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EFFICIENT OPTIMIZATION AND CONCEPTUAL BARRIERS IN VARIATIONAL FINITE PROJECTED ENTANGLED-PAIR STATES

Grenoble – 07.07.2026

Reliable numerics is essential to accompany experiments:

- * to predict expected physics for given platform geometry and parameter regime,
- * to validate and to benchmark quantum simulator output
- * to identify parameter regimes of particular physical interest
- * to interpret output and to distinguish genuine from artefacts

Particularly challenging is the situation in mesoscopic 2D...

A MENU OF TENSOR NETWORKS FOR 2D

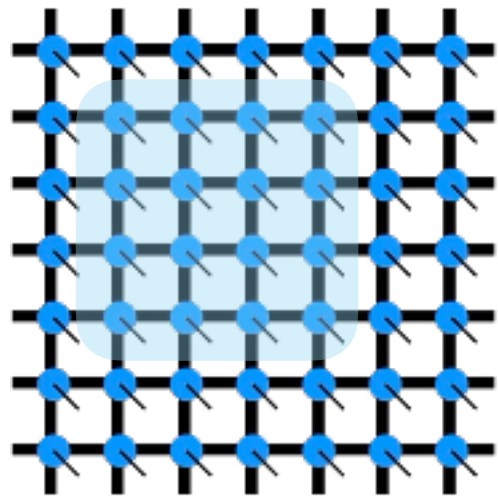
3

★ Physics in 2D is very interesting & challenging

? What tensor networks should we use to study it?

Good theory tells:

PEPS



Verstraete & Cirac, cond-mat/0407066v1

- ✓ entang. boundary law
- no canonical form
- very costly contraction
- tricky approx. optimization

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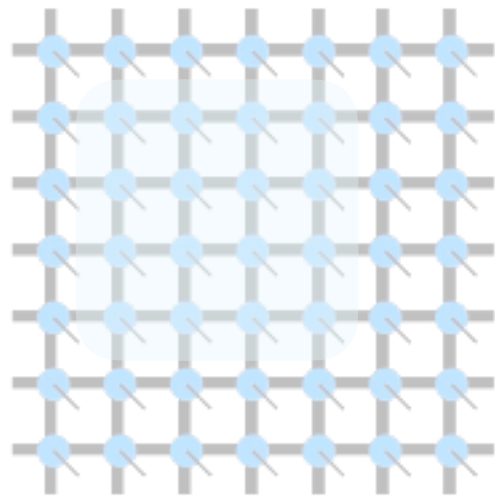
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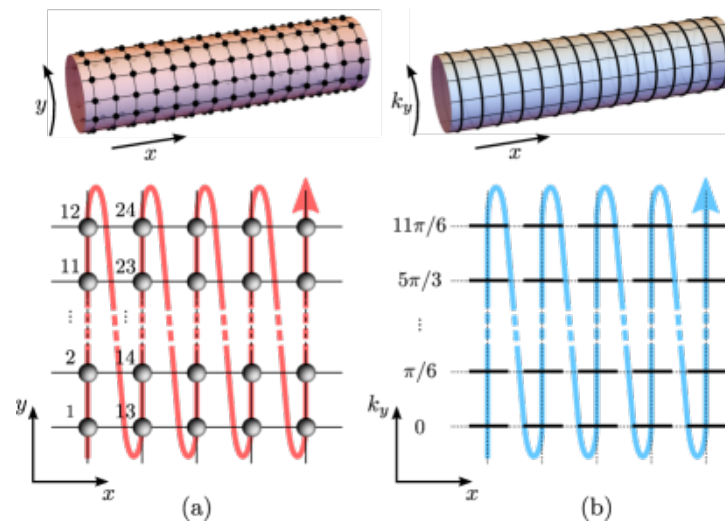
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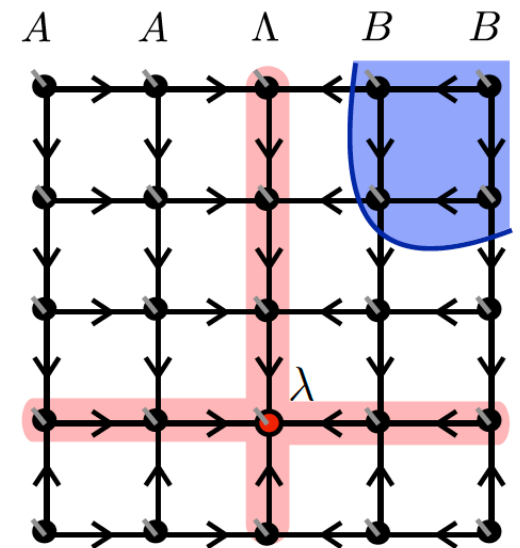
Practise often turns out to be:

cylinder-MPS



Motruk et al, PRB 93, 155139 ('16)

isoTNS



*Zaletel & Pollmann,
PRL 124, 037201 ('20)*

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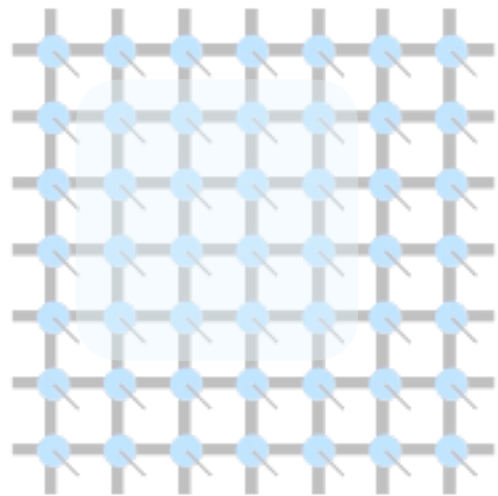
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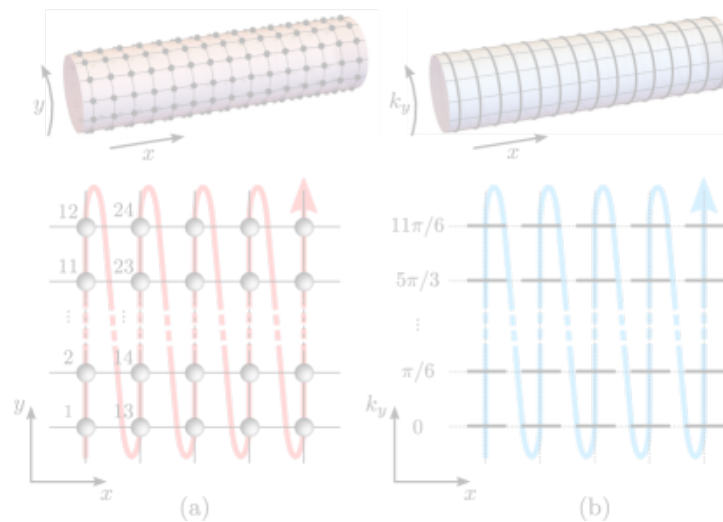
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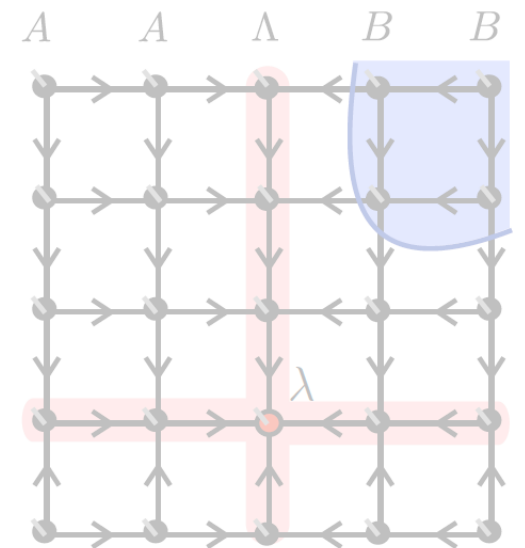
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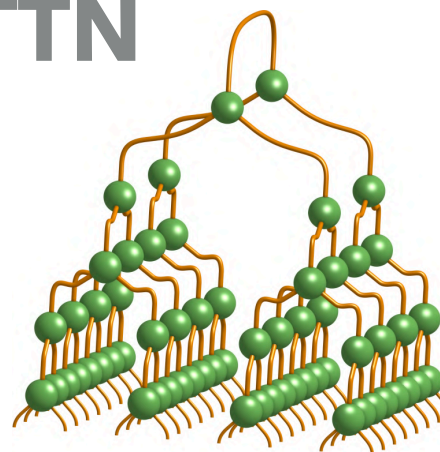
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TTN



- ~ area law only on average
- ✓ canonical form
- ✓ cheap contraction $O(\chi^4)$
- ✓ MPS-like optimization
- ✓ PBC at no extra cost

A MENU OF TENSOR NETWORKS FOR 2D

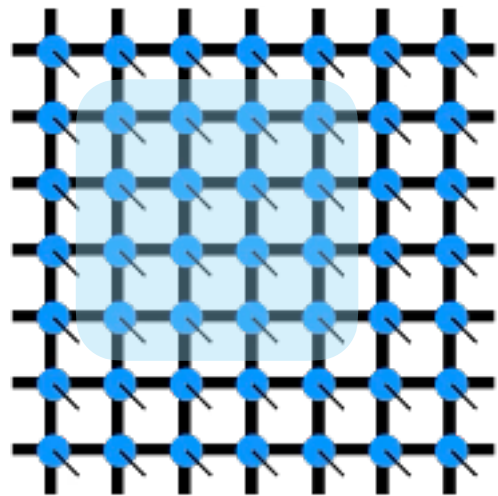
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- ★ Physics in 2D is very interesting & challenging
- ? What tensor networks should we use to study it?

Disclaimer:
no NQS here :-)

Good theory tells:

PEPS

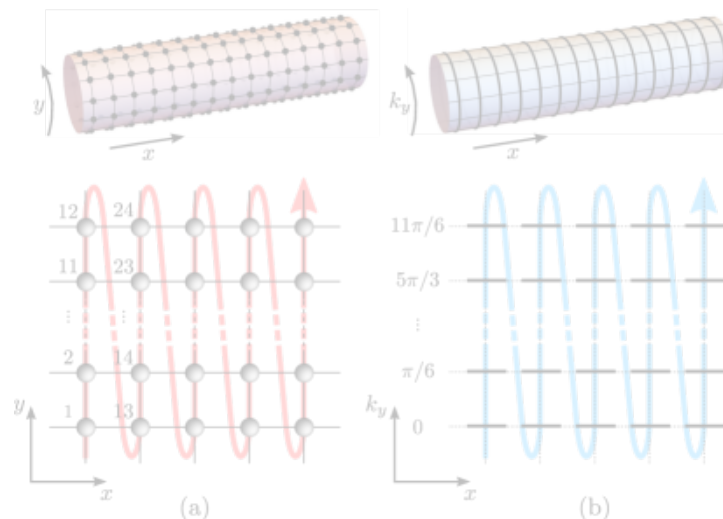


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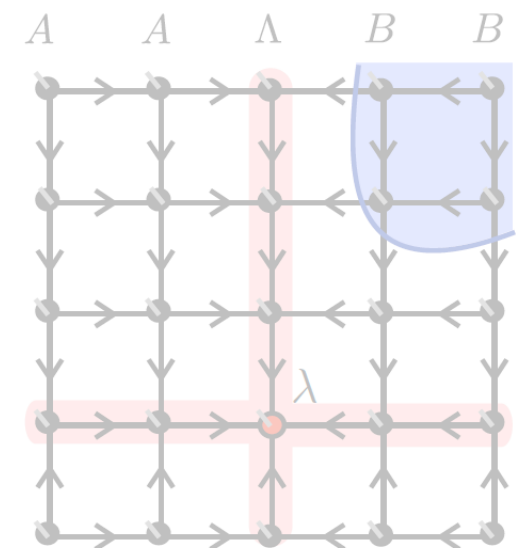
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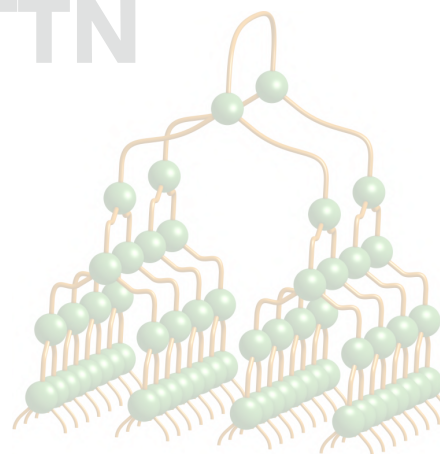
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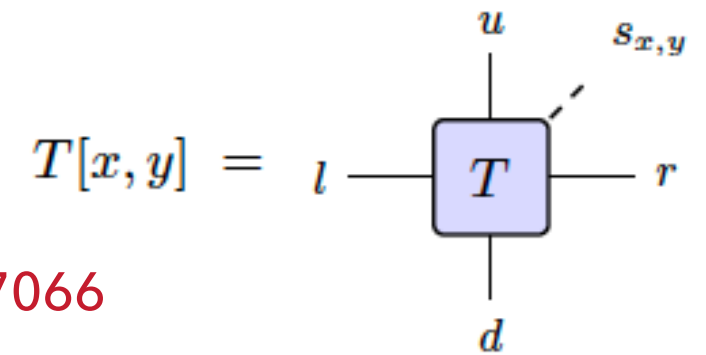
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FINITE PEPS: BASICS & POSSIBLE SUBTLETIES

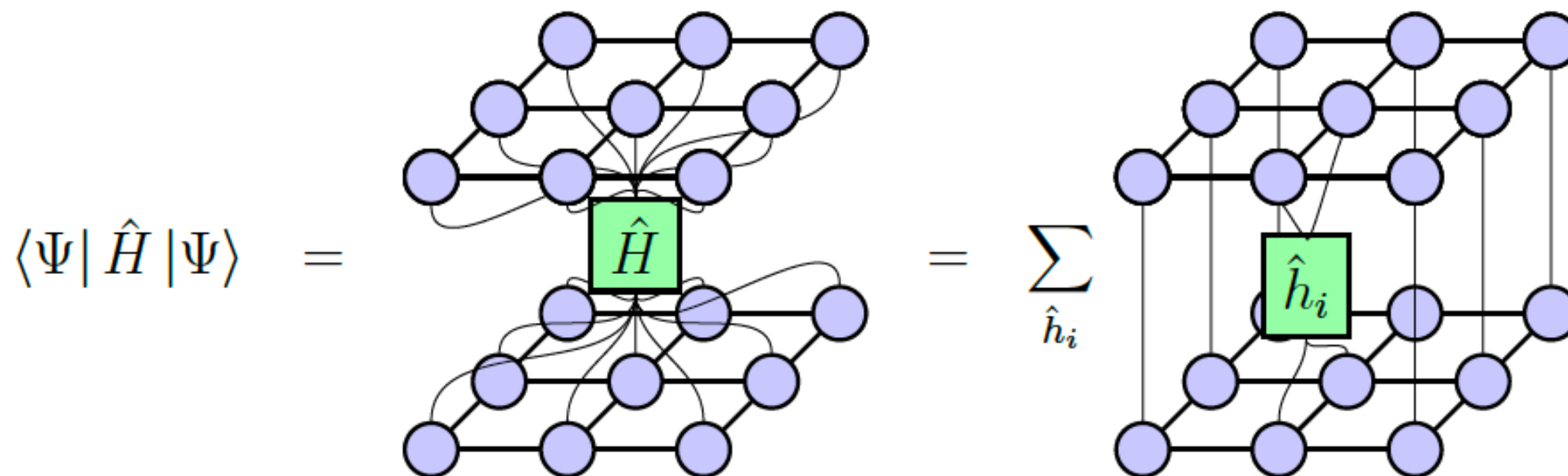
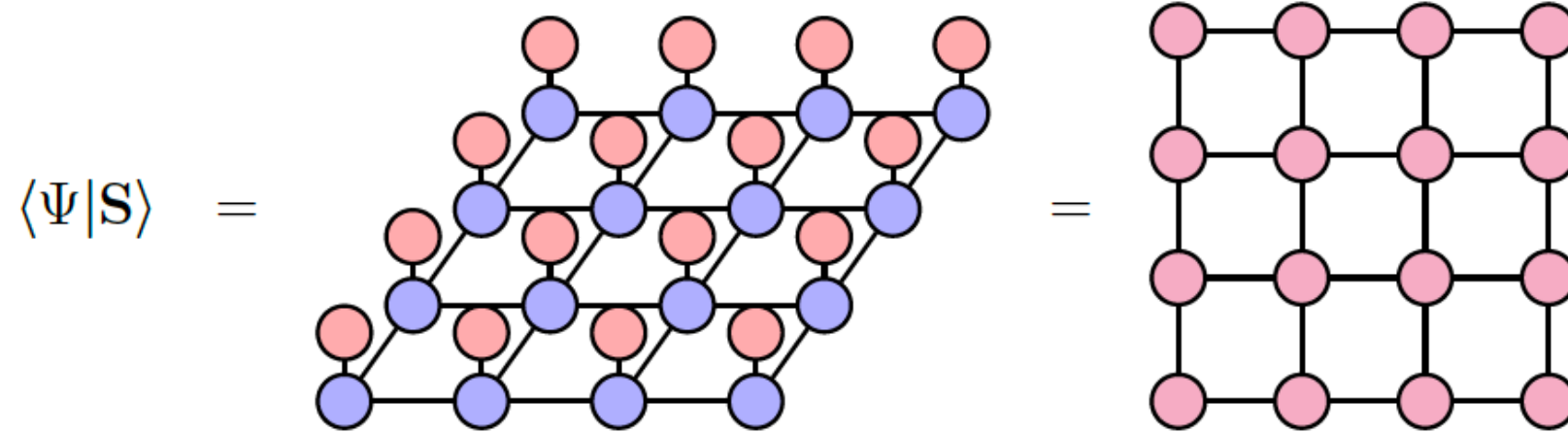
FINITE PEPS: BASICS

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$$|\Psi\rangle = \sum_{s_{1,1} \cdots s_{L_x, L_y}} \text{Tr}(T[1,1] \cdots T[L_x, L_y]) |s_{1,1} \cdots s_{L_x, L_y}\rangle$$

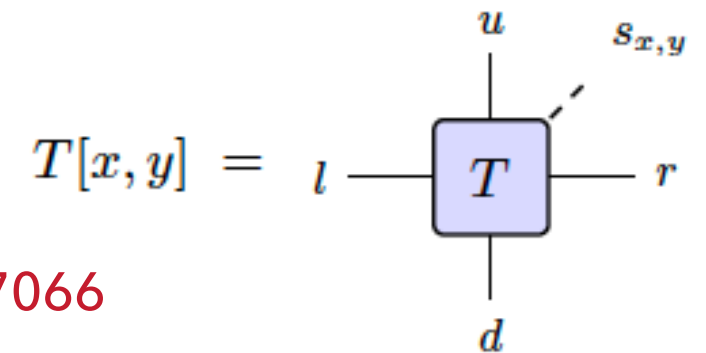


Verstraete & Cirac, cond-mat/0407066

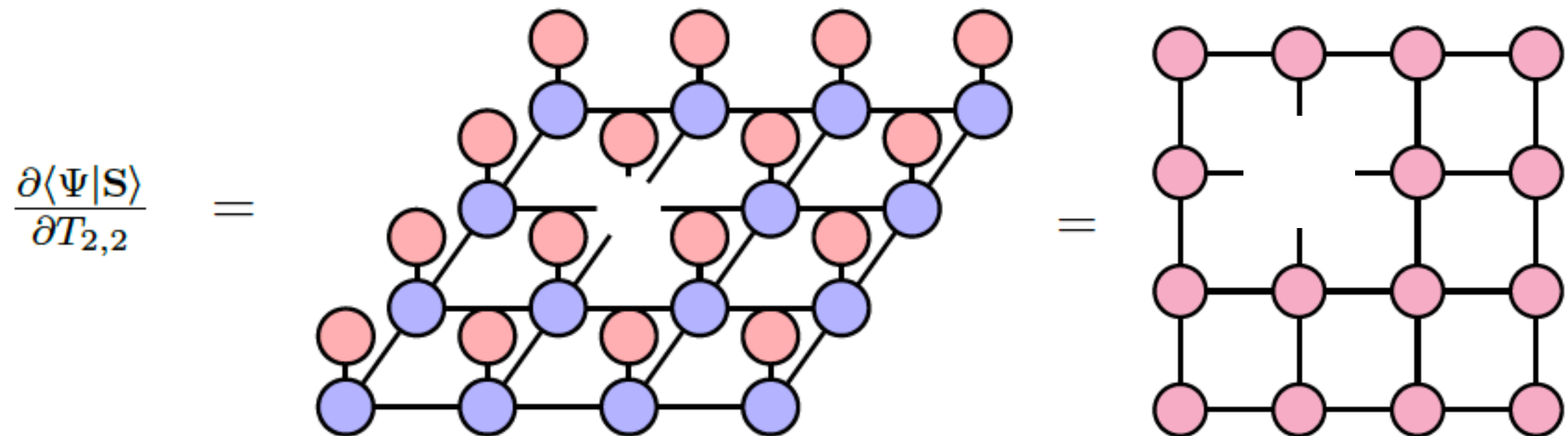


$$|\Psi\rangle = \sum_{s_{1,1} \cdots s_{L_x, L_y}} \text{Tr}(T[1, 1] \cdots T[L_x, L_y]) |s_{1,1} \cdots s_{L_x, L_y}\rangle$$

Verstraete & Cirac, cond-mat/0407066



✓ Multilinear Ansatz: easy derivatives!



✗ Loopy graph: #p-hard contractions! Schuch et al, PRL 98, 140506 (2007)

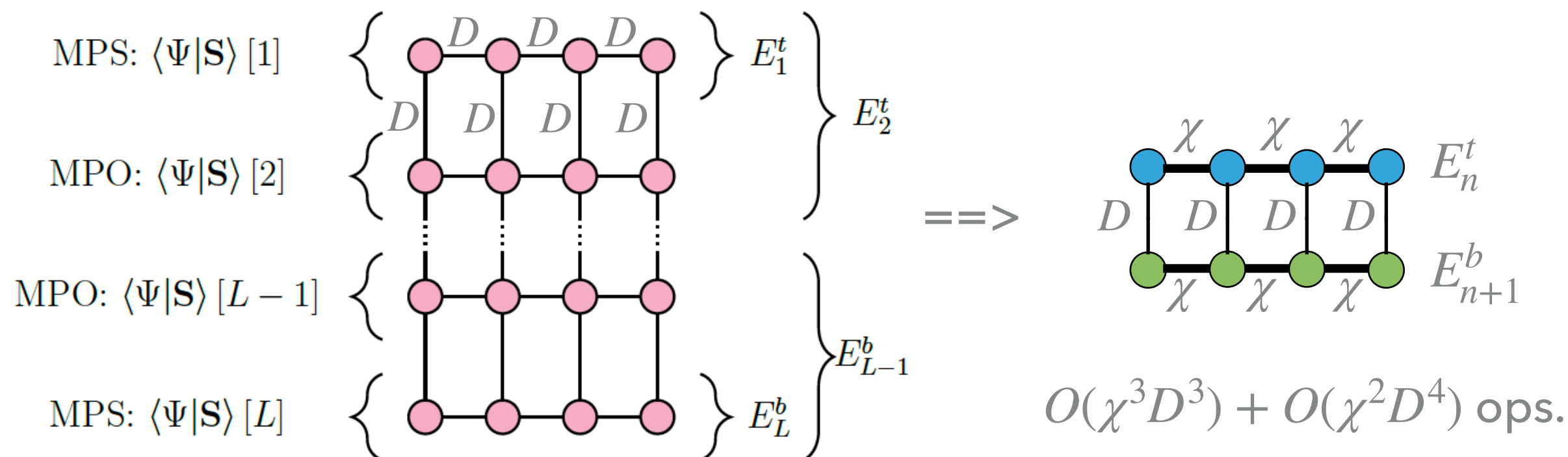
FINITE PEPS: BASICS

7

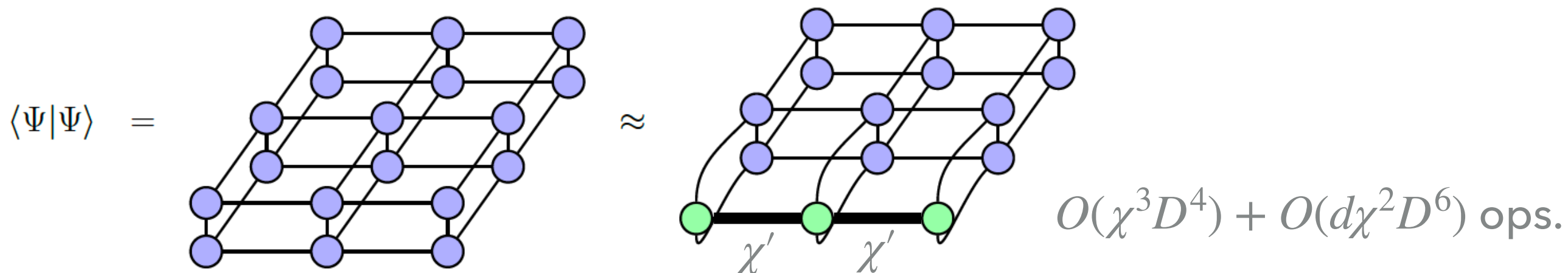
✗ Loopy graph: #p-hard contractions! Schuch et al, PRL 98, 140506 (2007)

💡 Boundary MPS method helps to approximate them!

Introduce another bond dimension χ



Similarly for double layer contractions (even more expensive):



✗ Loopy graph: #p-hard contractions! Schuch et al, PRL 98, 140506 (2007)

💡 Boundary MPS method helps to approximate them!

⚠ Computational-complexity phase transition (*random PEPS*)
 González-García, et al., PRB 109, 325102 (2024) Chen et al., PRX Quantum 6, 010312 (2025)
 (*links to quantum circuits, too*) McGinley, et al., PRX 15, 021059 (2025)

🔧 i) geometric entanglement $S_G(|\psi\rangle) = -\frac{1}{N} \log_2 \max_{|\phi\rangle \in \text{product states}} |\langle \phi | \psi \rangle|^2$

ii) relative contraction error $\Delta\psi(D_c, D_c^{\max}) = \frac{\psi(D_c^{\max}) - \psi(D_c)}{\psi(D_c^{\max})} \quad D_c \equiv \chi$

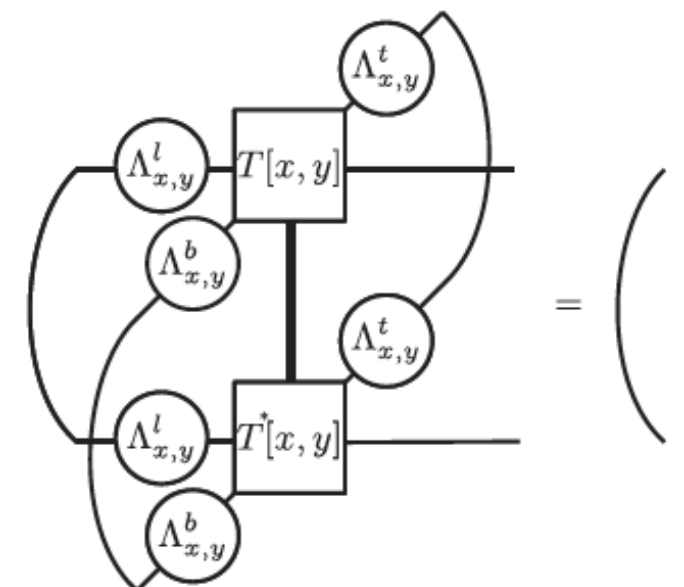
iii) average spectral entropy in Vidal gauge

$$H_{\text{spec}} = -\frac{1}{4} \sum_{\alpha \in \text{bonds}} \sum_k \Lambda_{\alpha,k}^2 \log \Lambda_{\alpha,k}^2$$

Vidal, PRL 91, 147902 (2003)

Ran et al., PRB 86, 134429 (2012)

Tindall et al, SciPost Phys. 15, 222 (2023)

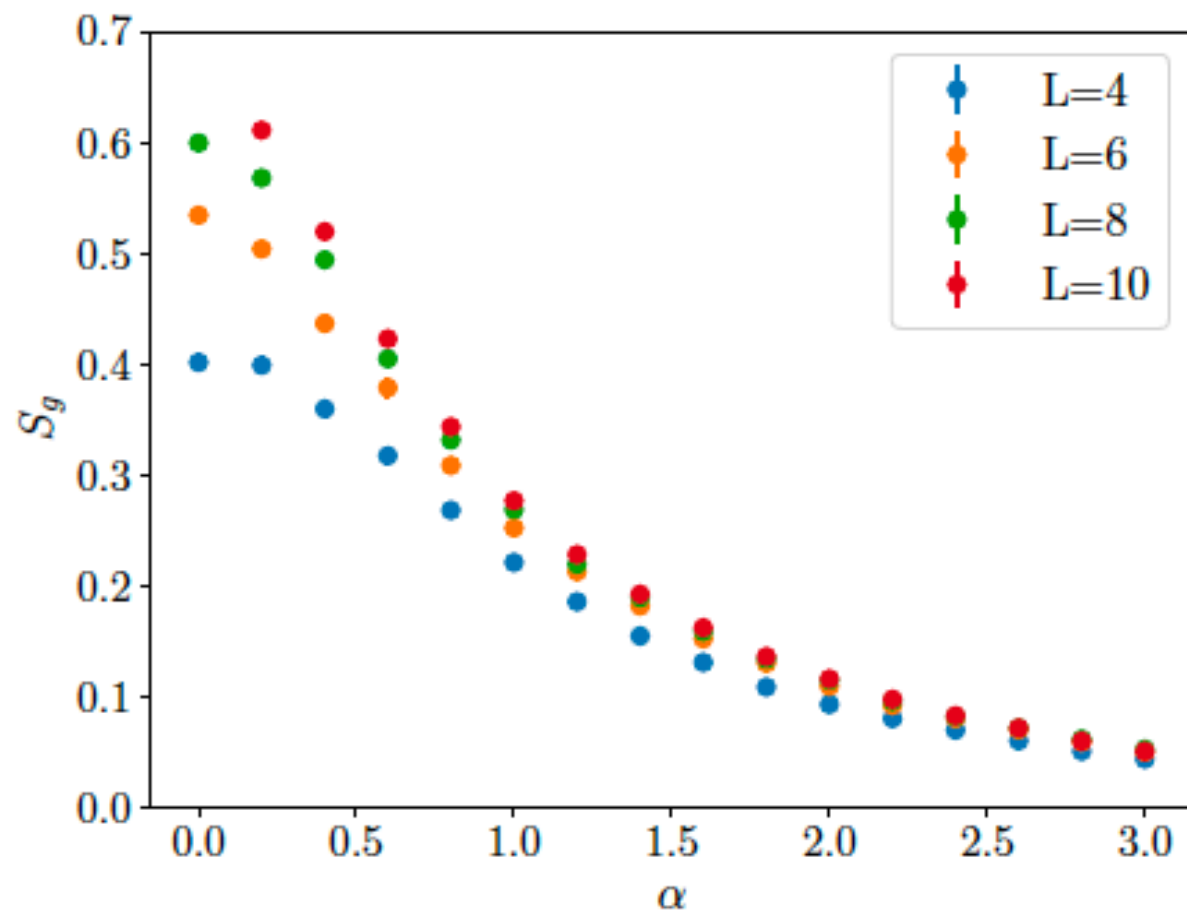
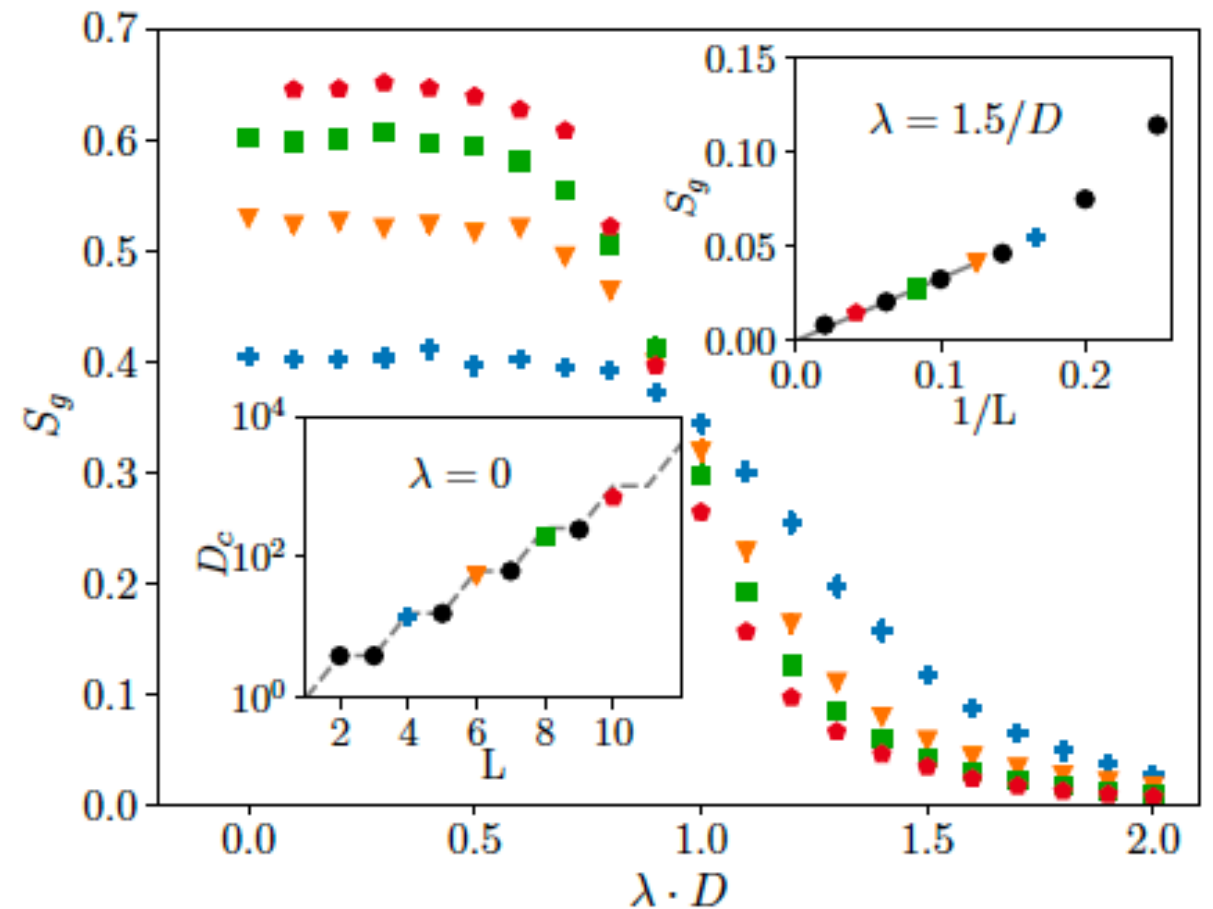


FINITE PEPS: CONTRACTION COMPLEXITY

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[Alcalde Puente, et al. \(MR\), PRB 111, 195120 \('25\)](#)

Haar random tensors
with shifted mean λ



power-law damped entries

$$S(\alpha)_{i,j} \propto \delta_{i,j}/i^\alpha$$

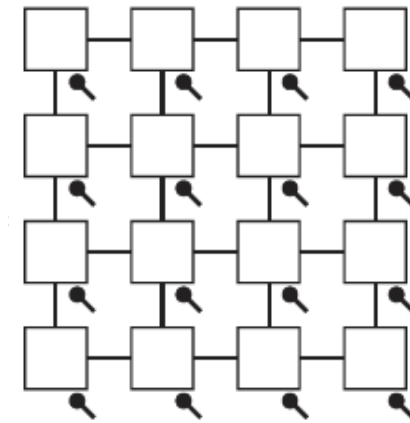
$$T(\alpha) = (S(\alpha)^{\otimes 4})T ; T(\alpha) =$$

FINITE PEPS: CONTRACTION COMPLEXITY

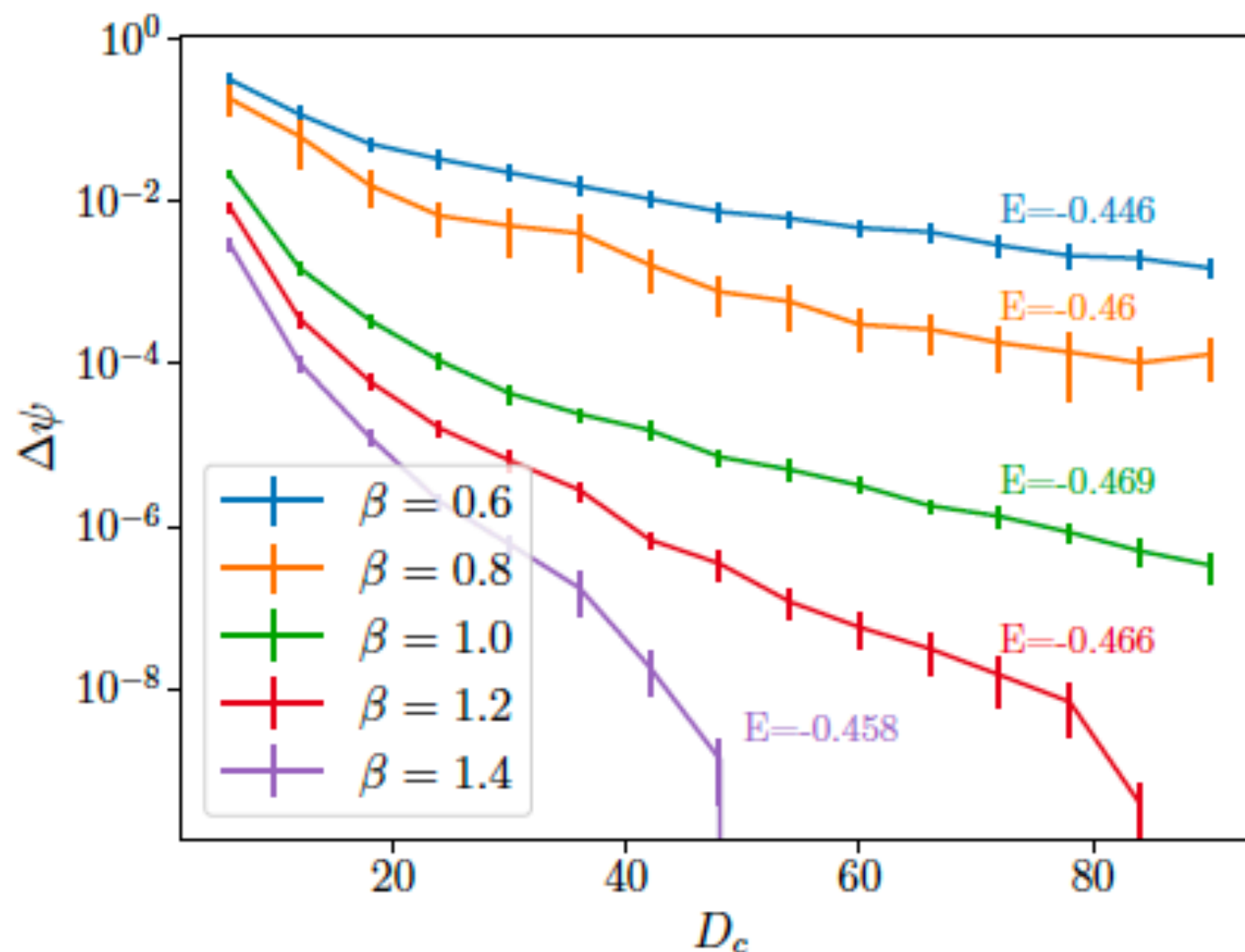
10

[Alcalde Puente, et al. \(MR\), PRB 111, 195120 \('25\)](#)

Transition cannot only depend on entanglement properties of the state, e.g.



Take “physical” PEPS & rescale Vidal spectra: $\{\Lambda\}_{\text{bonds}} \longrightarrow \{\Lambda^\beta\}_{\text{bonds}}$



$\beta < 1$ flattens

$\beta = 1$ original

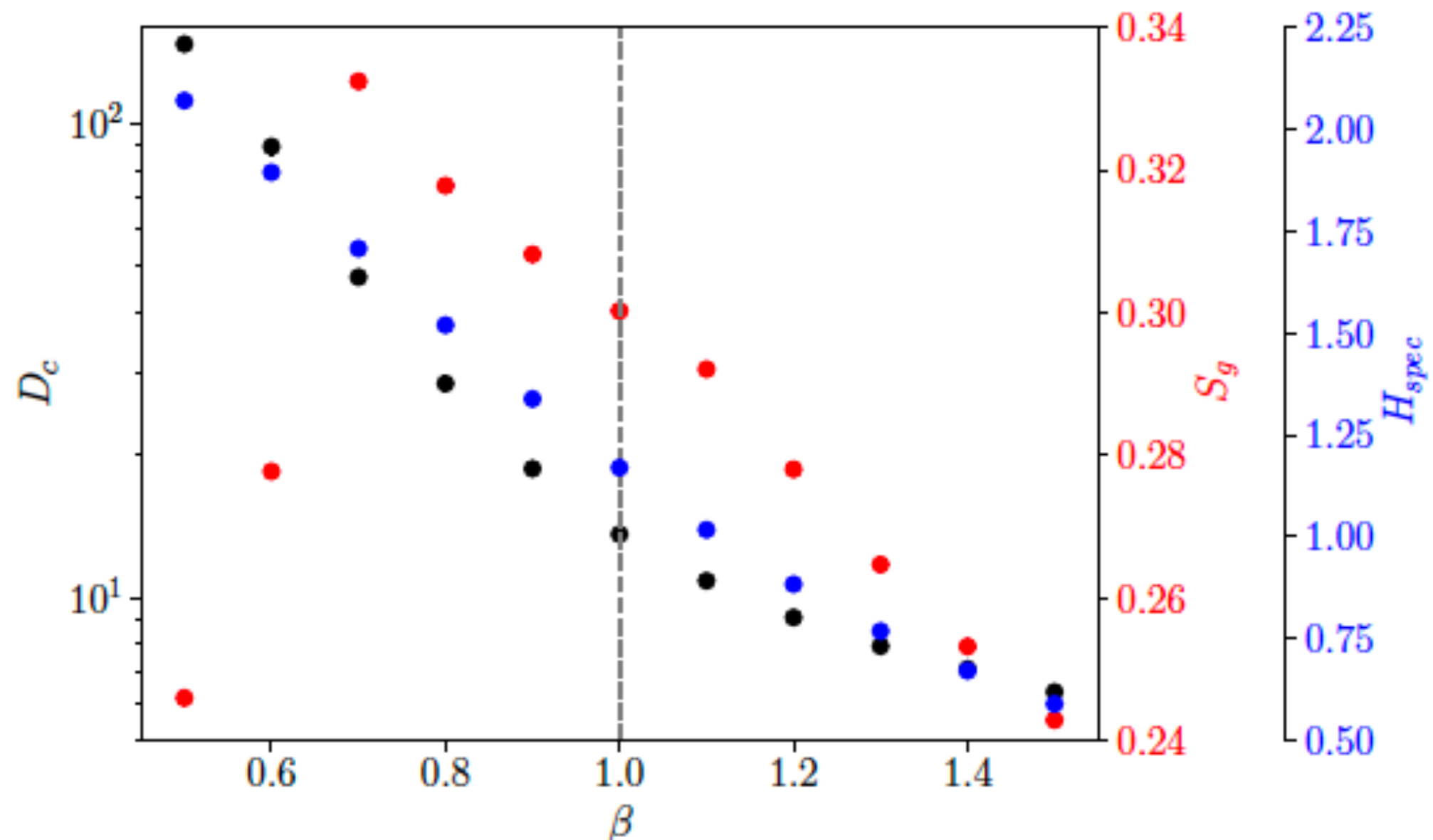
$\beta > 1$ sharpens

FINITE PEPS: CONTRACTION COMPLEXITY

11

[Alcalde Puente, et al. \(MR\), PRB 111, 195120 \('25\)](#)

Average spectral entropy in Vidal gauge
is a much better indicator than
geometric entanglement

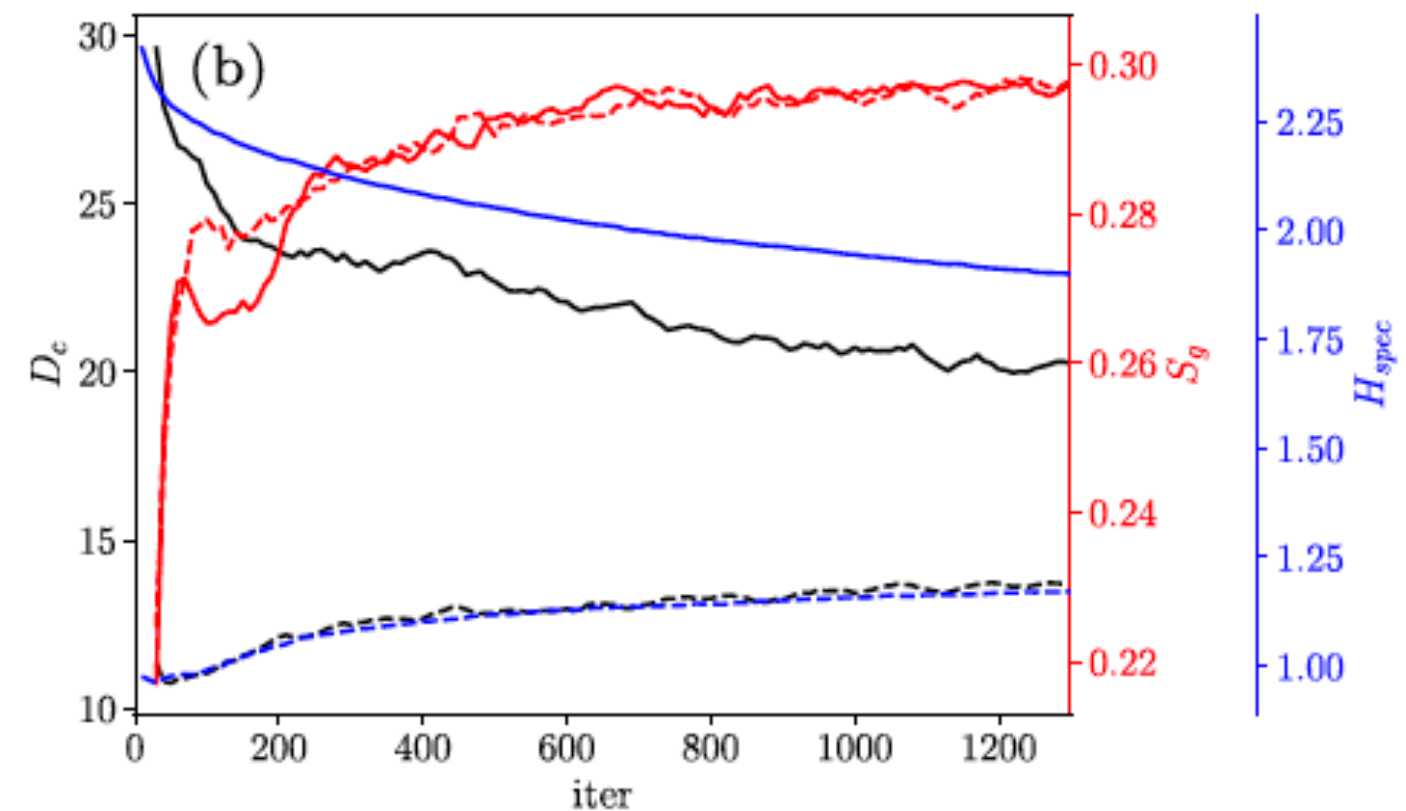
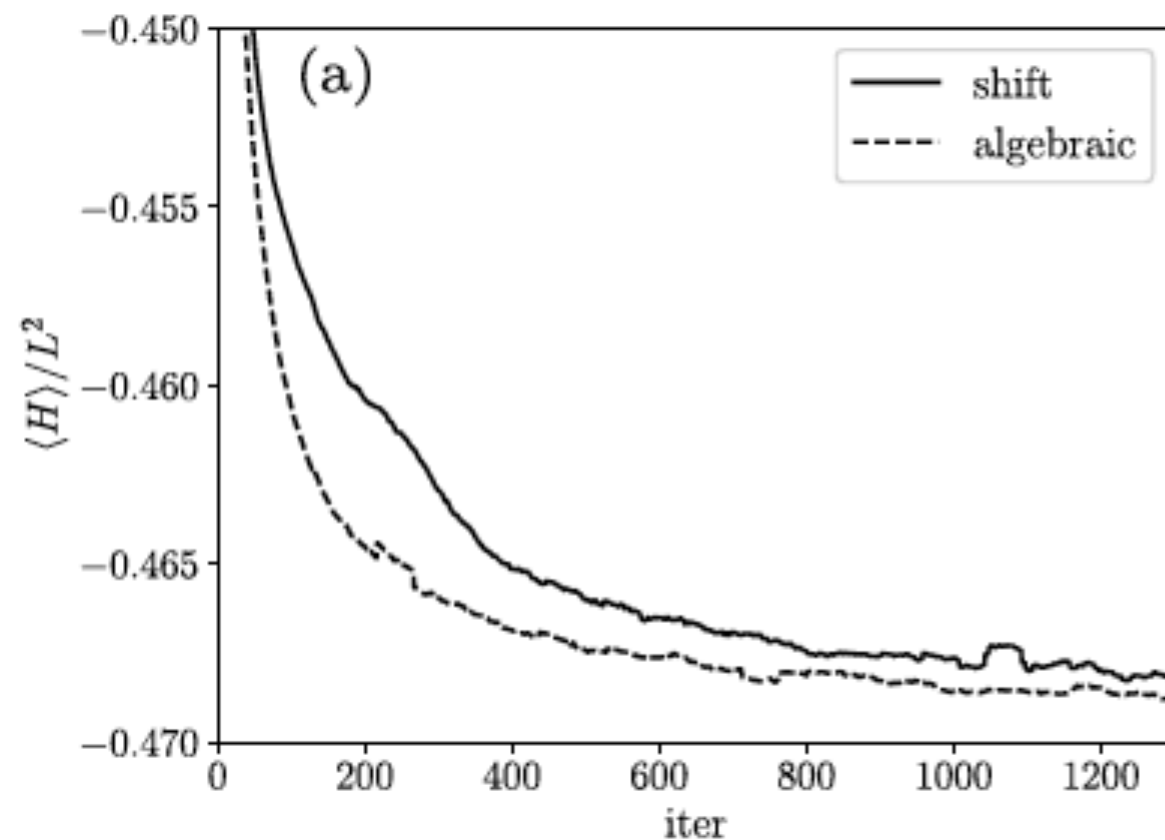


FINITE PEPS: CONTRACTION COMPLEXITY

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[Alcalde Puente, et al. \(MR\), PRB 111, 195120 \('25\)](#)

Regularisation in action: algebraic rescale is much better!



PROJECTED ENTANGLED PAIR STATES (PEPS) AS VARIATIONAL WAVEFUNCTIONS

[Alcalde Puente, et al. \(MR\), PRB 111, 195120 \('25\)](#)



Imaginary-**TDVP** (a.k.a. **natural gradient**) for N_P param. θ (tensor entries)

$$|\dot{\Psi}(\theta)\rangle = -H |\Psi(\theta)\rangle \longrightarrow \sum_i \underbrace{\frac{\partial \langle S | \Psi(\theta) \rangle}{\partial \theta_i}}_{\tilde{O}_{S,i}} \dot{\theta}_i = - \underbrace{\langle S | H | \Psi(\theta) \rangle}_{\tilde{E}_S^{\text{loc}}}, \quad \forall S \in \mathcal{H}$$

not (exactly) solvable, since $N_P \ll \dim(\mathcal{H})$



Best approx. by N_S relevant **samples** in $\mathcal{H}$

$$\min_{\dot{\theta}} \sum_{\{S\}} \frac{|\langle \Psi | S \rangle|^2}{\langle \Psi | \Psi \rangle} \left\| \sum_i \underbrace{\frac{\tilde{O}_{S,i}}{\langle \Psi | S \rangle}}_{O_{S,i}} \dot{\theta}_i + \underbrace{\frac{\tilde{E}_S^{\text{loc}}}{\langle \Psi | S \rangle}}_{E_S^{\text{loc}}} \right\|^2$$

$\frac{1}{N_S} \sum_{S \sim p_\Psi} \rho_\Psi(S)$

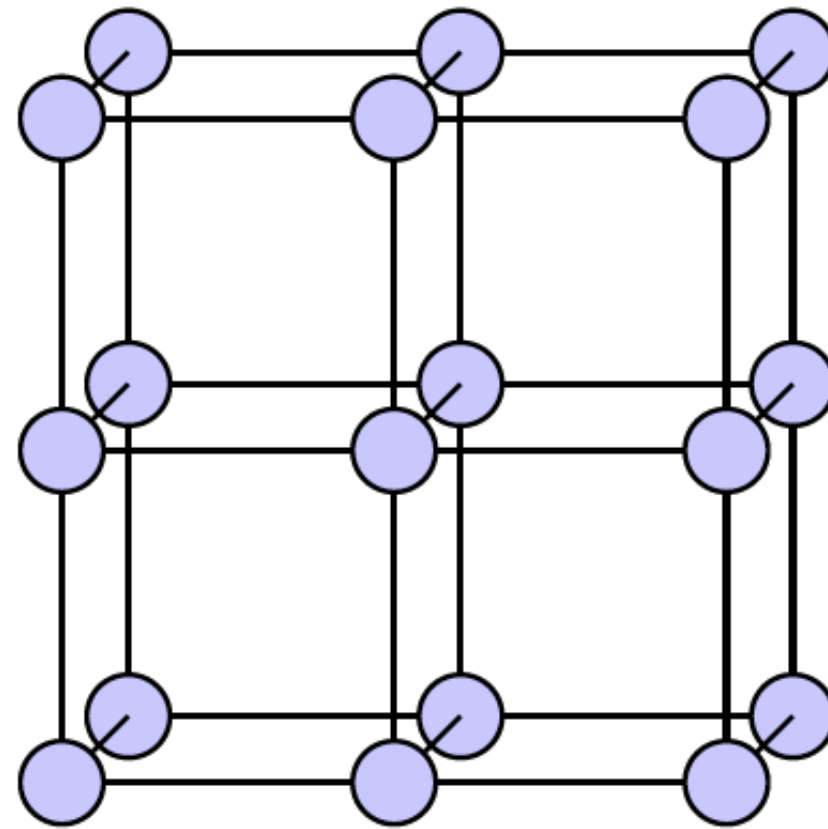


smart pseudo-inversion by **minSR** [$N_S \ll N_P$]
(minimum-step Stochastic Reconfiguration)

$$\dot{\theta} = -O^\dagger \underbrace{(OO^\dagger)^{-1}}_T E_{\text{loc}}$$

Chen, Heyl,
Nat. Ph. 20, 1476 ('24)

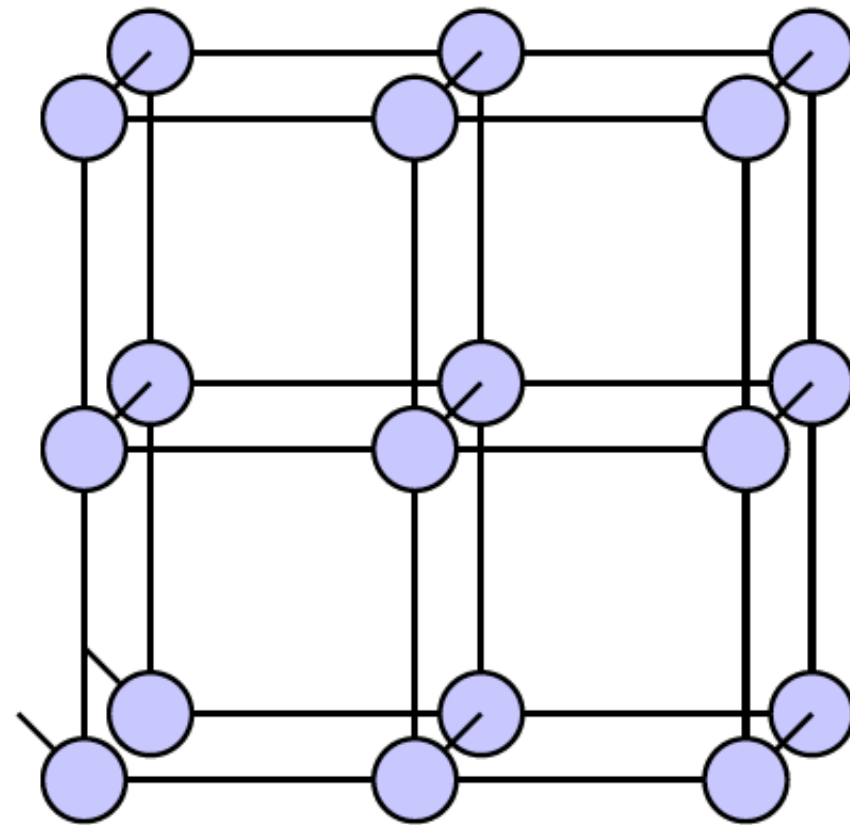
Vieijra, et al., PRB 104, 235141 ('21)



$$\langle \Psi | \Psi \rangle$$

Vieijra, et al., PRB 104, 235141 ('21)

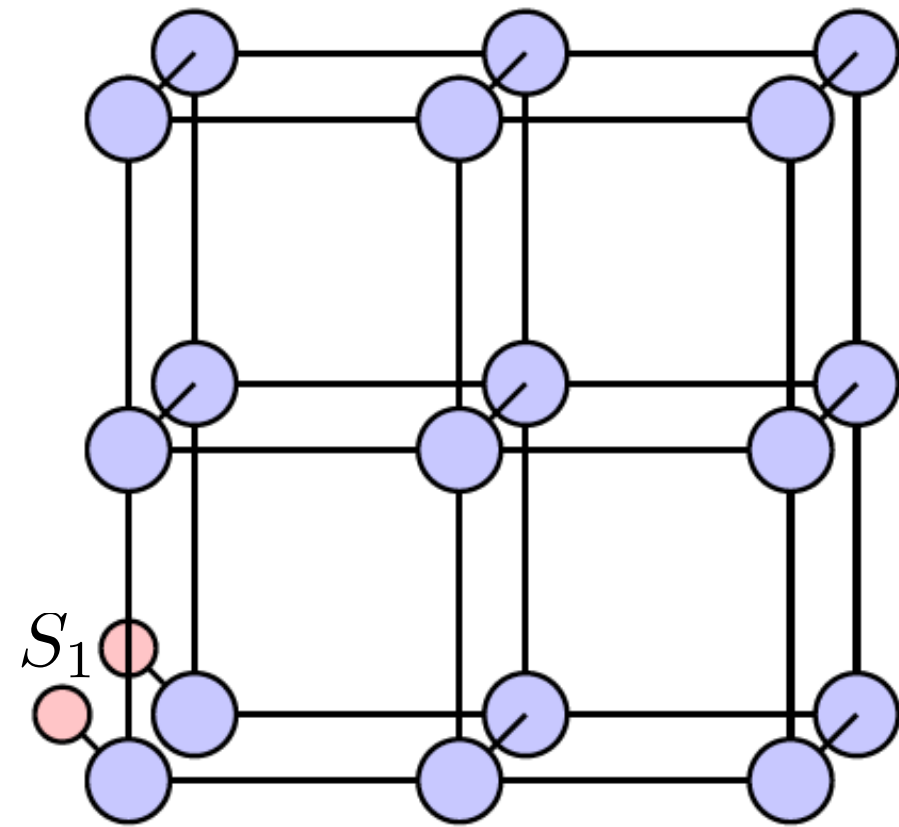
A Compute $\rho(S_1)$



$\rho(S_1)$

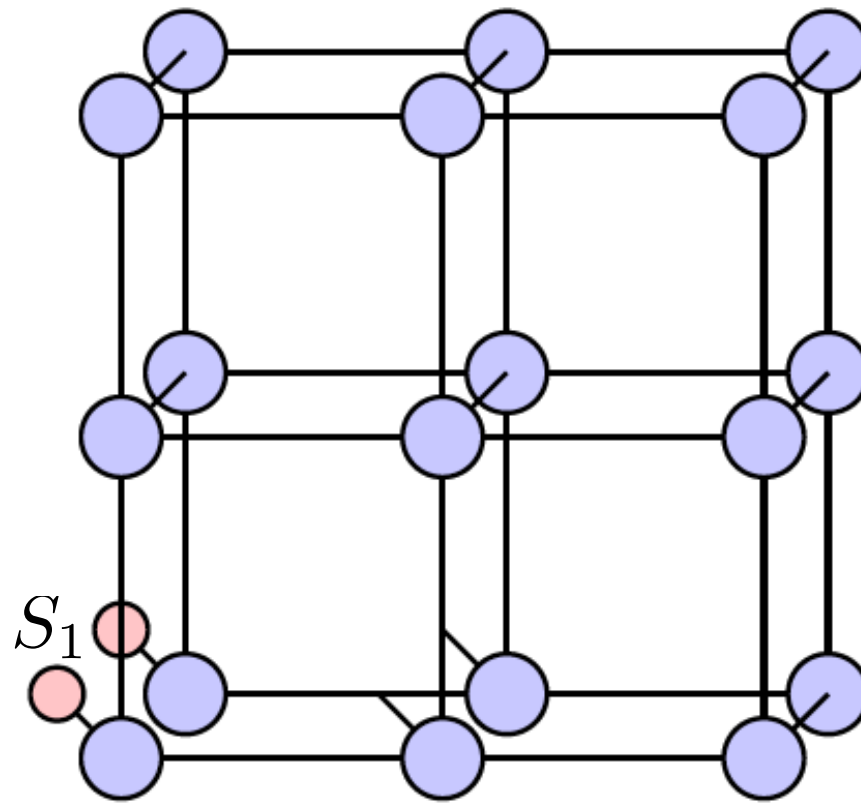
Vieijra, et al., PRB 104, 235141 ('21)

- A Compute $\rho(S_1)$
- B Sample S_1 accordingly



Vieijra, et al., PRB 104, 235141 ('21)

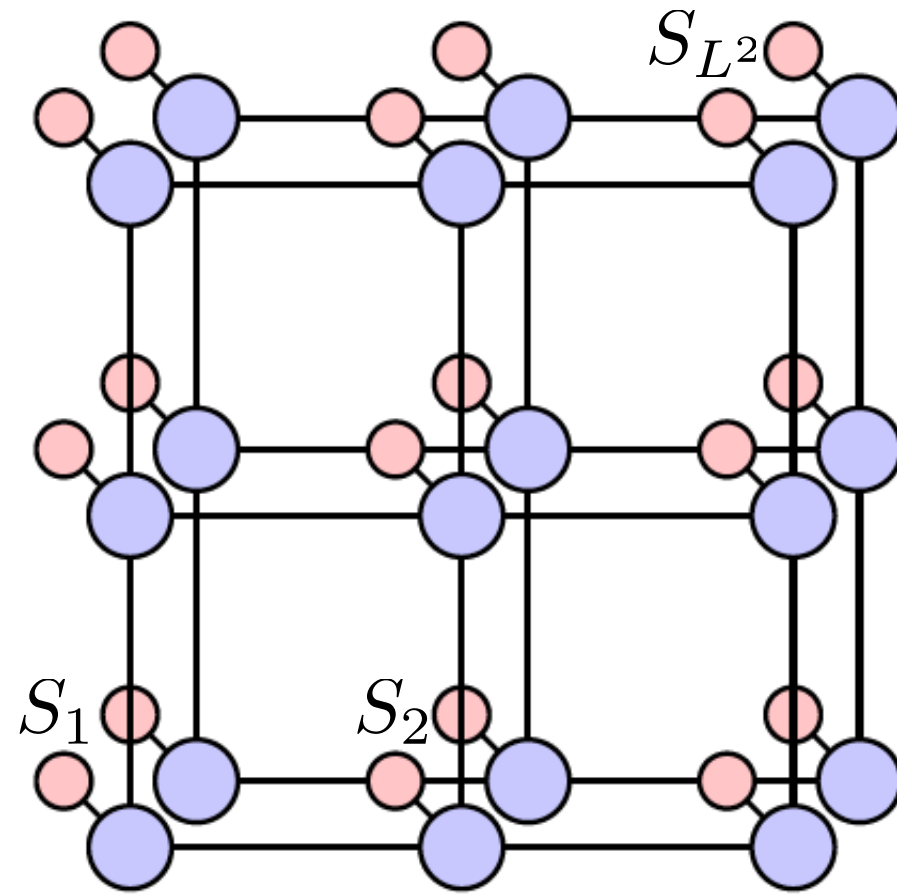
- A** Compute $\rho(S_1)$
- B** Sample S_1 accordingly
- C** Compute $\rho(S_2 | S_1)$



Vieijra, et al., PRB 104, 235141 ('21)

- A** Compute $\rho(S_1)$
- B** Sample S_1 accordingly
- C** Compute $\rho(S_2 | S_1)$
- D** Repeat until S_{L^2}

**No autocorrelation
& parallelizable !!!**



$\rho \implies$ (expensive) *double-layer* $\implies$ small χ' for getting a proxy p_c of p_ψ

$\psi(\mathbf{S}) \implies$ (cheaper) *single-layer* $\implies$ larger χ for more precise O & E^{loc}

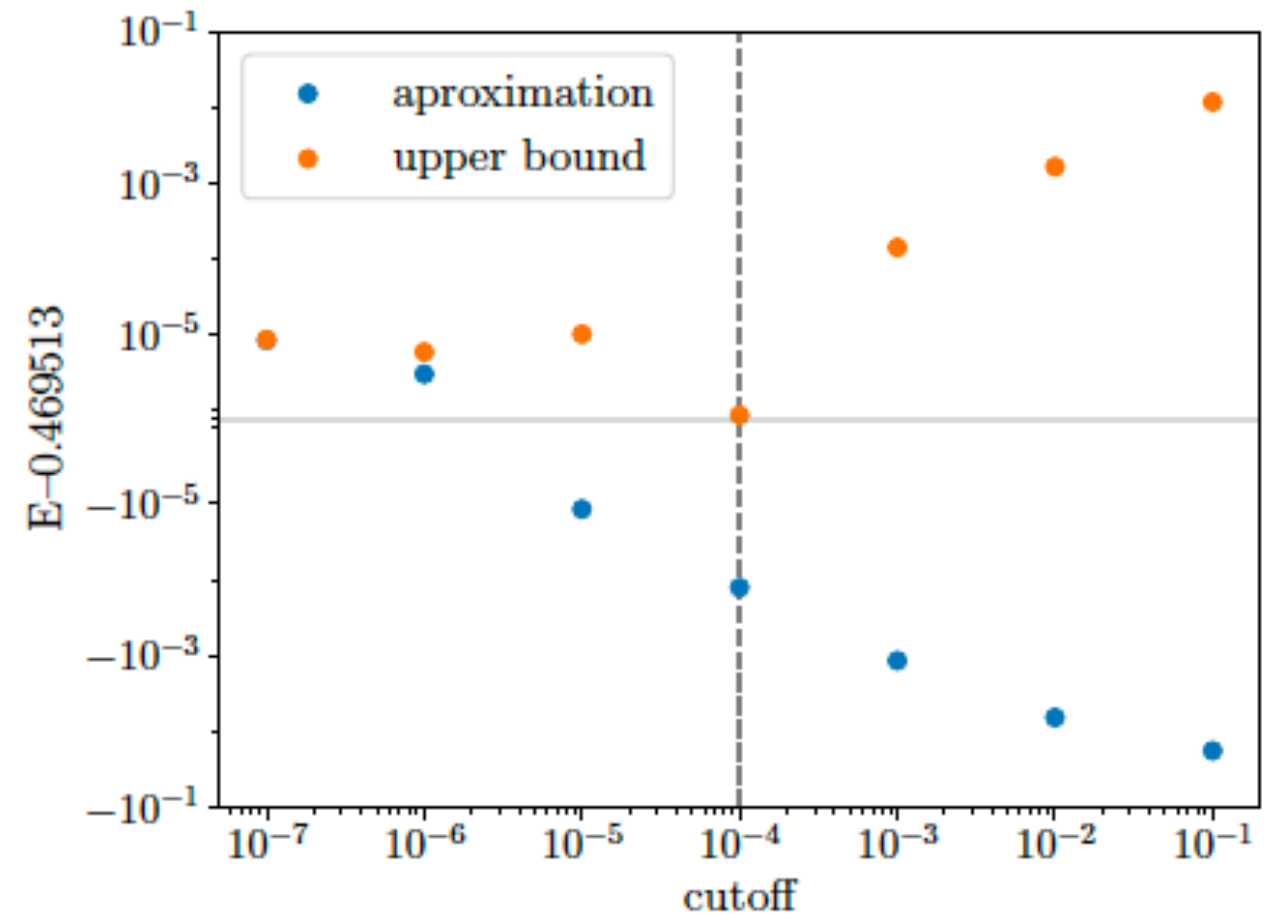
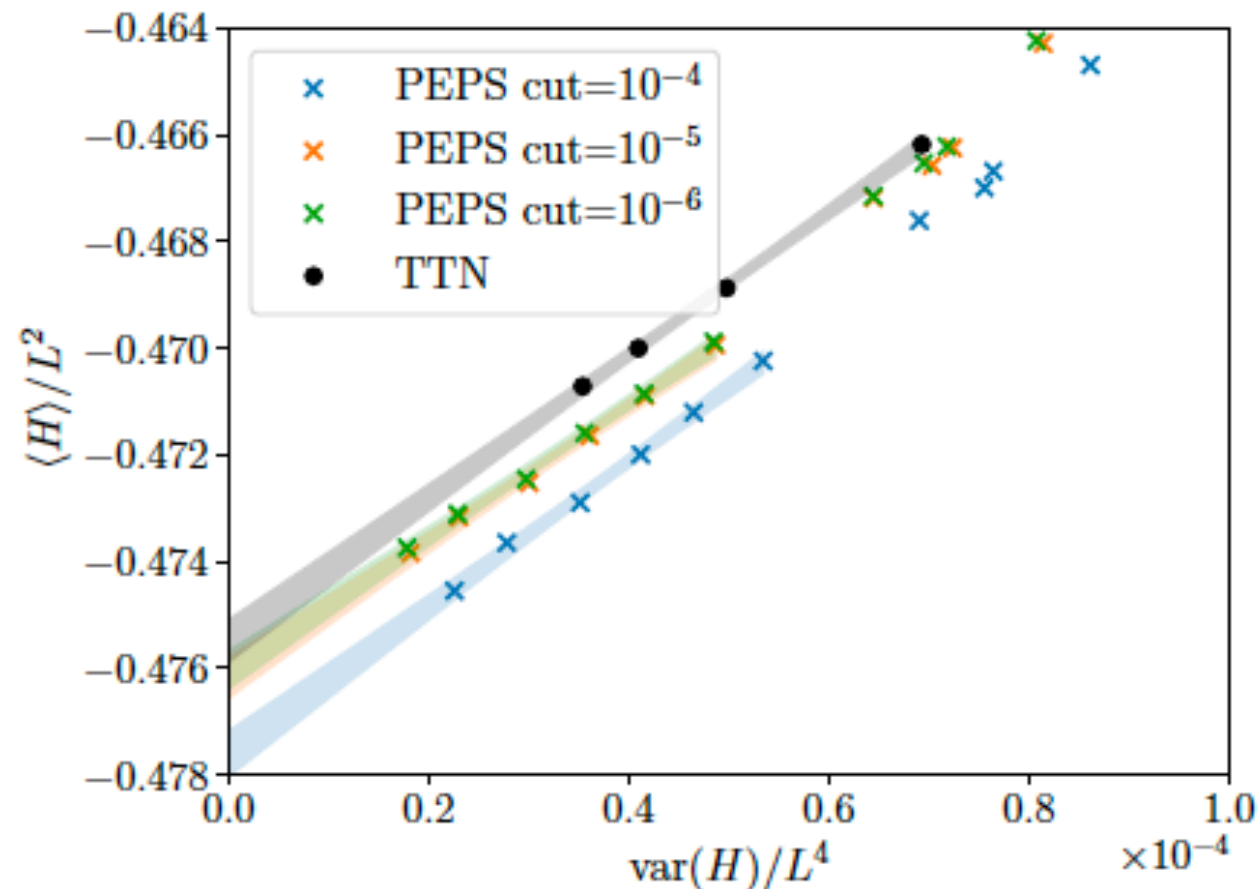
i.e., use importance weights: $\omega_{\mathbf{S}} \approx \frac{|\Psi(\mathbf{S})|^2 / p_c(\mathbf{S})}{\frac{1}{N} \sum_{\mathbf{S}' \sim p_c} \frac{|\Psi(\mathbf{S}')|^2}{p_c(\mathbf{S}')}}$

FINITE PEPS: ENERGY ESTIMATION

16

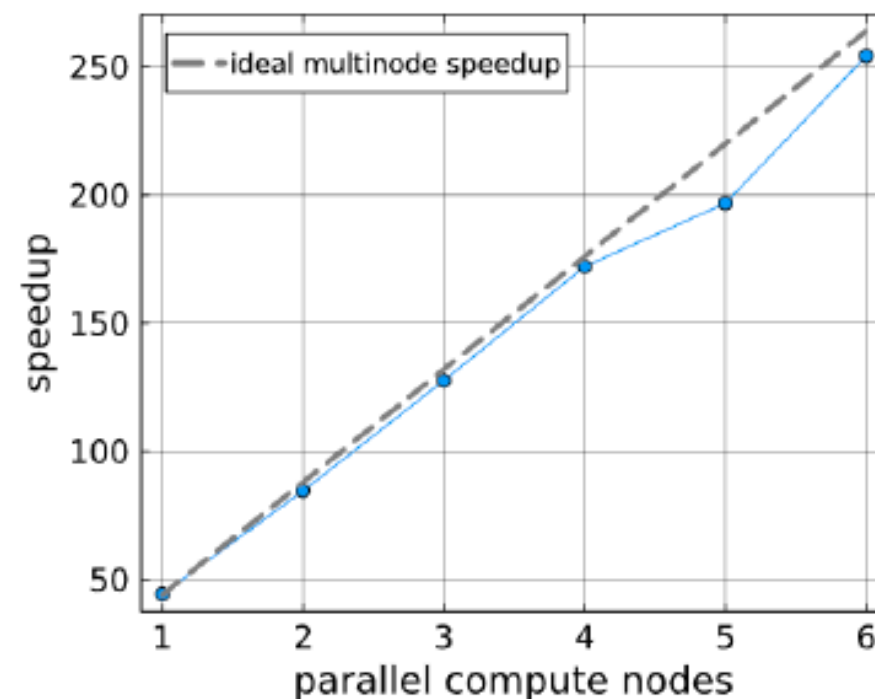
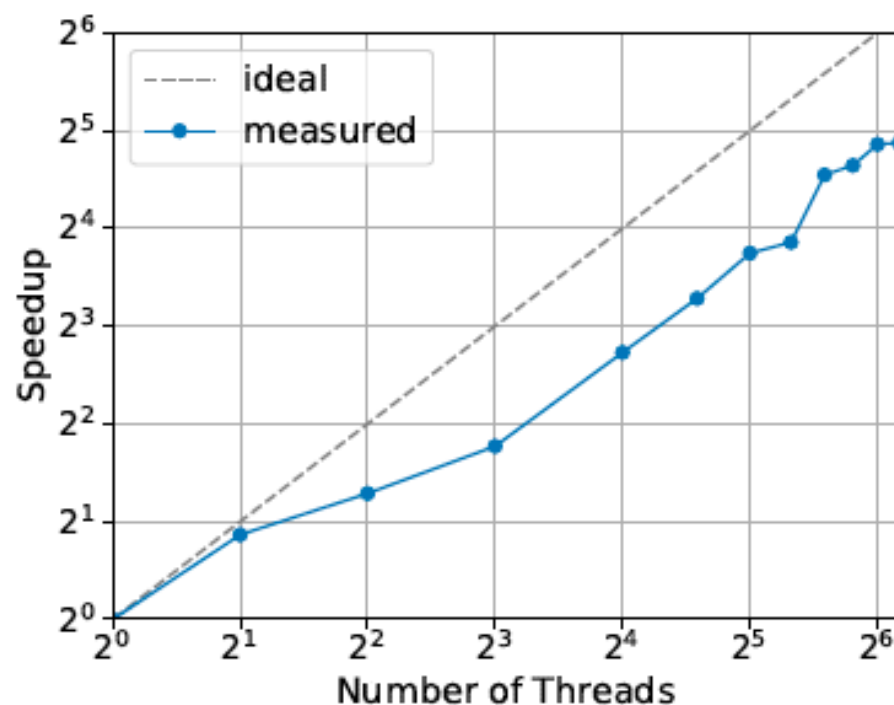
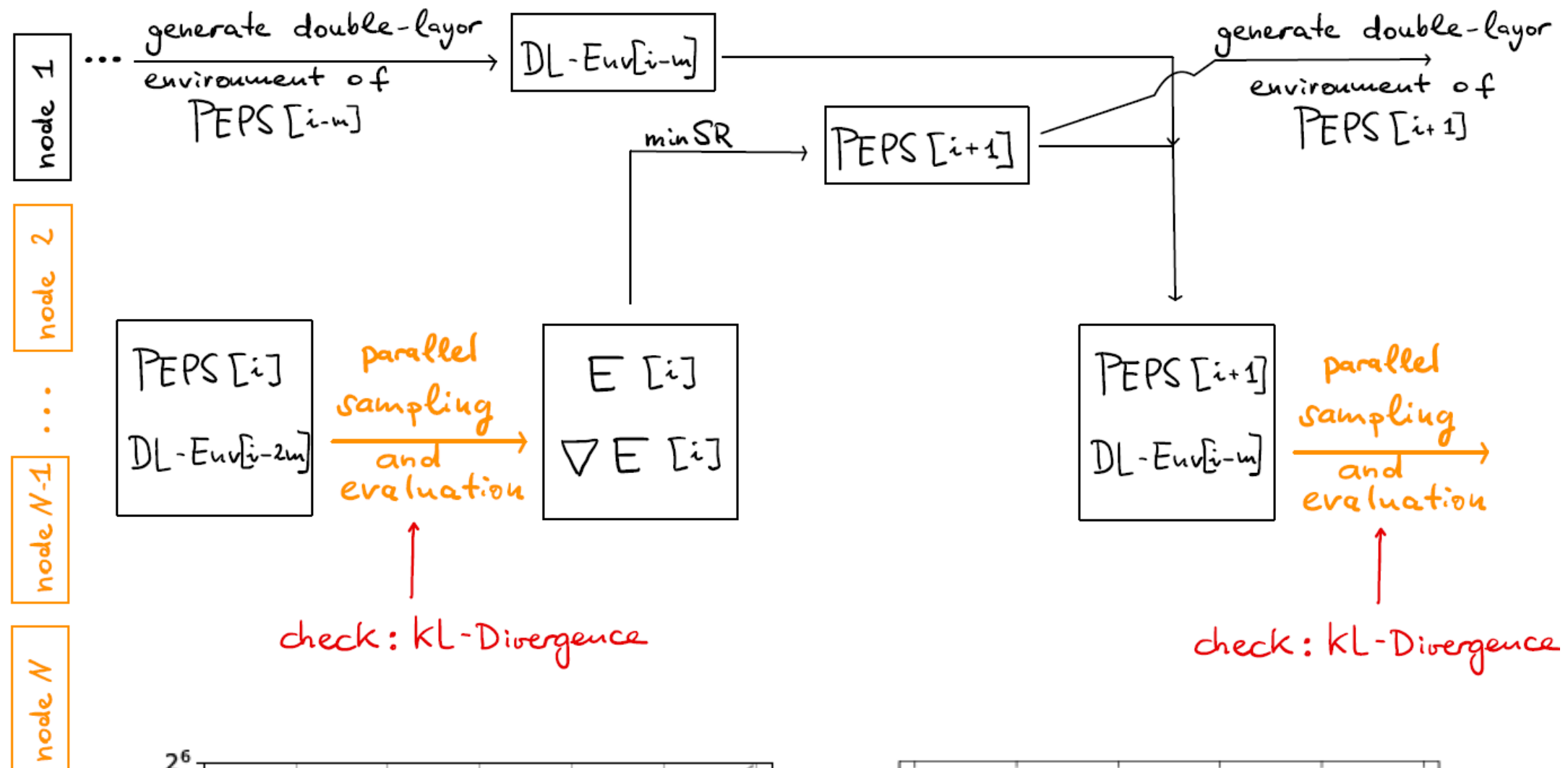
Alcalde Puente, et al. (MR), PRB 111, 195120 ('25)

possibility of defining
a strict bound on energy,
**avoiding the exploitation of
approximations for fake low energy**



**systematic extrapolation
against energy variance**

FINITE PEPS: PARALLELIZATION



FIRST BENCHMARKS

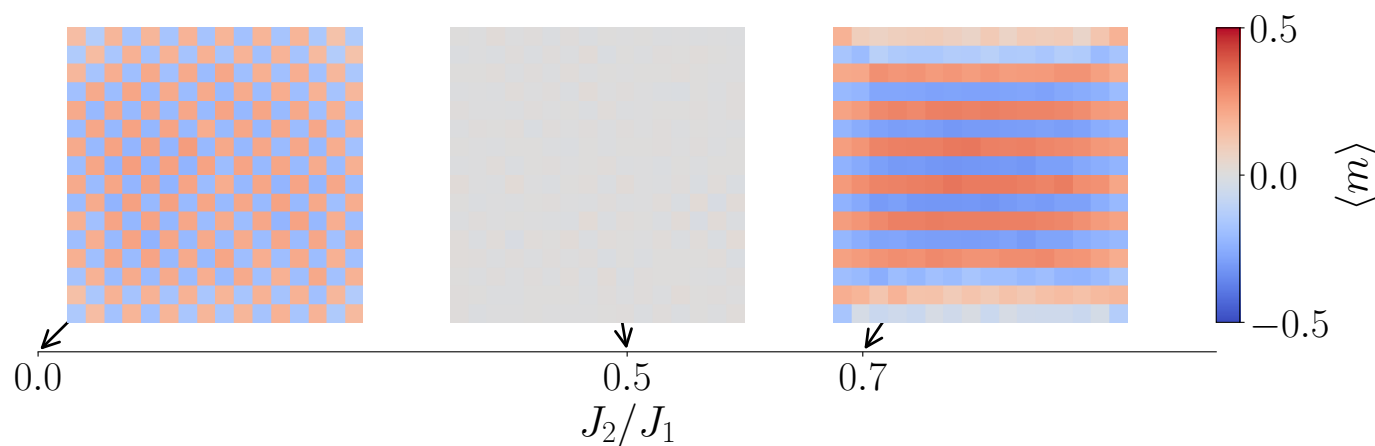
FINITE-PEPS: FIRST BENCHMARKS

19

Alcalde Puente, et al. (MR), PRB 111, 195120 ('25)

Frustrated $J_1 - J_2$ model on square lattice

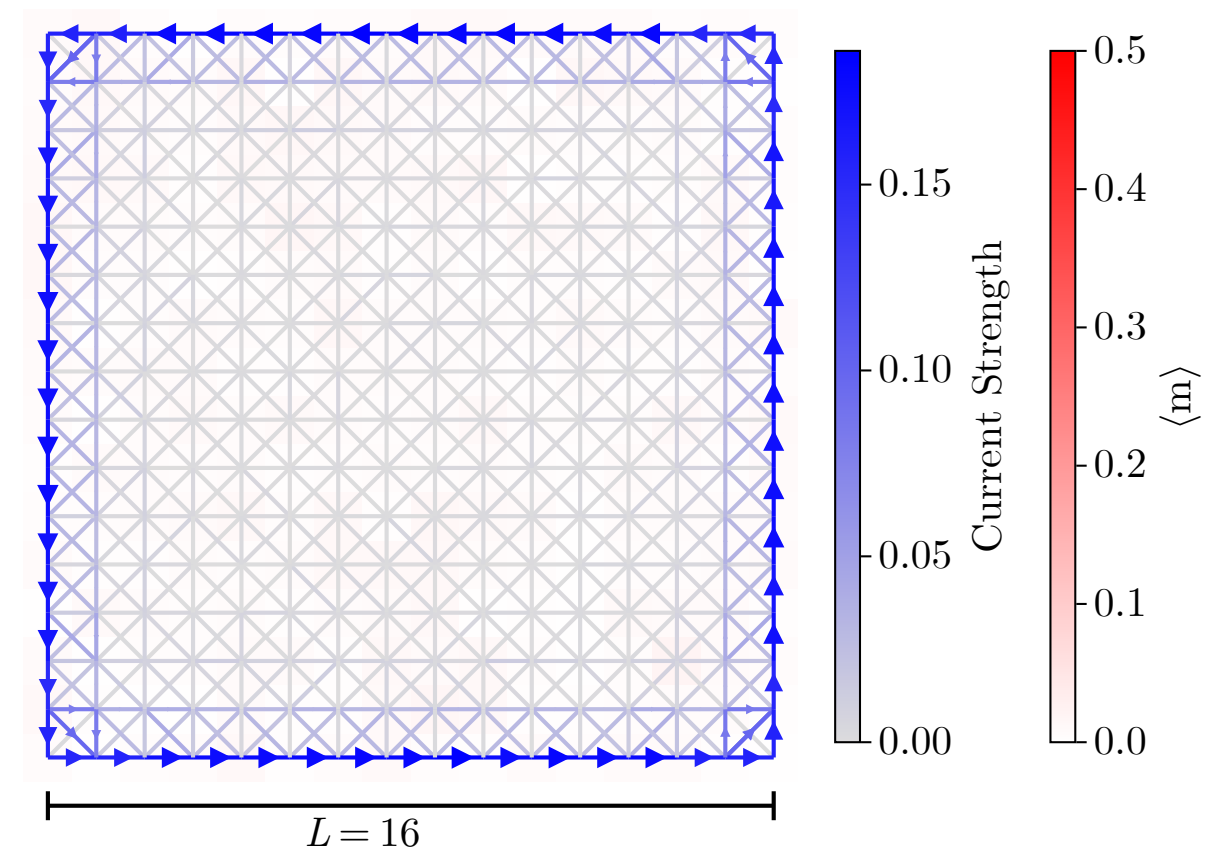
$$\hat{H}_{\text{frust}} = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$



Additional 4-body cyclic term to stabilise a **chiral spin liquid**

A.E. Nielsen et al. Nat. Comm. 4, 2864

$$\hat{H}_{\text{CSL}} = \hat{H}_{\text{frust}} + i\lambda \sum_{\square} (P_{ijkl} - P_{ijkl}^{-1})$$

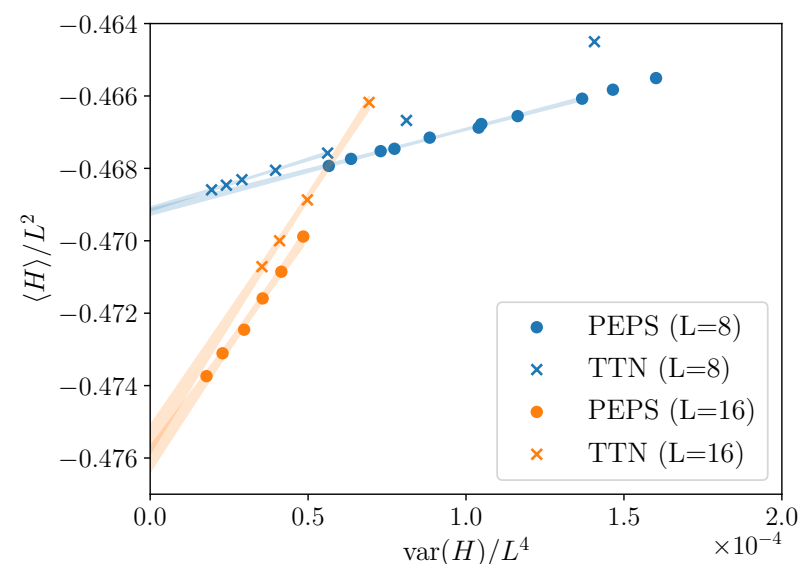


$$E = -0.9697 \pm 0.0005$$

$$E_{\text{bulk}} = -0.993 \pm 0.004$$

$$E_{\infty}^{\text{ex}} = -1$$

Systematic extrapolation of energy estimates & errors



FINITE-PEPS: FIRST BENCHMARKS

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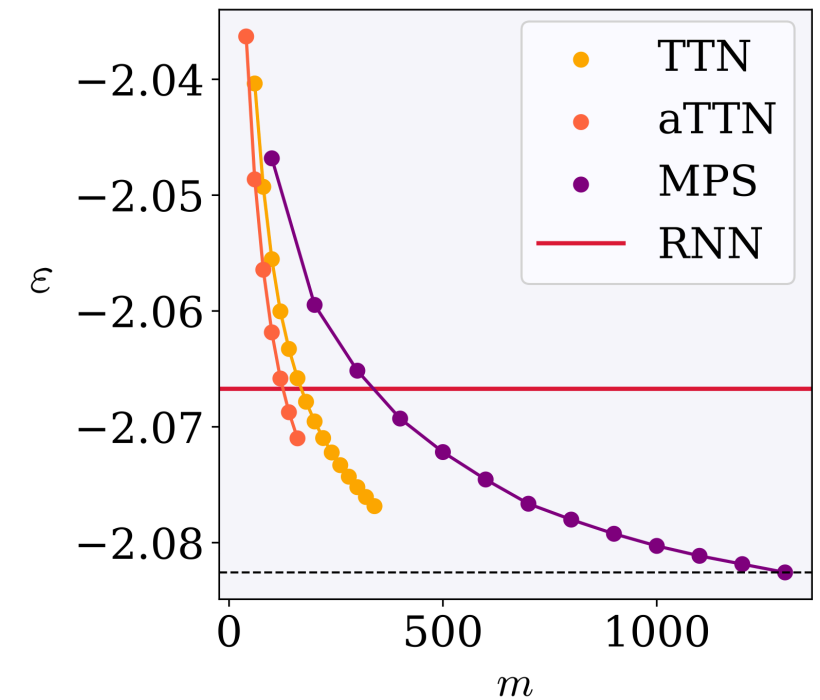
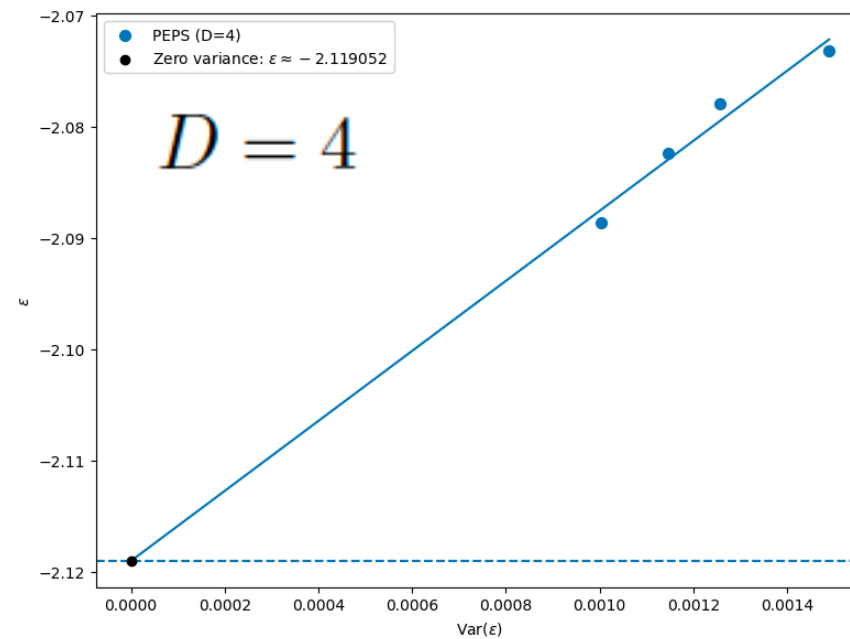
A. Dubey & MR (unpublished)

Antiferro Heisenberg model on triangular lattice (**Frustrated**)

$$L = 16,$$

$$\epsilon_{\text{PEPS}} = -2.0886 \pm 4 \times 10^{-4}$$

$$\epsilon_{\text{extrapolated}} = -2.119052$$

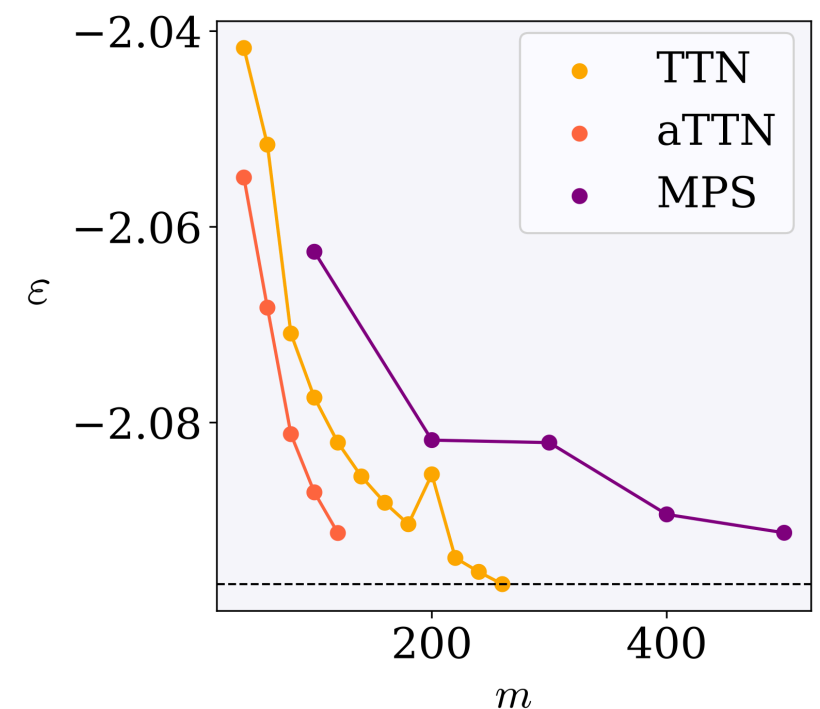
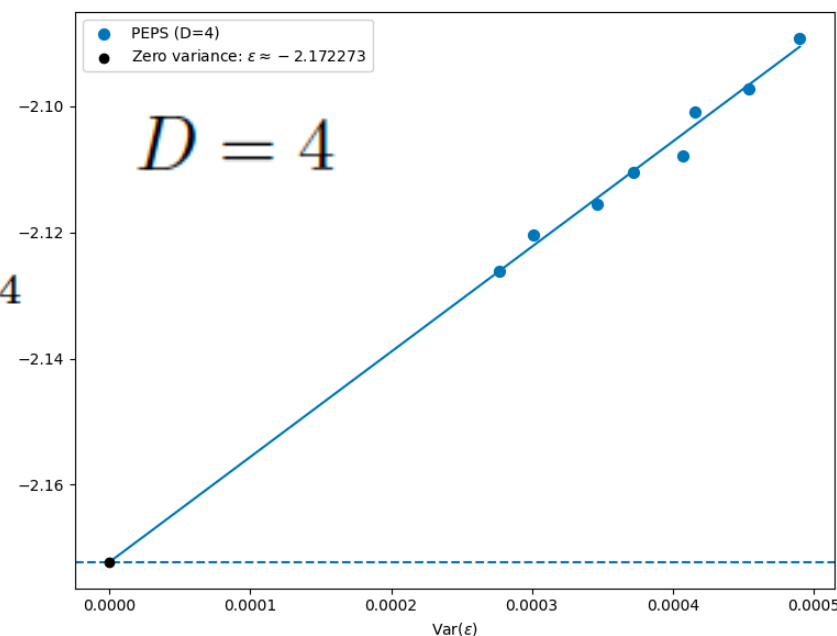


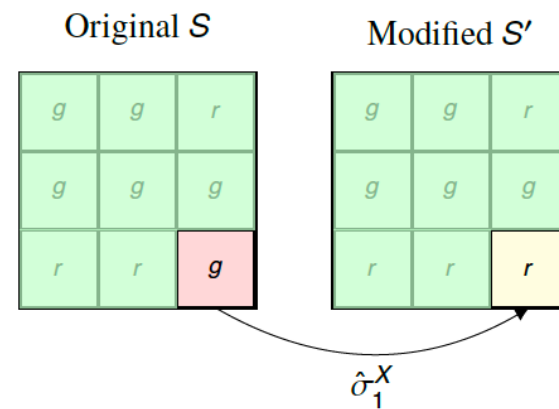
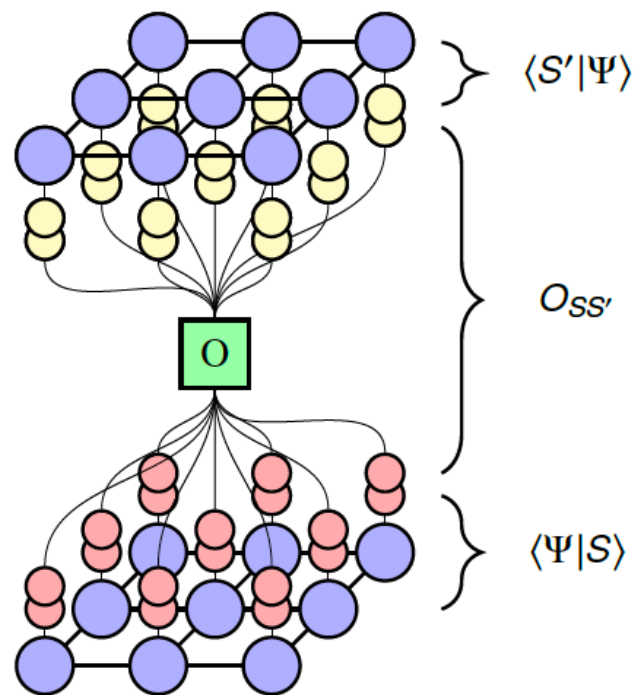
Reinić et al, arXiv:2507.21236v1

$$L = 32$$

$$\epsilon_{\text{PEPS}} = -2.1262 \pm 2 \times 10^{-4}$$

$$\epsilon_{\text{extrapolated}} = -2.172273$$



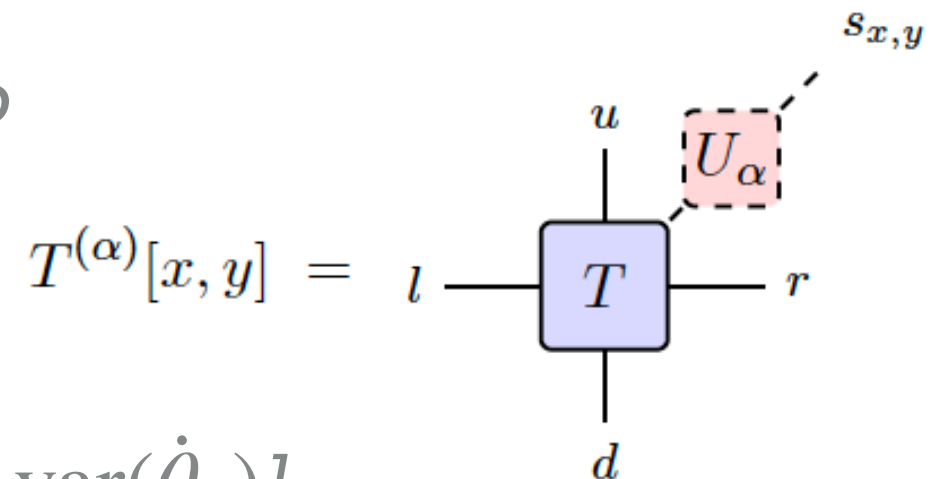


**Rydberg interactions
at no extra cost !!!**

$$\hat{H} = \frac{1}{2} \sum_i \sigma_i^x - \Delta \sum_i n_i + \sum_{i \neq j} \frac{1}{((\mathbf{r}_i - \mathbf{r}_j)/R_b)^6} n_i n_j$$

Other long-range terms by basis rotation, too

$$\hat{H}_{\alpha,\alpha} = \sum_{i < j} J_{\hat{d}}(i, j) U_{\alpha}^{\dagger} S_i^z S_j^z U_{\alpha} \quad \alpha \in \{x, y, z\}$$



[a bit more expensive sampling: $\text{var}(\dot{\theta}) = \sum_{\alpha} \text{var}(\dot{\theta}_{\alpha})$]

Long-range tails of the interaction are crucial for stability of phases!

FINITE-PEPS: RYDBERG ATOMS

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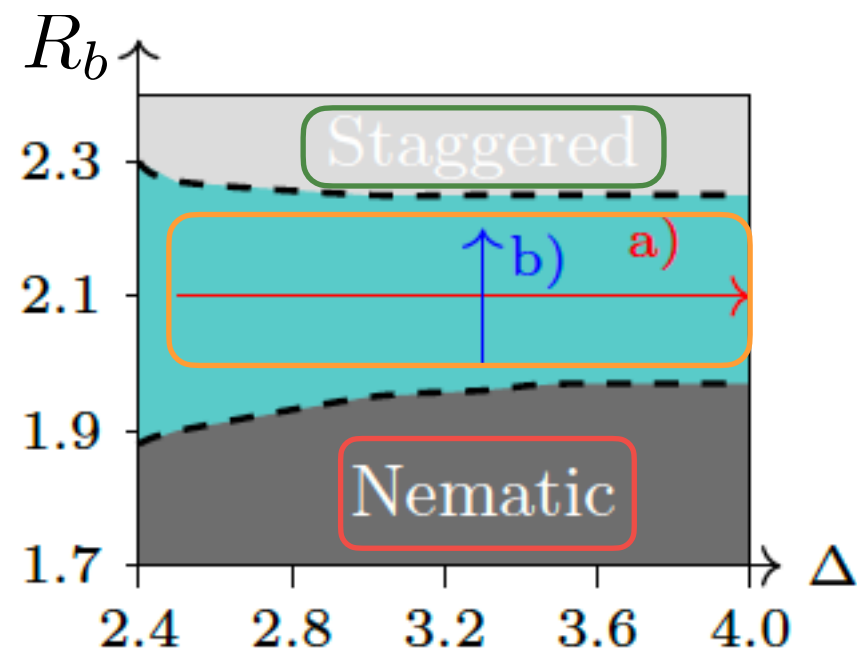
Schröder, Weerda, MR, in preparation

Long-range tails of the interaction are crucial for stability of phases!

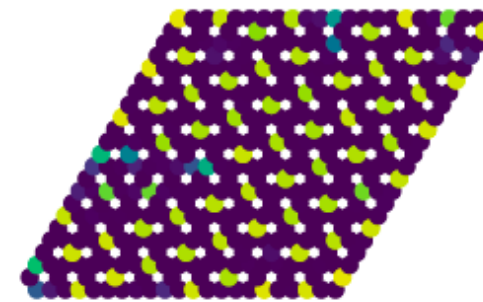
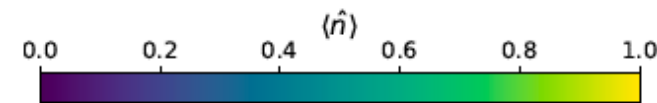
e.g., spin-glass on Kagome lattice!?

Yan et al., PRL 130, 206501 ('23)

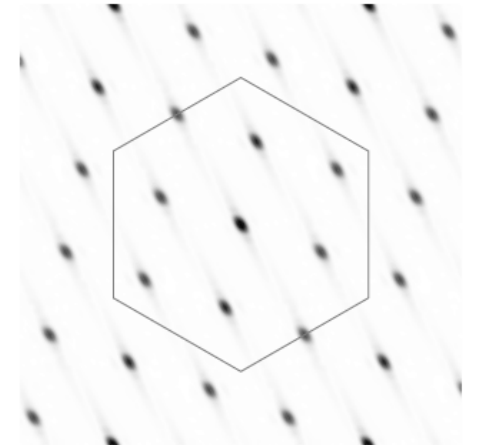
Hibat-Allah, et al., Comm. Ph. 8, 308 ('25)



real-space density



structure factor

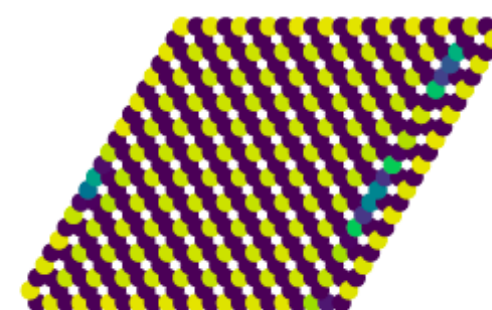
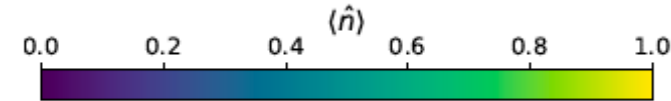


glassy or disordered?

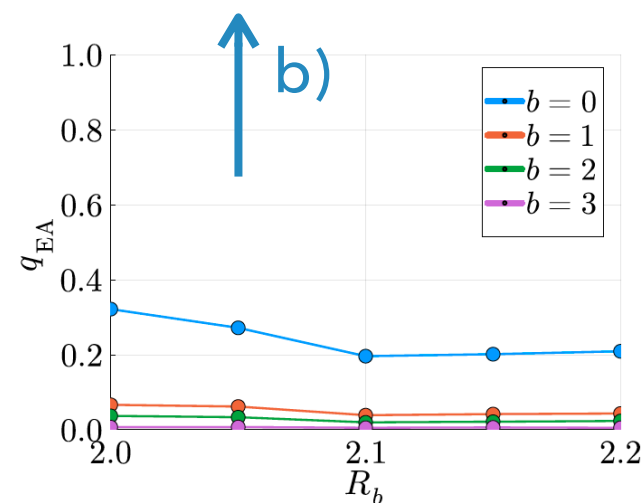
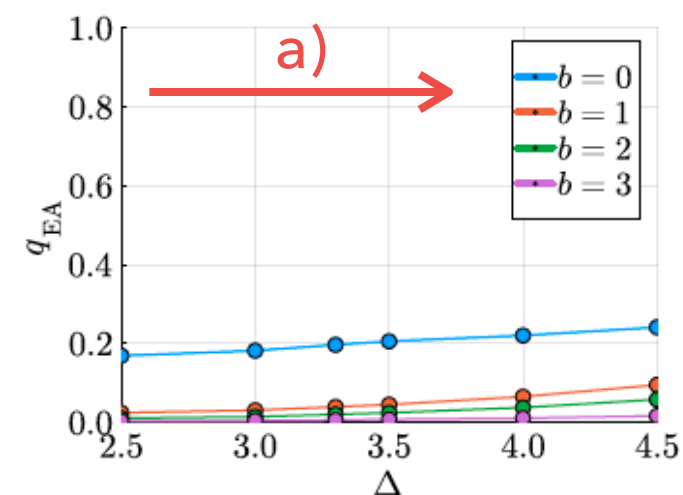
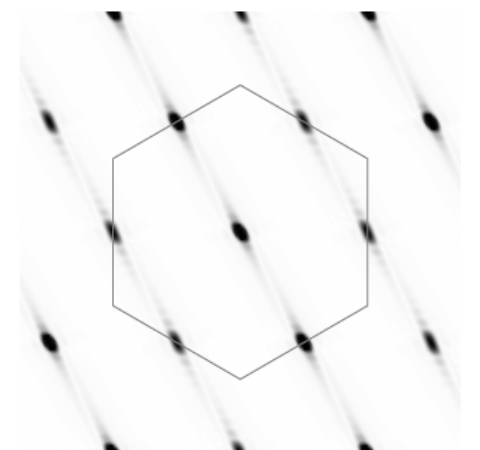
$$q_{\text{EA}} = \sum_{i=1}^N \frac{\langle \hat{n}_i - \rho \rangle^2}{N \rho (1 - \rho)}$$

$$\rho = \sum_{i=1}^N \frac{\langle \hat{n}_i \rangle}{N}$$

real-space density



structure factor



FINITE-PEPS: RYDBERG ATOMS

23

Schröder, Weerda, MR, in preparation

Long-range tails of the interaction are crucial for stability of phases!

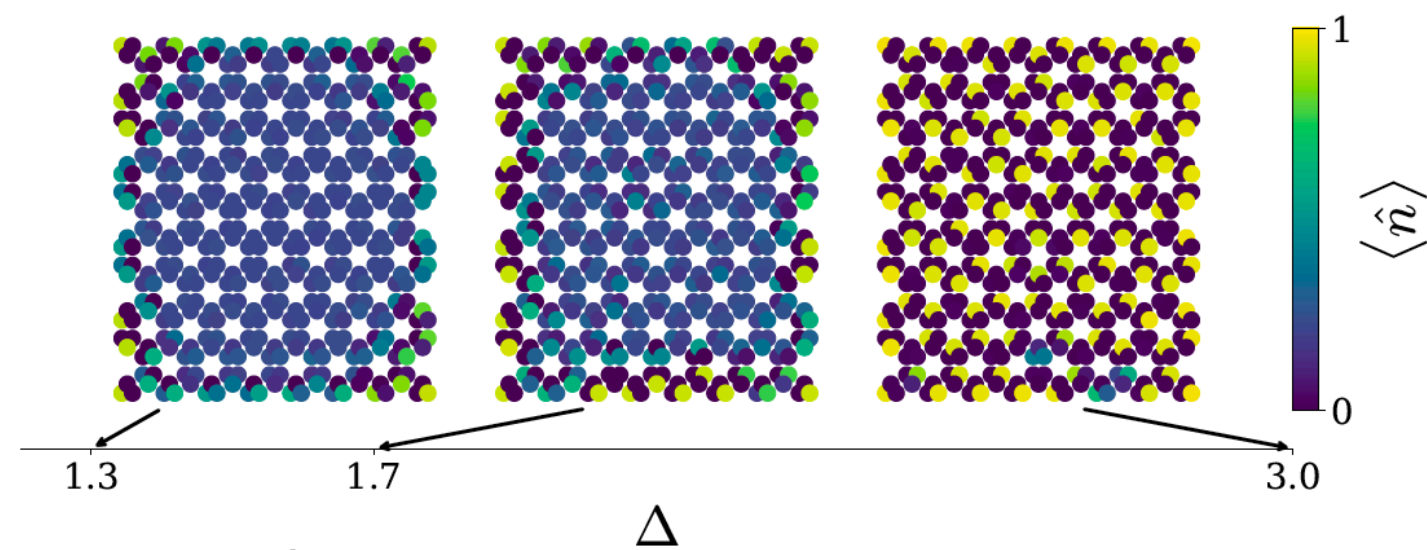
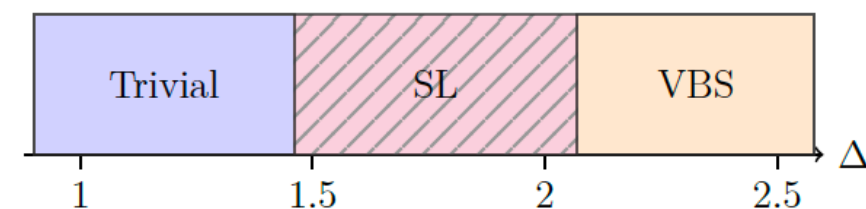
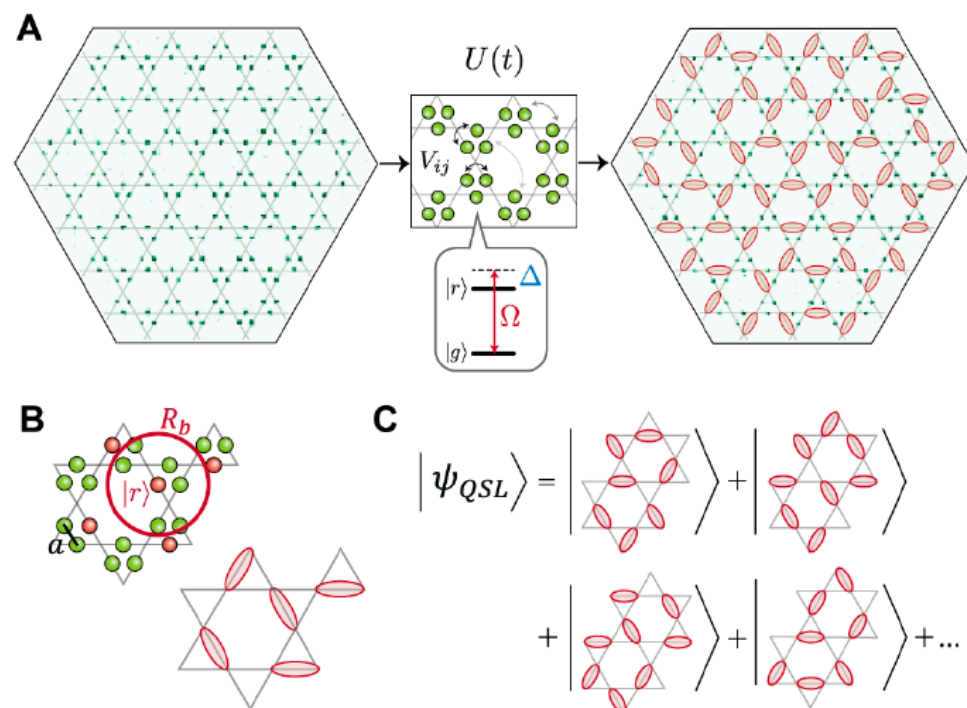
e.g., spin-liquid on Ruby lattice !?

Verresen et al. Phys. Rev. X 11, 031005 ('21)

Semeghini, et al., Science 374, 1242 ('21)

'PXP'-model

$$V(r) = \begin{cases} +\infty, & r \leq 2a \\ 0, & r > 2a \end{cases}$$



Fredenhagen-Marcu order params.
to detect anyon condensation

$$\hat{T}(\Gamma^*) = \prod_{i \in \Gamma^*} \hat{\sigma}_i^Z$$

$$\hat{W}(\Gamma) = \prod_{i \in \Gamma} \hat{\sigma}_i^X$$

$$W_{\text{FM}}(\Gamma) = \frac{\langle \hat{W}(\Gamma) \rangle}{\sqrt{|\langle \hat{W}(\tilde{\Gamma}) \rangle|}}, \dots$$

$$W_{\text{FM}} \neq 0$$

$$T_{\text{FM}} = 0$$

$$W_{\text{FM}} = T_{\text{FM}} = 0$$

$$W_{\text{FM}} = 0$$

$$T_{\text{FM}} \neq 0$$

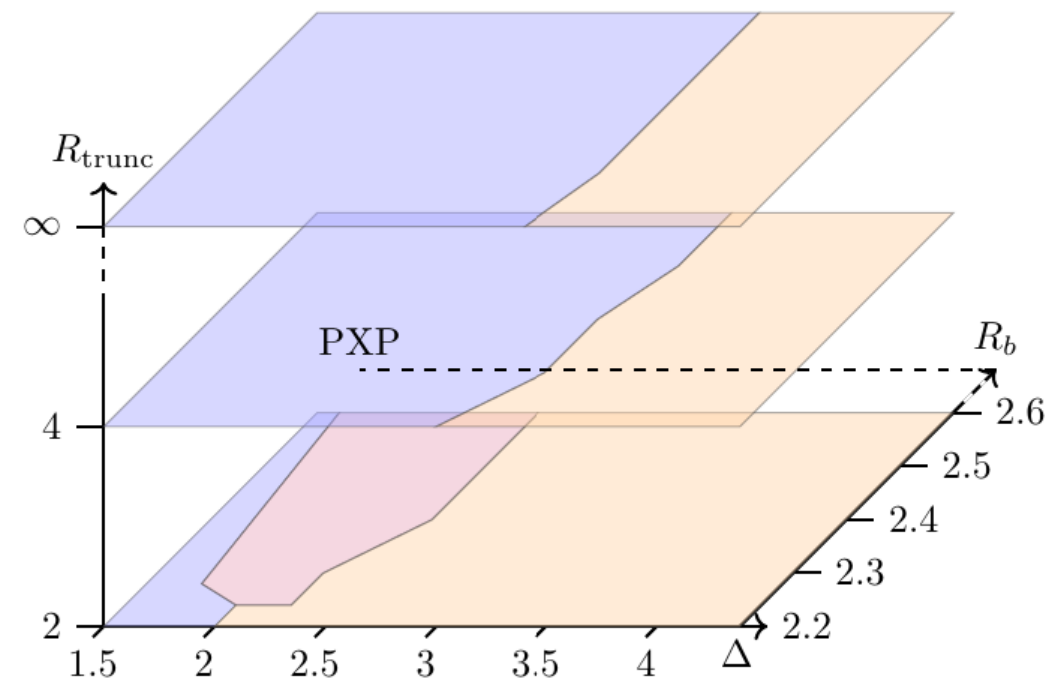
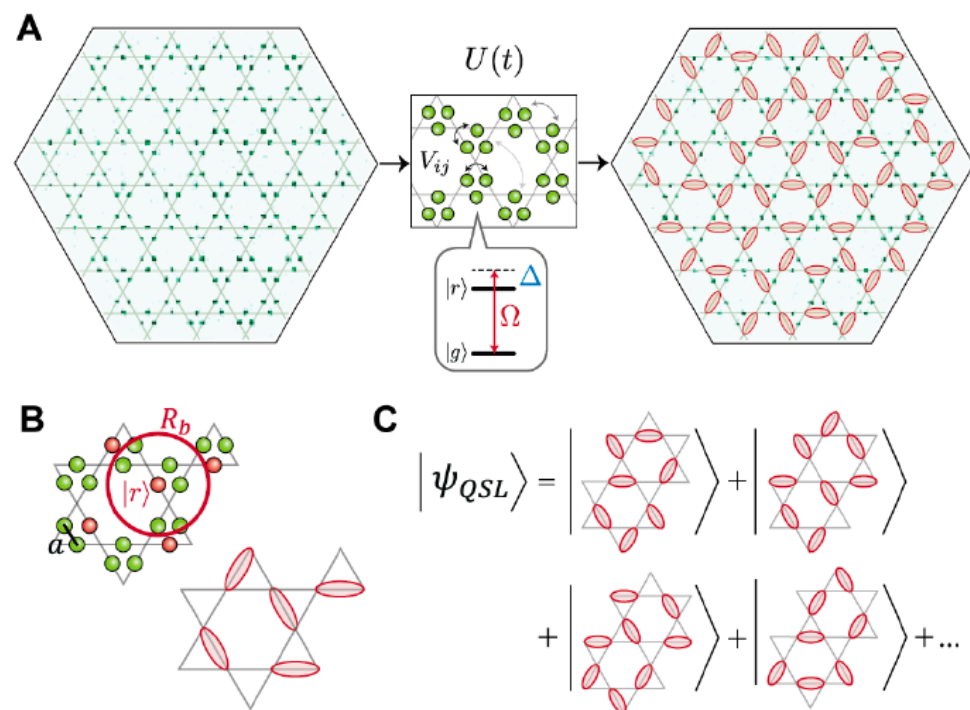
Schröder, Weerda, MR, in preparation

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Verresen et al. Phys. Rev. X 11, 031005 ('21)

Semeghini, et al., Science 374, 1242 ('21)

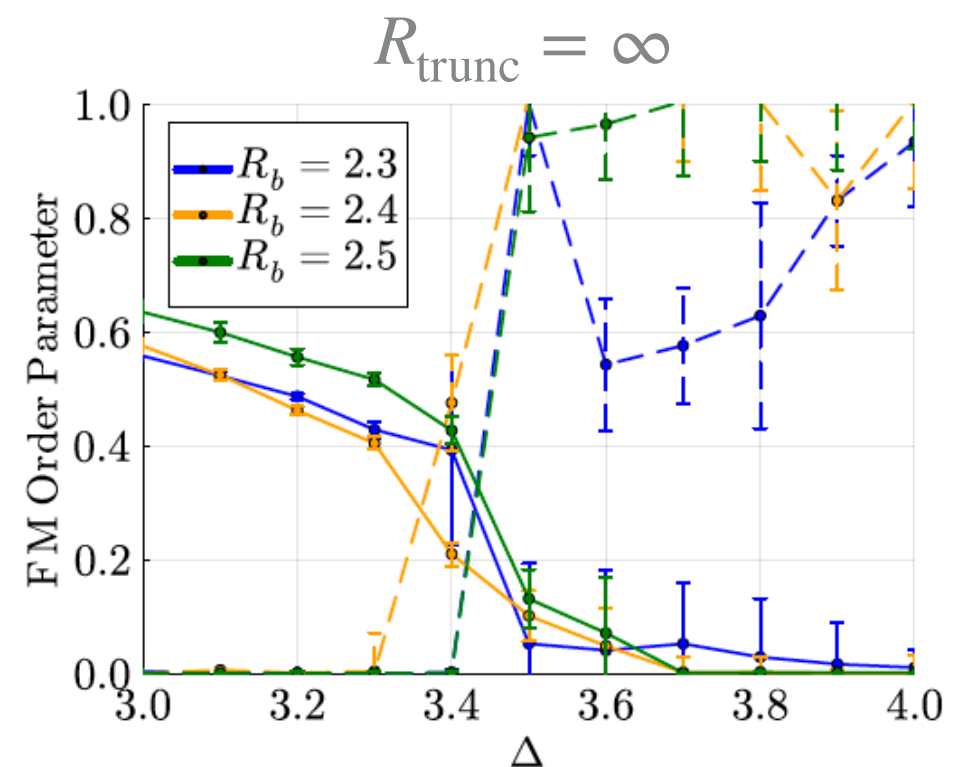


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$$W_{\text{FM}}(\Gamma) = \frac{\langle \hat{W}(\Gamma) \rangle}{\sqrt{|\langle \hat{W}(\tilde{\Gamma}) \rangle|}}; \dots$$



EXPLORING PHASE DIAGRAMS WITH REDUCED BASIS METHODS

PHASE DIAGRAMS VIA REDUCED BASIS

25

Brehmer, Herbst, Wessel, **MR**, Stamm, PRE 105, 045303 ('22) & 108, 025306 ('23)

i) Hamiltonian depends on few parameters $\mu \in \mathbb{P}$ $\hat{H}(\mu) = \sum_{q=1}^Q \theta_q(\mu) \hat{H}_q$



extensive scans via “snapshots”: very expensive!

ii) # phases $\ll$ # points in parameter space

iii) inside each phase, states are similar!



is it possible to reconstruct phase diagrams
from a few expensive snapshots (e.g., PEPS)
via some smart interpolation strategy?



YES! via “Reduced **B**asis” (surrogate) methods
extensive literature in applied math (also for PDE solutions)

PHASE DIAGRAMS VIA REDUCED BASIS

26

Brehmer, Herbst, Wessel, **MR**, Stamm, PRE 105, 045303 ('22) & 108, 025306 ('23)

affine decomposition in few terms

$\mu \in \mathbb{P} \equiv$ parameter space

$$\hat{H}(\mu) = \sum_{q=1}^Q \theta_q(\mu) \hat{H}_q$$

$$\hat{O}(\mu; p) = \sum_{r=1}^R \alpha_r(\mu; p) \hat{O}_r$$

Reduced **B**asis of few "snapshots"

$$N := \dim \mathbb{V}_n \leq M := \sum_{j=1}^n m_j$$

$$\mathbb{V}_n := \text{span}\{|\Psi(\mu_1)\rangle, \dots, |\Psi(\mu_n)\rangle\}$$

$$\hat{H}(\mu_j) |\Psi(\mu_j)\rangle = E(\mu_j) |\Psi(\mu_j)\rangle \quad \forall j$$

Rayleigh-Ritz Variational Ansatz
over "training grid"

$$|\Phi_{\text{RB}}(\mu)\rangle = \arg \min_{|\Phi\rangle \in \mathbb{V}_n} \frac{\langle \Phi | \hat{H}(\mu) | \Phi \rangle}{\langle \Phi | \Phi \rangle}, \quad \forall \mu \in \Xi_{\text{train}}$$

$$|\Phi_{\text{RB}}(\mu)\rangle = B \varphi_{\text{RB}}(\mu) \\ B: \mathbb{V}_n \rightarrow \mathcal{H}$$

$$b = B^\dagger B$$

$$h(\mu) = \sum_{q=1}^Q \theta_q(\mu) B^\dagger \hat{H}_q B$$

effective eigenvalue problem

$$h(\mu) \varphi_{\text{RB}}(\mu) = E_{\text{RB}}(\mu) b \varphi_{\text{RB}}(\mu)$$

"greedy" search for new snapshots
based on some "error estimator"

$$\mu_{n+1} = \arg \max_{\mu \in \Xi_{\text{train}}} \text{Err}_n(\mu)$$

- ✓ affine decomposition in few terms?
almost all Hamiltonian models of interest :-)

- ✓ efficient overlap between snapshots?

“dual” sampling

X. Waintal et al., unpublished

$$\langle \phi | \psi \rangle = \sqrt{\langle \tilde{\phi} \rangle_{\psi} \langle \tilde{\psi} \rangle_{\phi}} \exp \left(i \arg \langle \tilde{\psi} \rangle_{\phi} \right)$$

$$\tilde{\psi}(s) := \psi(s) / \phi(s) \quad \tilde{\phi}(s) := \phi(s) / \psi(s)$$

- ✓ efficient error estimator?

~~$$\text{Res}_n(\boldsymbol{\mu}) := \left\| \hat{H}(\boldsymbol{\mu}) |\Phi_{\text{RB}}(\boldsymbol{\mu})\rangle - E_{\text{RB}}(\boldsymbol{\mu}) |\Phi_{\text{rb}}(\boldsymbol{\mu})\rangle \right\|$$~~

“residual” perfect for 1D,
but too expensive in 2D

$$\Delta_n(\boldsymbol{\mu}) := \left\| \varphi_{\text{RB}}(\boldsymbol{\mu}) \right\|_{\ell^1}$$

Lebesgue function indicator:
only looser bounds,
but cheaper and reliable

Y. Chen, J. Jiang, A. Narayan,
Comp. Math. w. App. 77.7, 1963 (2019)

FINITE-PEPS + REDUCED BASIS

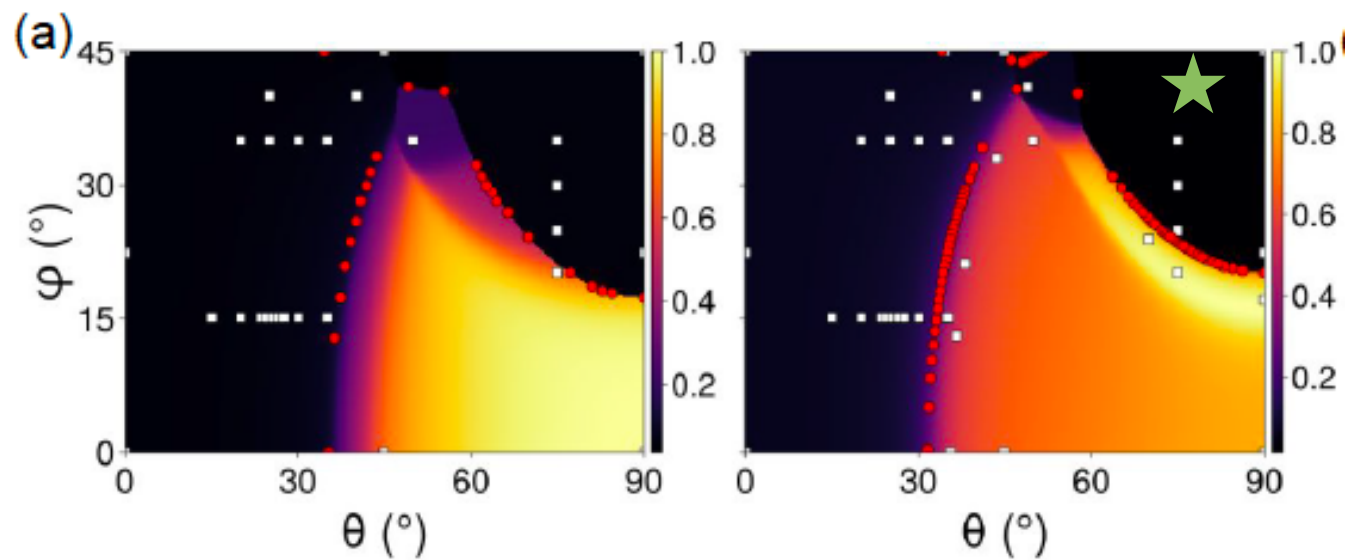
28

Spin-1/2 dipolar XXZ (e.g., NV centers) Dubey, Dannenfeld, **MR**, et al., in preparation

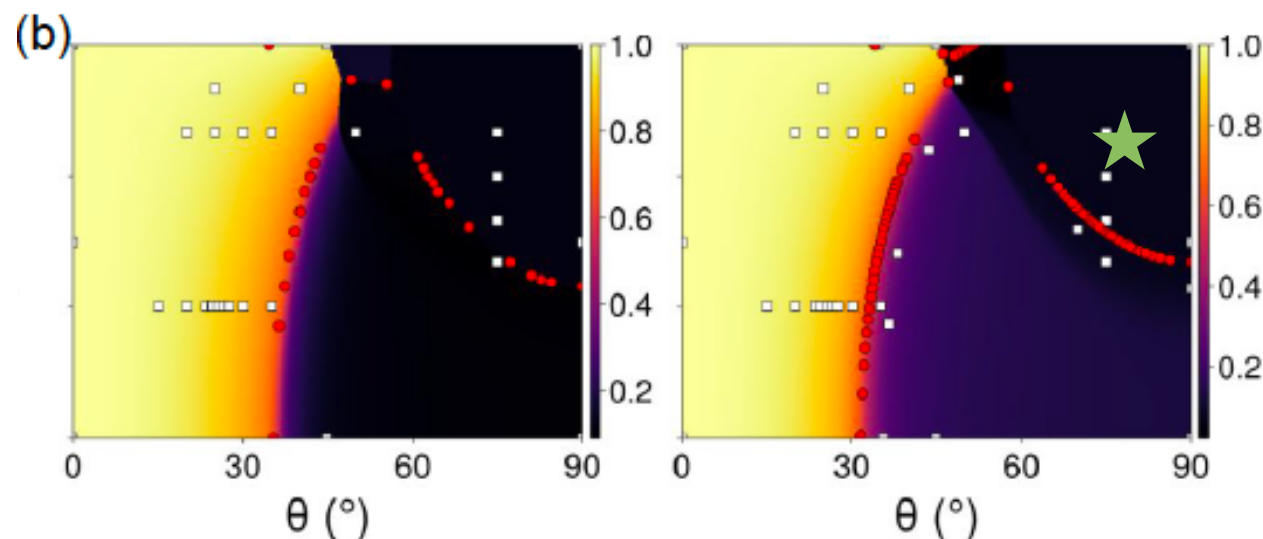
$$\hat{H} = \sum_{i < j} J_{\hat{d}}(i, j) \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \Delta \hat{S}_i^z \hat{S}_j^z \right) \quad J_{\hat{d}}(i, j) = J[1 - 3(\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{d}})^2]/|\mathbf{r}_{ij}|^3$$

Phase diagram via structure factor

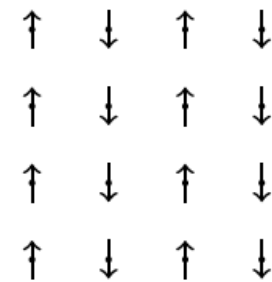
$$\mathcal{S}(\mathbf{k}) = \frac{1}{(L_x L_y)^2} \sum_{i, j} e^{-i\mathbf{k} \cdot \mathbf{r}_{ij}} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j.$$



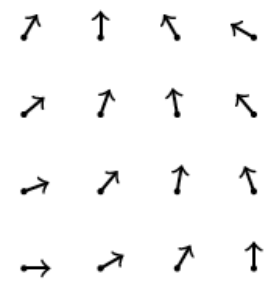
increasing N



$$\mathcal{S}(\pi, 0)$$

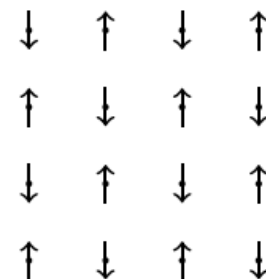


Stripe

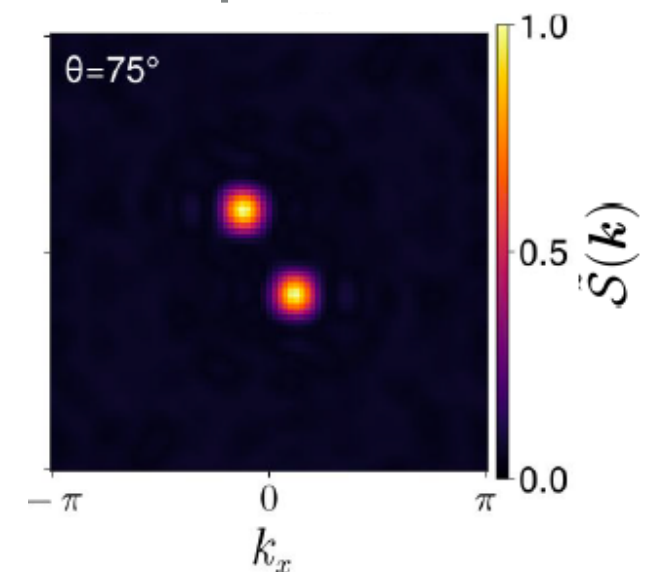


★ Spiral

$$\mathcal{S}(\pi, \pi)$$



Néel



OUTLOOK ON REAL-TIME DYNAMICS

~~Imaginary~~ **TDVP** (a.k.a. **natural gradient**) for N_P param. θ (tensor entries)
Real

$$|\dot{\Psi}(\theta)\rangle = -\dot{\mathbf{i}}H|\Psi(\theta)\rangle \longrightarrow \sum_i \underbrace{\frac{\partial \langle S|\Psi(\theta)\rangle}{\partial \theta_i}}_{\tilde{O}_{S,i}} \dot{\theta}_i = -\underbrace{\dot{\mathbf{i}}\langle S|H|\Psi(\theta)\rangle}_{\tilde{E}_S^{\text{loc}}}, \quad \forall S \in \mathcal{H}$$

Schmitt, Heyl,
PRL 125, 100503 ('20)
& many more!

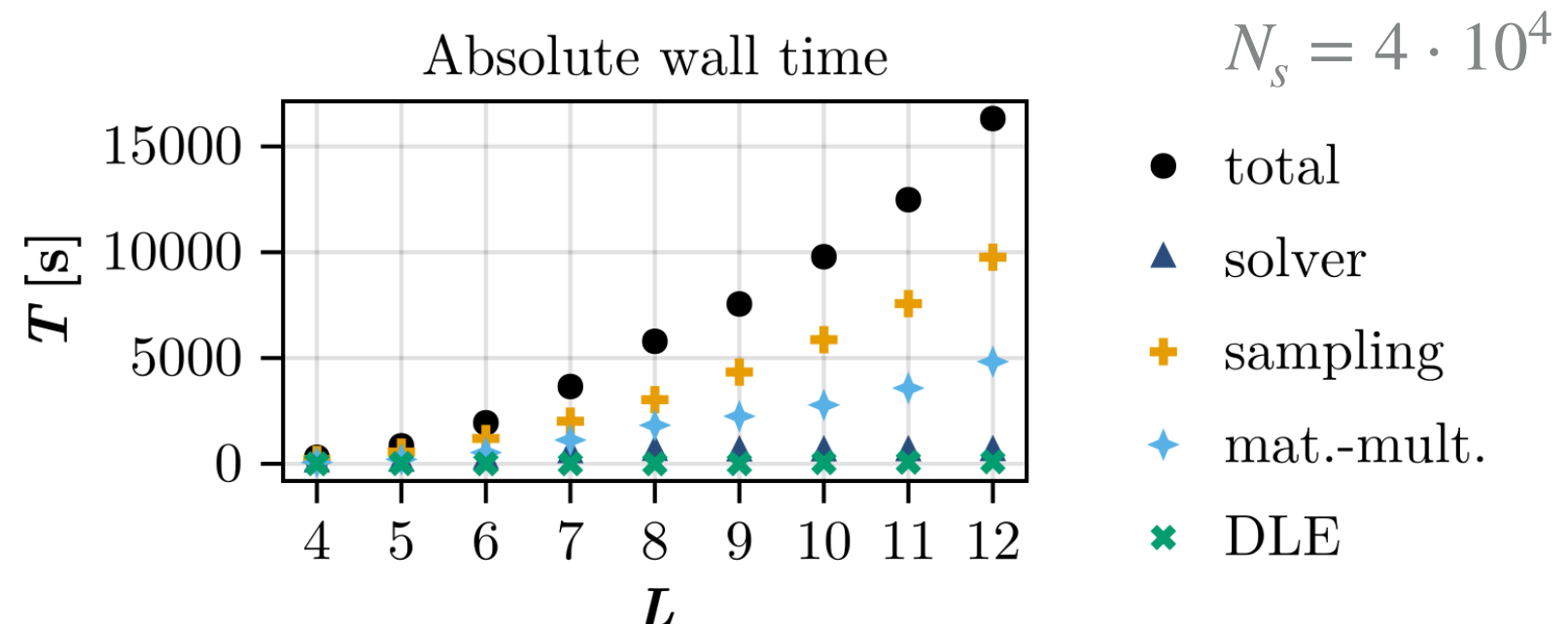
NQS use this for real-time evolution...

...why don't we try for finite-PEPS as well?

Y. Wu, J. Nys, arXiv.2512.06768
previous talk :-)



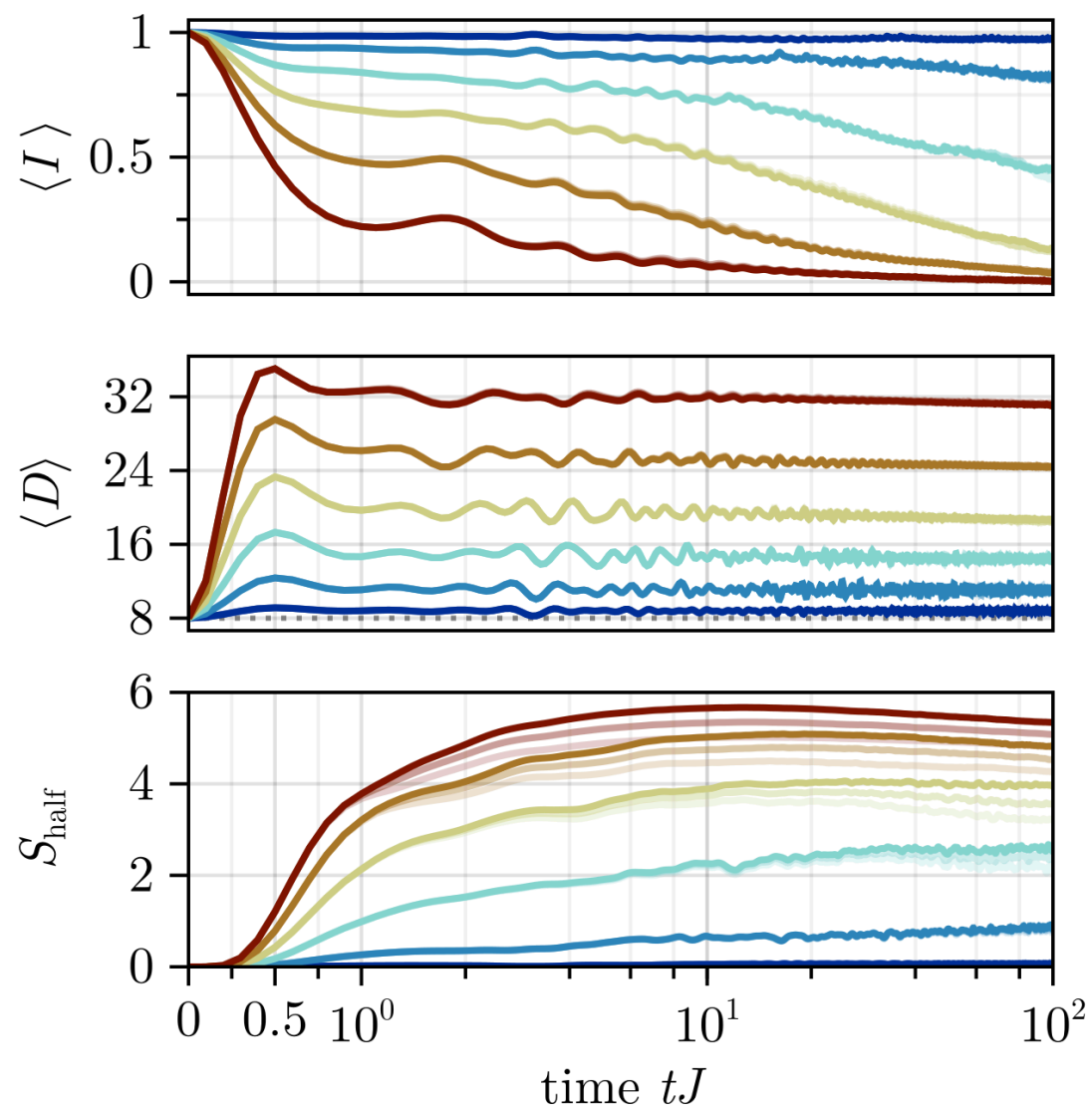
More sampling needed
to get reliable gradients
*(imaginary evolution is
way more permissive...)*



FINITE-PEPS & REAL DYNAMICS

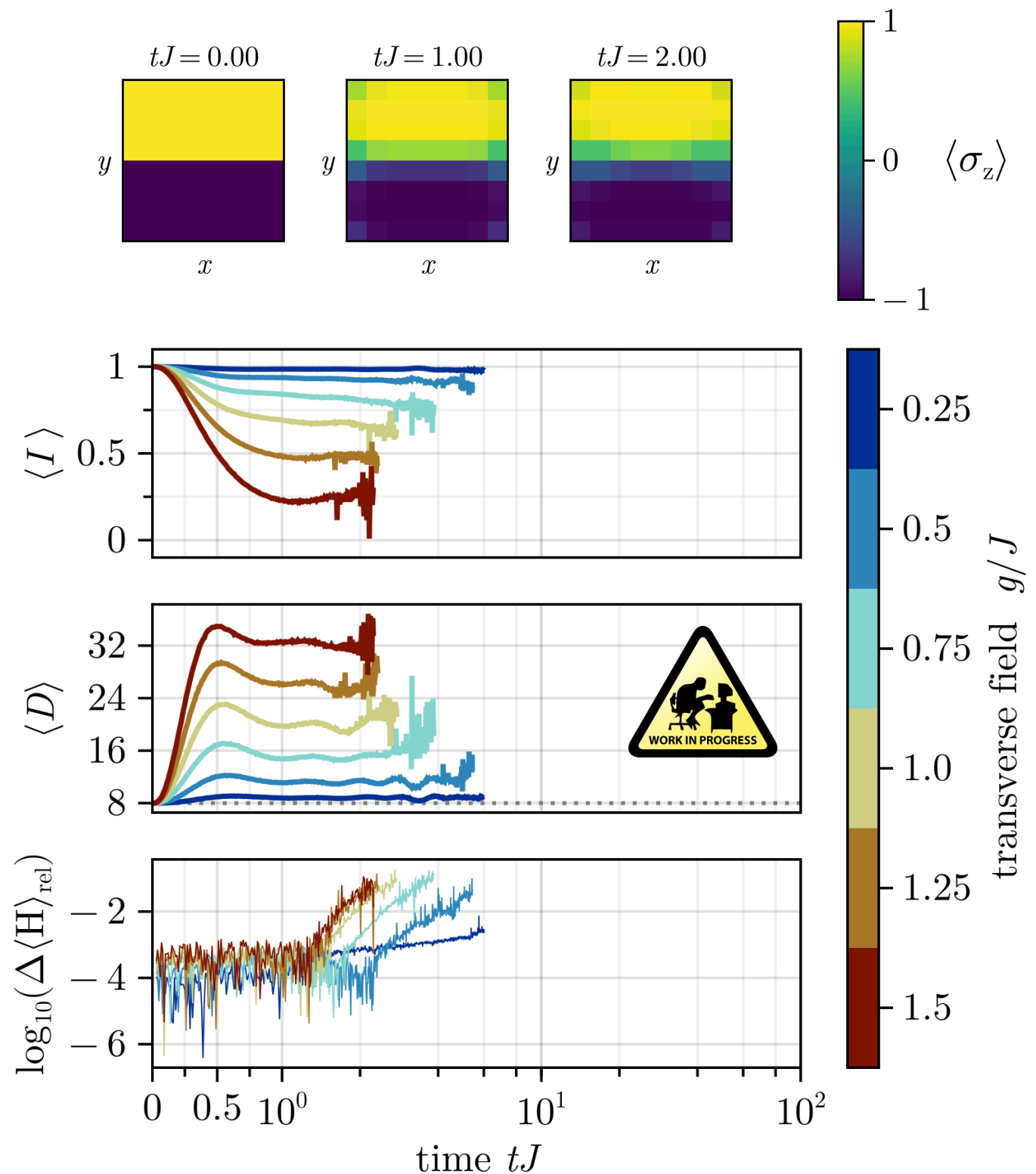
31

Benchmark on roughening dynamics of 2D Ising (8×8)
(quench at $g \neq 0, h = 0$)



Krinitzin, et al, (**MR**), PRL 134, 240402 (2025)

TTN $\chi \simeq 400$



Hartwich, Weerda, **MR**, et al., in preparation

PEPS $D = 5$

CONCLUSIONS

*"Never give up on a dream just because of
the time it will take to accomplish it.
The time will pass anyway."*

[Earl Nightingale]

SPECIAL THANKS TO...

33



E. Weerda



D. Alcalde



N. Tausendpfund



P. Geraghty



J. Nguyen



A. Dubey



K. Schröder



N. Dannenfeld



N. Elbracht



L. Reich



Markus Schmitt



W. Krinitsin

Uni-Regensburg/FZJ

... and to all other collaborators, too!
(J. Naumann, P. Schmoll, J. Eisert, S. Montangero, M. Heyl, ...)

- * Projected Entangled Pair States (PEPS):
 - * natural 2D choice
 - * tough contraction problems (& complexity transitions)
 - * stochastic methods (TDVP+ minSR) help considerably
 - * long-range interactions for free (almost)
 - * reduced basis models for cheaper phase diagrams
 - * amenable to study real-time dynamics
- * Brain-storming very welcome :-)
(e.g., combo with Belief Propagation / exp. time-grids / etc.)

- * check out our codebase,
based on iTensors
[Alcalde Puente, et al. \(MR\), PRB 111, 195120 \('25\)](#)
- * stay tuned for results soon on arXiv :-)
- * if you are curious about 2D loop-less
Tree Tensor Network techniques...
[Krinitzin, et al. \(MR\), PRL 134, 240402 \('25\)](#)
[Krinitzin, et al. \(MR\), PRB 112, 134310 \('25\)](#)



THANKS!