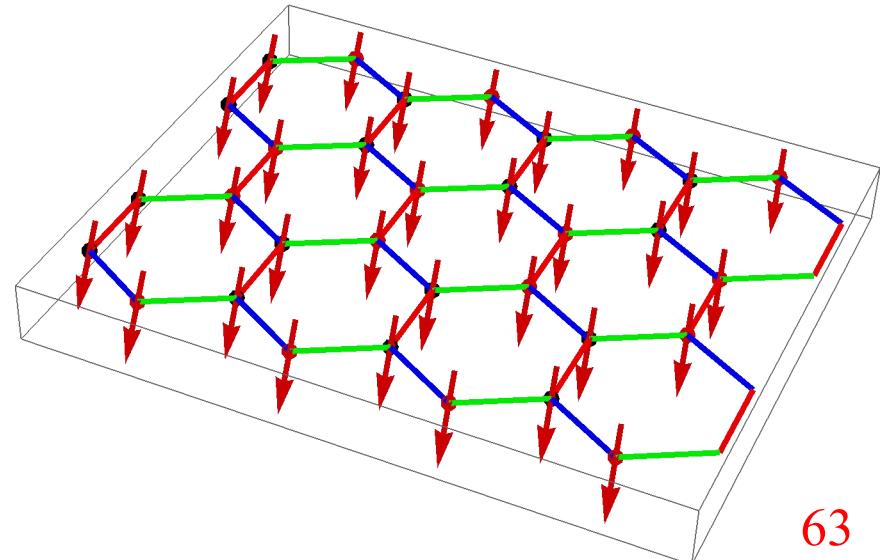
E = -0.65990

M[1,1] = [0.04685, -0.22688, -0.2248]

M[2,1] = [0.0485, -0.22538, -0.22486]

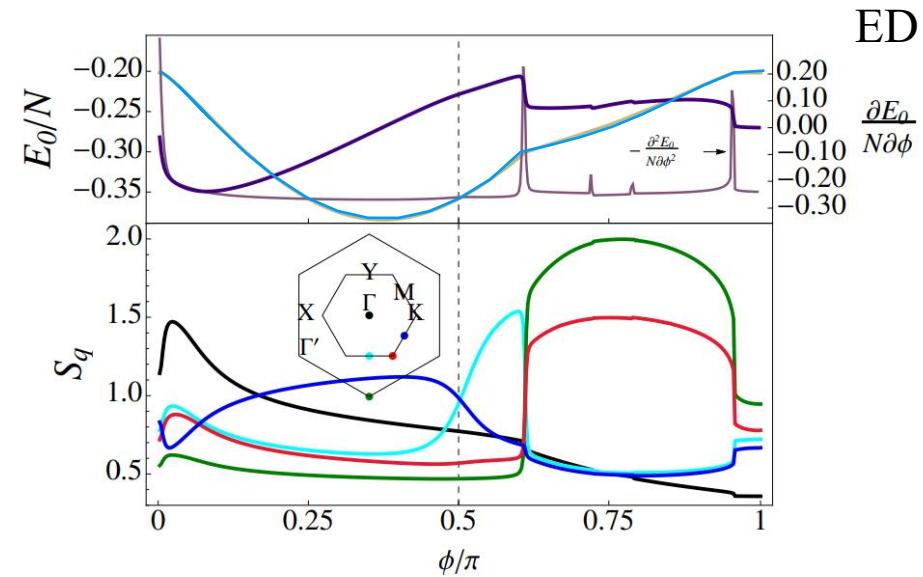
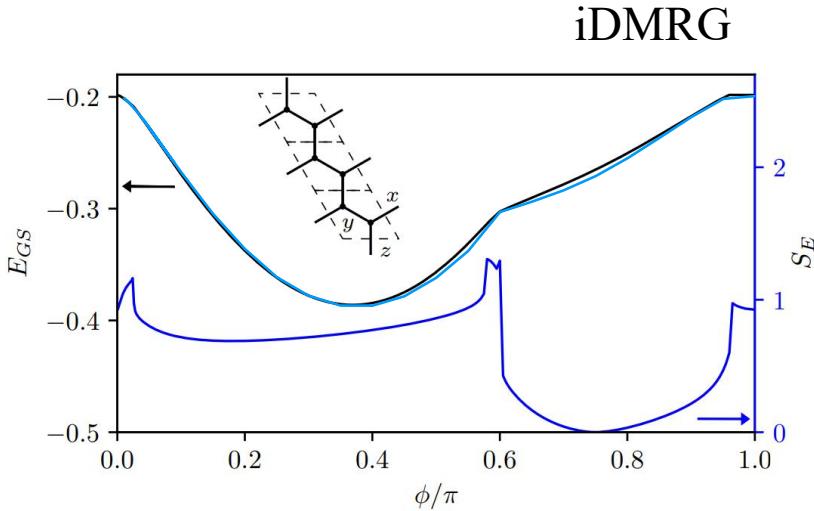
M[1,2] = [0.04673, -0.22765, -0.22405]

M[2,2] = [0.04794, -0.22497, -0.2246]

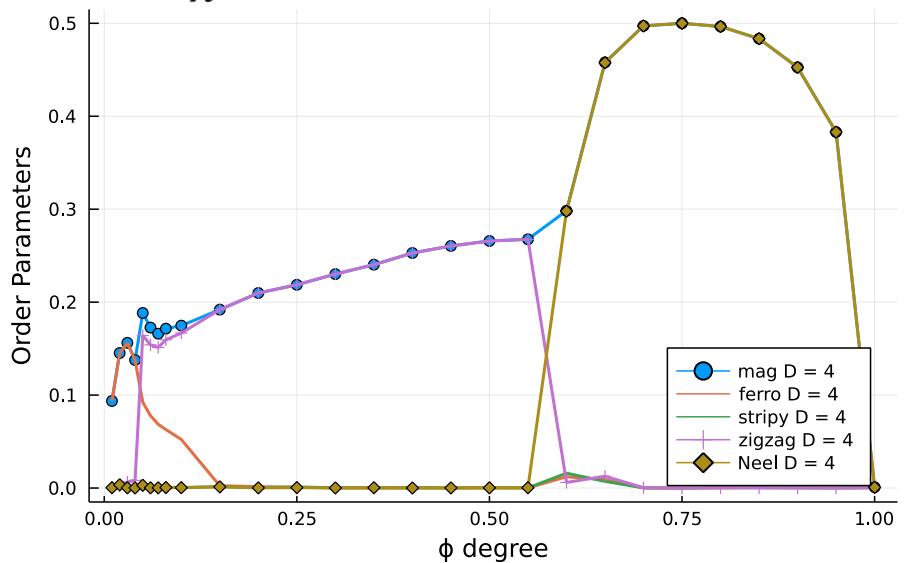


# $K - \Gamma$

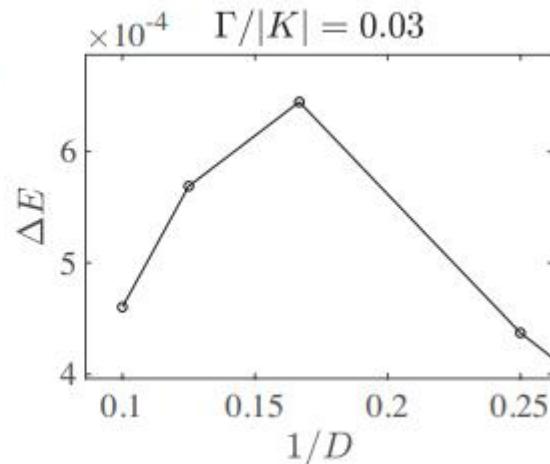
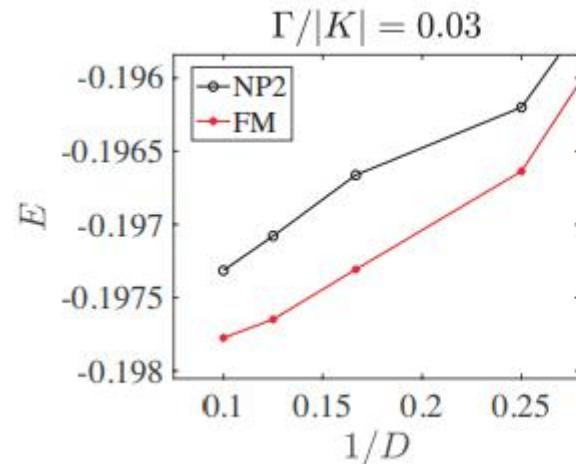
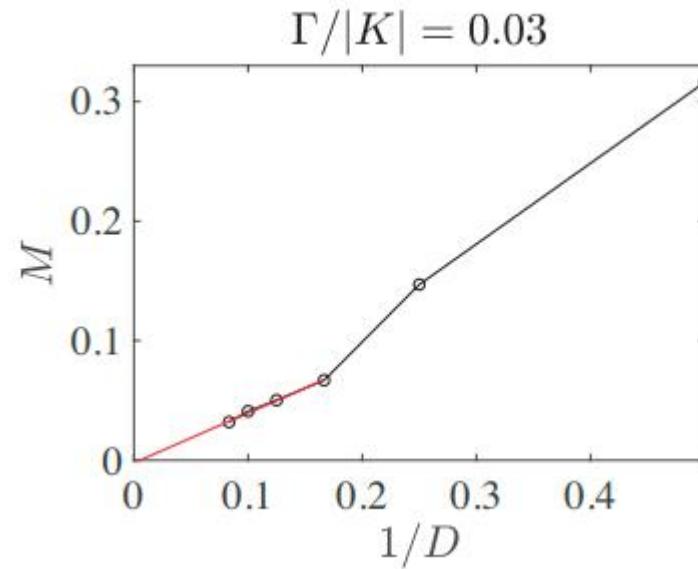
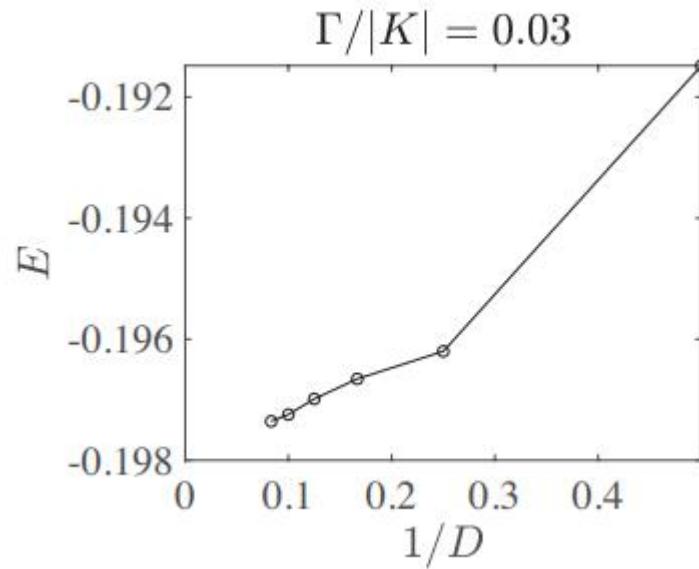
$K = -\cos \varphi$  and  $\Gamma = \sin \varphi$



$D = 4 \chi = 20$

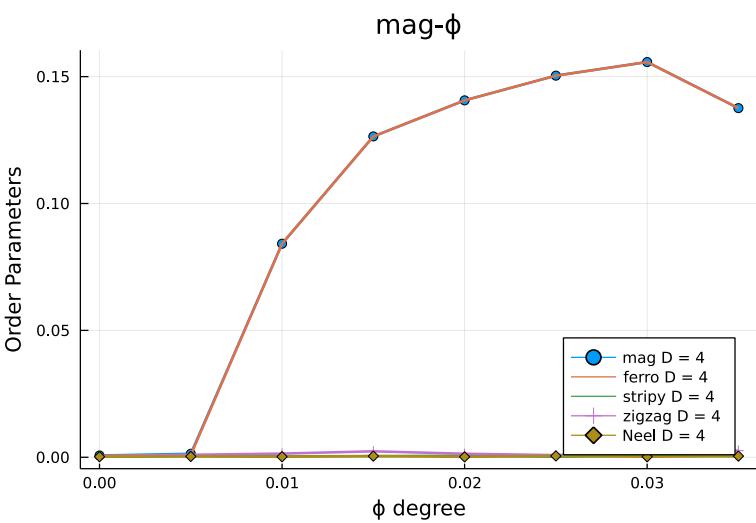


# FM or NP?

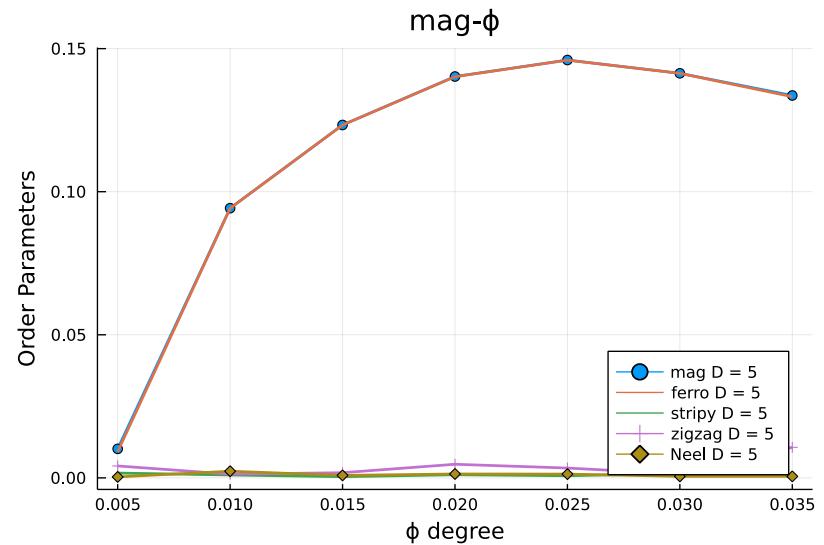


# $K - \Gamma$

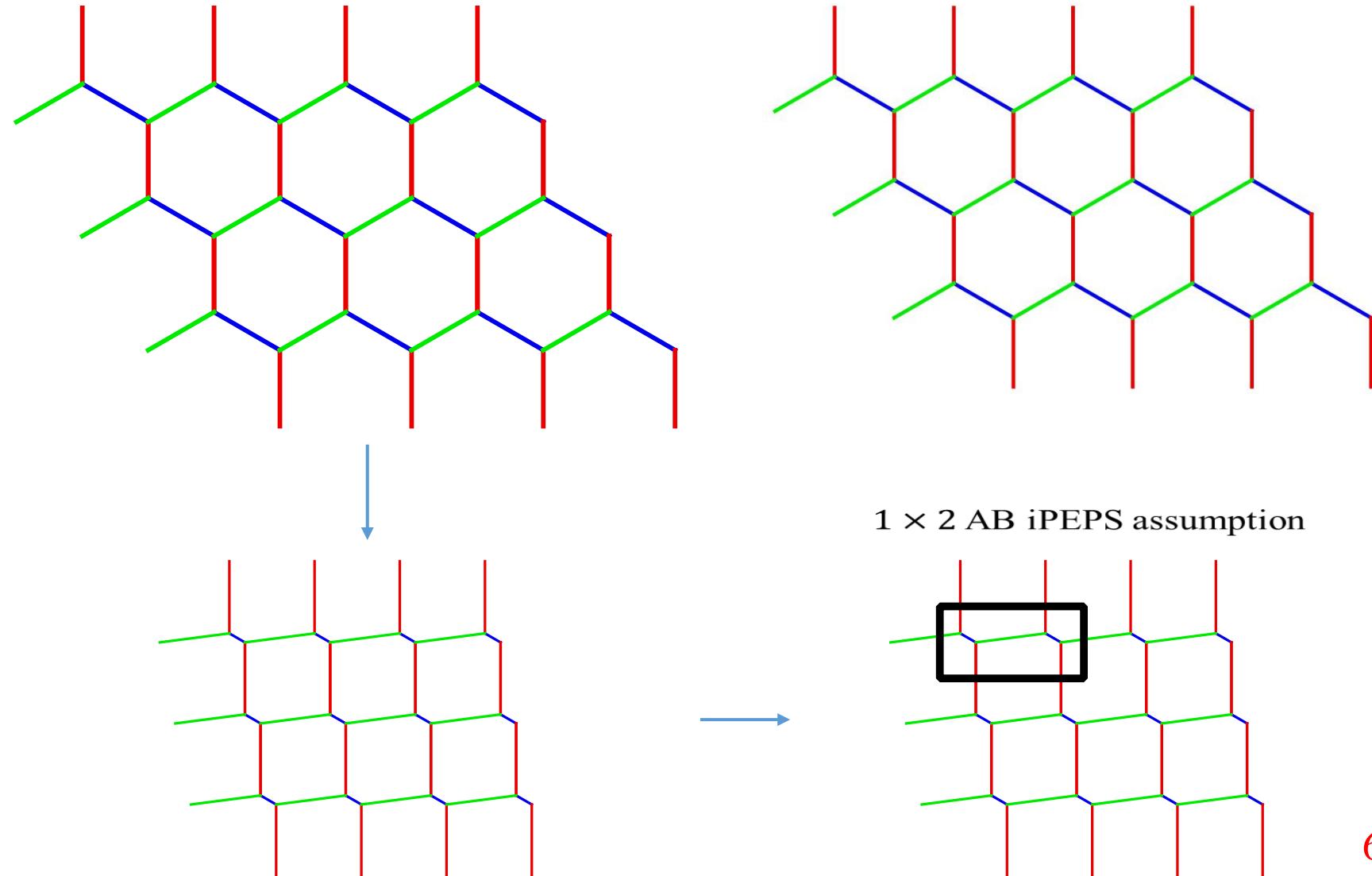
$D = 4 \chi = 30$  direct 4



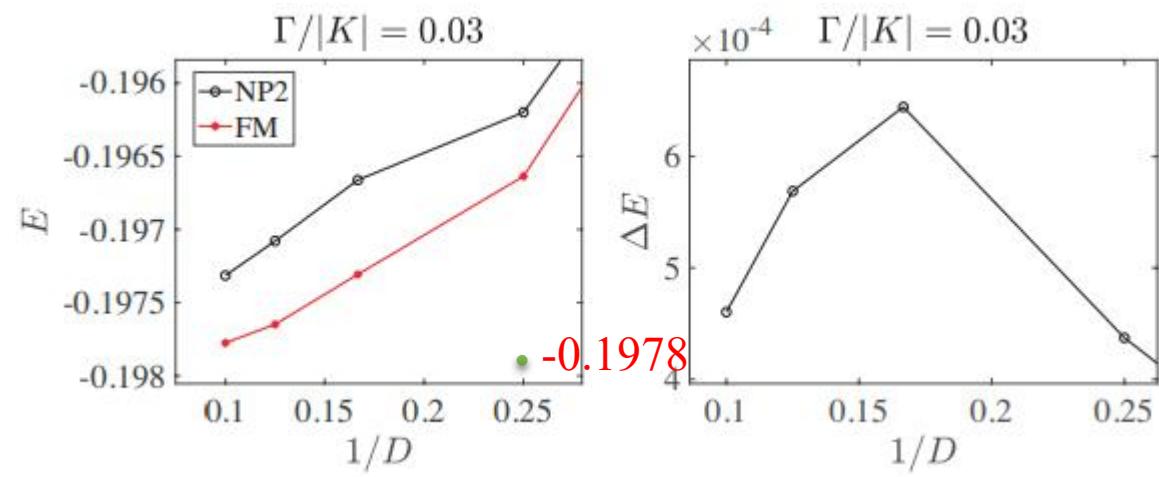
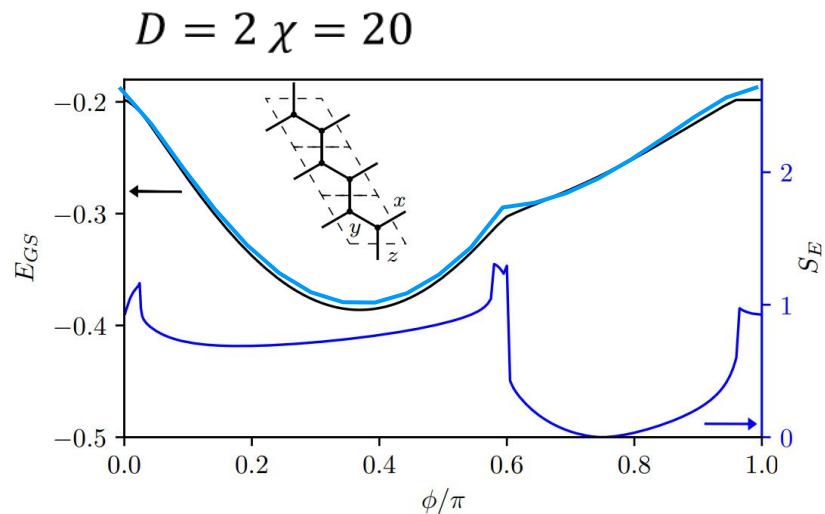
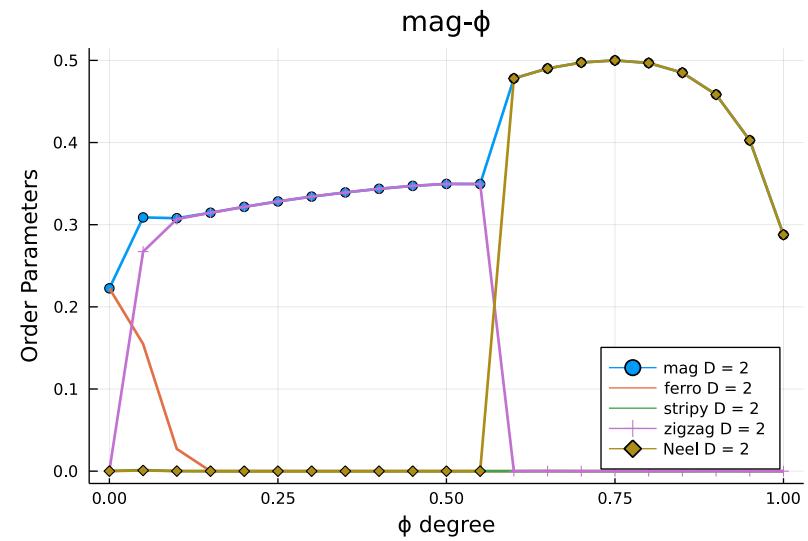
$D = 5 \chi = 80$  33 $\rightarrow$ 4



# Honeycomb lattice to $1 \times 2$ cell square



# $1 \times 2$ cell



# extrapolation

similar parameter  
3h for  $2 \times 2$

$D/\chi$	time	steps	E	mag
2/20	333.7s	33	-0.1941418207761279	0.22714278093309
3/20	23.6min	120	-0.1965226482022378	0.16773840372855753
4/30	1.3h	151	-0.19781799675211129	0.06719914675549436
4/50	0.7h	63	-0.19851218680018168	
4/80	1h	33	-0.19919462200323318	0.06876717784521033
5/50	2.1h	124	-0.19967101706414678	hy = -0.0615101 hx = -0.0684368
5/100	1.9h	21	-0.1980928366925278	hz = -0.0681459

