Generating Functions for Projected Entangled-Pair States

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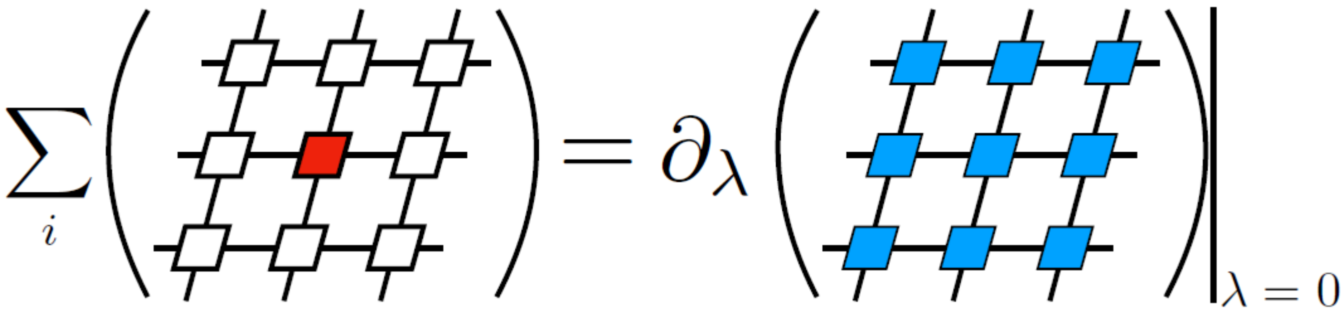
Graduate School of Science and Technology, Keio University



Physical Review B **103**, 205155 (2021)
PRX Quantum **5**, 010335 (2024)

SQAI
Center of Innovation for Sustainable Quantum AI

COI-NEXT

2024/11/16 Tensor Network 24
@Shiinoki Cultural Complex, Kanazawa

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TENSOR NETWORK 2024

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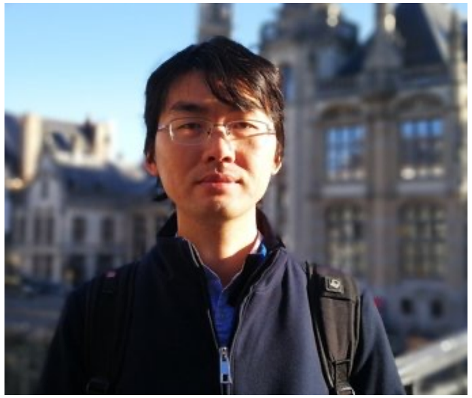

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Univ. of Maryland

Dr. Huan-Kuang Wu

Outline

- Introduction

- Tensor network – Ground state search

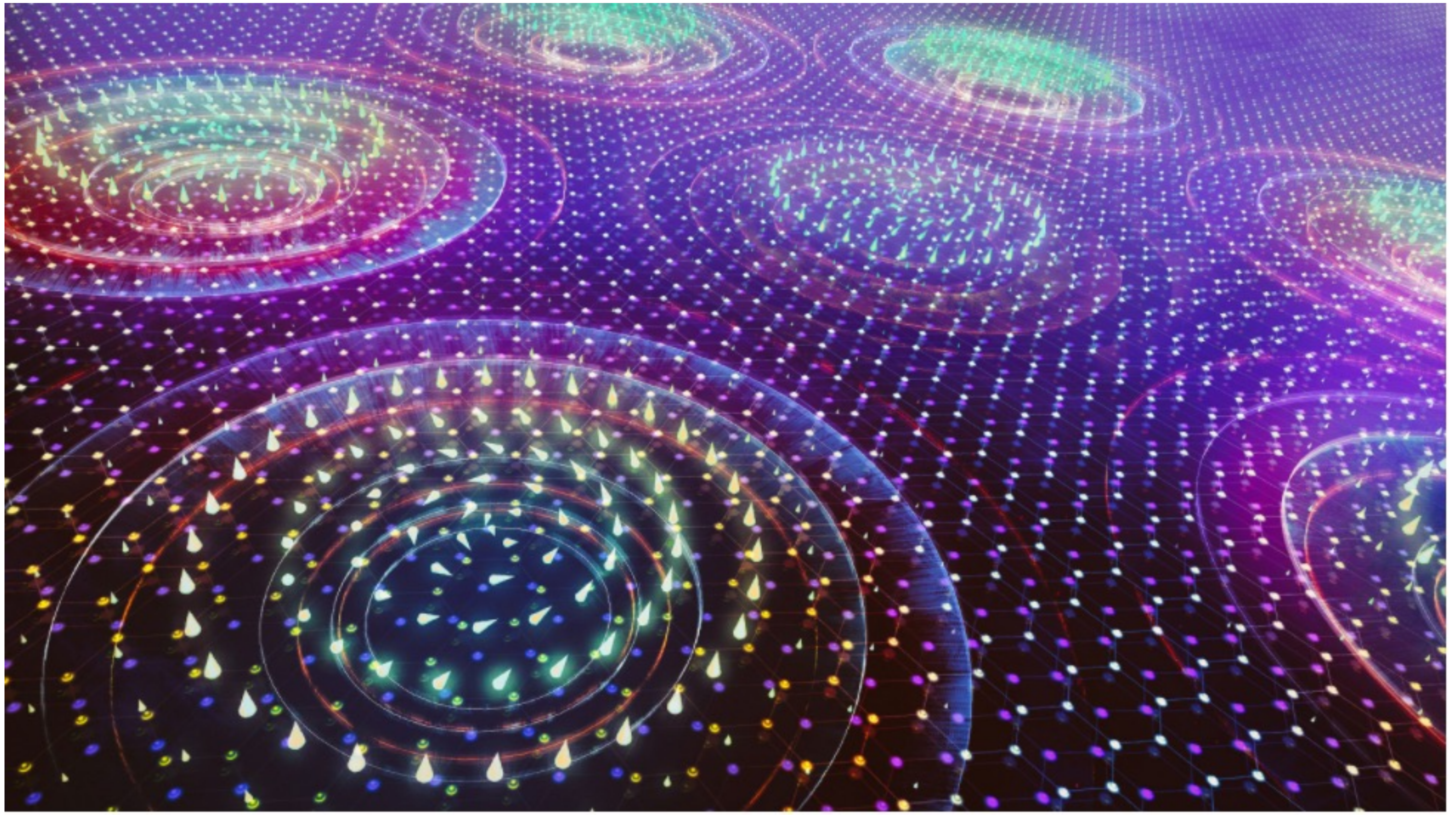
  - Variational optimization
  - Some results

- Tensor network – Excited state ansatz

  - One dimension (*Physical Review B* **103**, 205155 (2021))
  - Two dimensions (*PRX Quantum* **5**, 010335 (2024))

- Summary

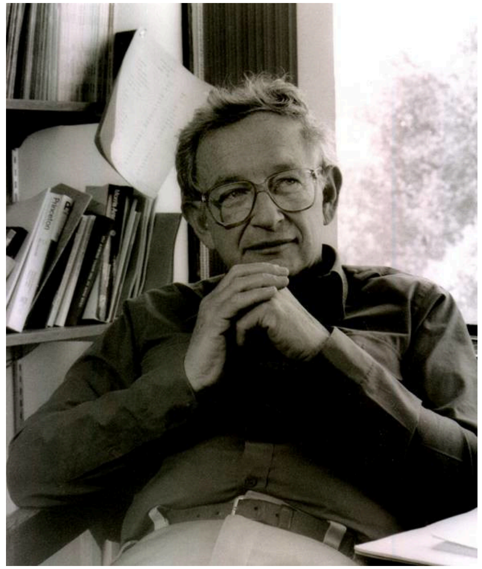
Quantum many-body physics



Skyrmions emerge from the collective behavior of scores of electrons, but they behave as individual particles.

Maciej Rebisz for Quanta Magazine

More is different



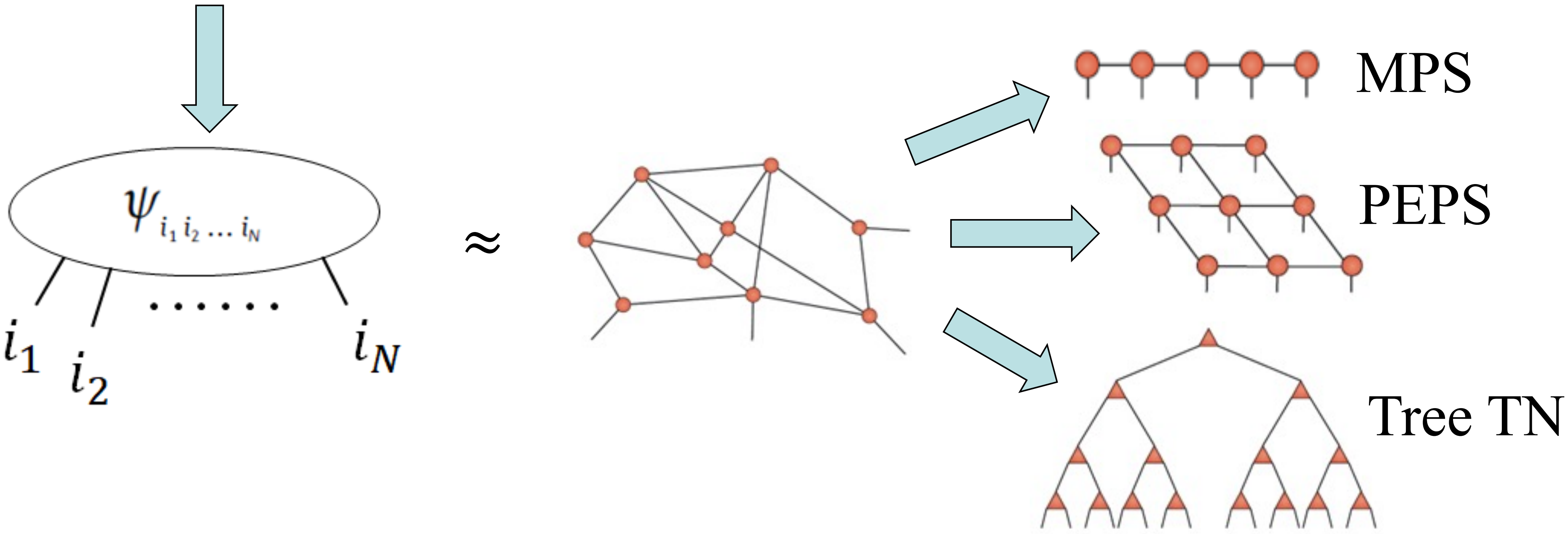
How to probe the low-energy states with some appropriate tools?

…and difficult

Tensor network algorithm

$$|\psi\rangle = \sum_{i_1, i_2, \ldots, i_N = 1} \psi_{i_1 i_2 \ldots i_N} |i_1\rangle |i_2\rangle \ldots |i_N\rangle$$

- Size of Hilbert space: d^N (d represents the number of possible local states)
- The question further reduces to representing $\psi_{i_1 i_2 \ldots i_N}$ in an efficient way



How to “train” the tensors?

R. Orus, *Nature Review Physics* **1**, 538 (2019)

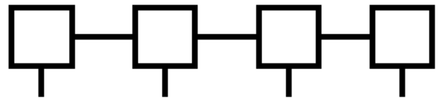
- Ground state optimization and characterization
  - MPS

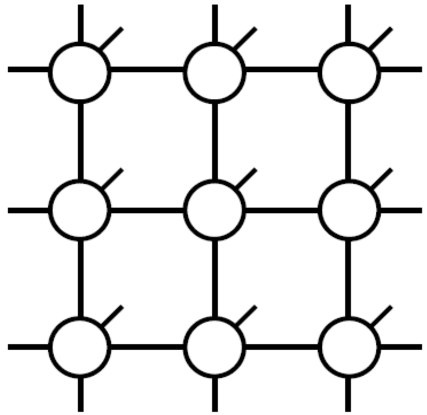
    optimization: DMRG, infinite DMRG, TEBD, VUMPS, etc.

    characterization: entanglement spectrum, fundamental theorem, etc.
  - PEPS

    optimization: simple update, (fast) full update, gradient optimization, AD, etc.

    characterization: ES, gauge symmetry, finite entanglement scaling, etc.





- Tensor networks describe ground states well
  - Symmetry breaking ordered phase
  - Non-chiral topological ordered phase
  - Quantum critical point
  - Gapless spin liquid
  - Chiral spin liquid
- Many experimentally accessible observables are excitations
  - Spin excitation: neutron scattering
  - Spin-dimer excitation: Raman scattering, RIXS
  - Fermion excitation: ARPES
- One way to bridge tensor networks to real experiments: excited state

Courtesy of Prof. Ji-Yao Chen

S. R. White, PRL 69, 2863 (1992); I. P. McCulloch, arXiv: 0804.2509 (2008); F. Verstraete and J. I. Cirac, arXiv: 0407066 (2004);
H. C. Jiang, Z. Y. Weng, and T. Xiang, PRL (2008); H. N. Phien, J. A. Bengua, et al. PRB (2015);
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J. I. Cirac, D. Poilblanc, N. Schuch, and F. Verstraete, PRB (2011); R. Chi, Y. Liu, Y. Wan, H.-J. Liao, and T. Xiang, PRL (2022)

Ground state search – variational optimization

Variational principle:

Target: minimize the energy $\langle\psi|H|\psi\rangle$

↓

Get gradients $\partial_a\langle\psi|H|\psi\rangle$

Central question:

How to obtain the gradients of a complex multi-variable function efficiently?

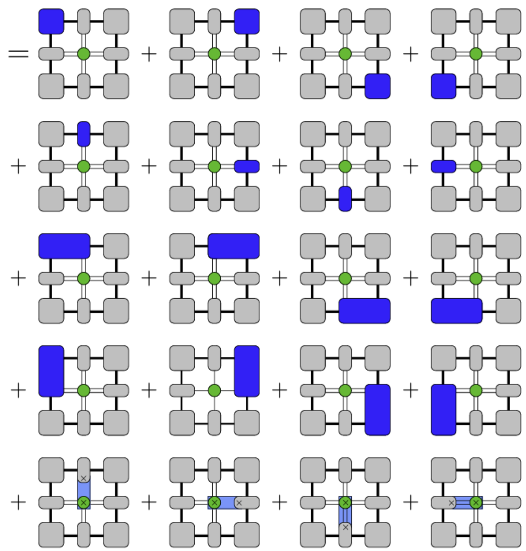
Option 1: finite difference

$$(\mathbf{g}_0)_i \approx \frac{E(\mathbf{x}_0 + h\mathbf{e}_i) - E(\mathbf{x}_0)}{h}$$

- Disadvantage: large error

Option 2: systematic summation

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



P. Corboz, *Physical Review B* **94**, 035133 (2016)

- Iteratively solving the eigenvalue problem for the lowest energy
- Disadvantage: complexity due to a summation of many different copies of tensor graph

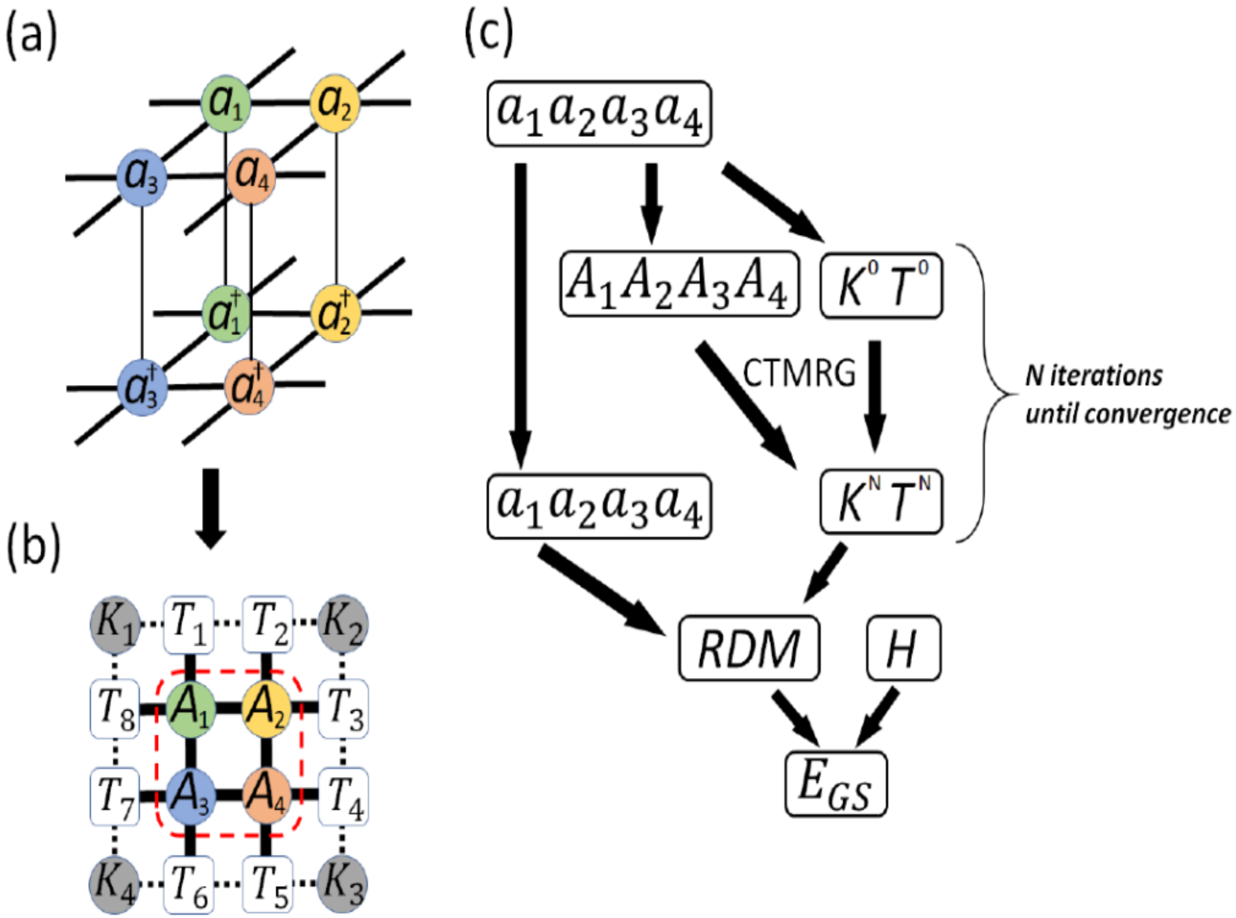
Option 3: automatic differentiation

H.-J. Liao, J.-G. Liu, L. Wang, and T. Xiang, *Physical Review X* **9**, 031041 (2019)

Frequently used for ML. A (numerically) exact gradient can be well approximated through the so-called back propagation!!

Update the tensors – variational optimization

For 2D iPEPS:



WLT, E.-G. Moon, K.-W. Lee, W. E. Pickett, and H.-Y. Lee, *Commun. Phys.* **5**, 130 (2022)

- The left plot shows the computational graph of one iteration for iPEPS.
- After each iteration, the gradient can be evaluated through AD.

$$\left(\frac{\partial E_{GS}}{\partial a_1}, \frac{\partial E_{GS}}{\partial a_2}, \frac{\partial E_{GS}}{\partial a_3}, \frac{\partial E_{GS}}{\partial a_4}\right) \rightarrow (a'_1, a'_2, a'_3, a'_4)$$

- After *N* iterations a well approximated ground-state ansatz can be constructed.

$$(a'_1, a'_2, a'_3, a'_4)$$

$$\vdots \quad \Big\} \; N \text{ steps}$$

$$(a^f{}_1, a^f{}_2, a^f{}_3, a^f{}_4)$$

Our previous results

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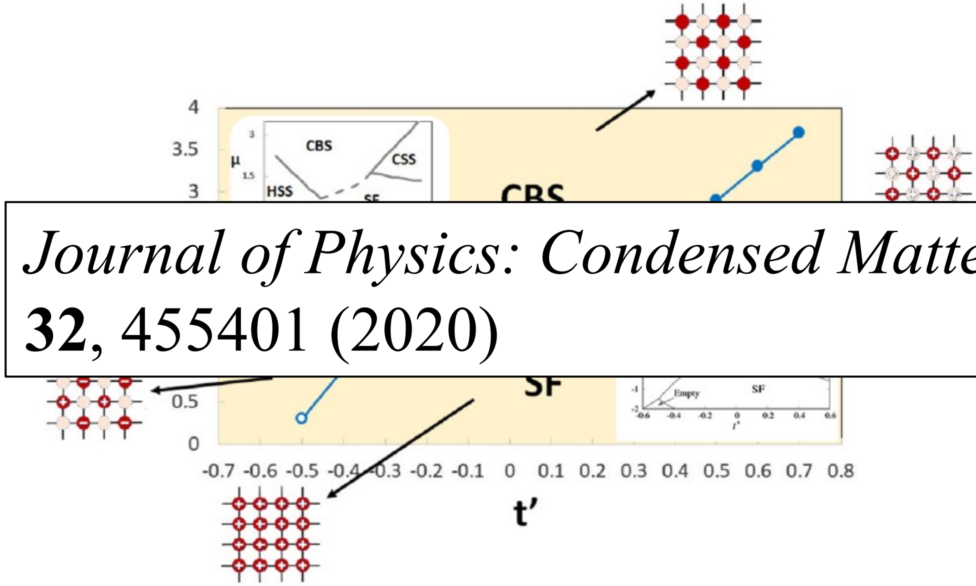
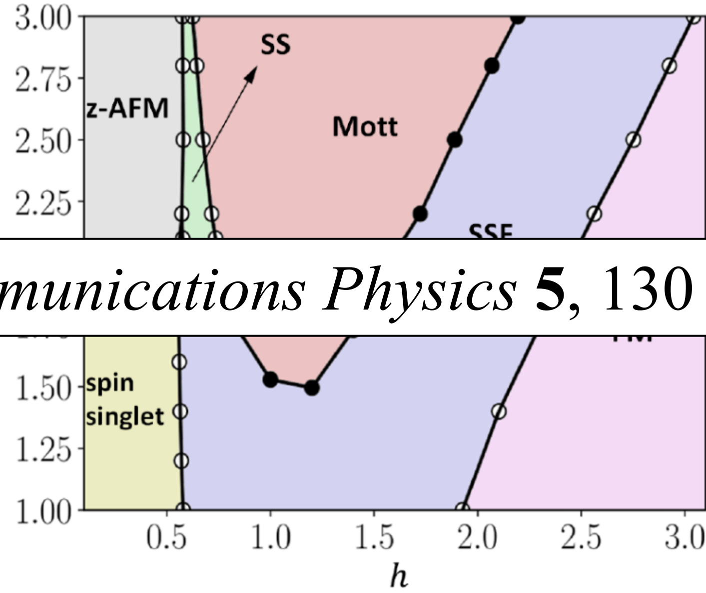
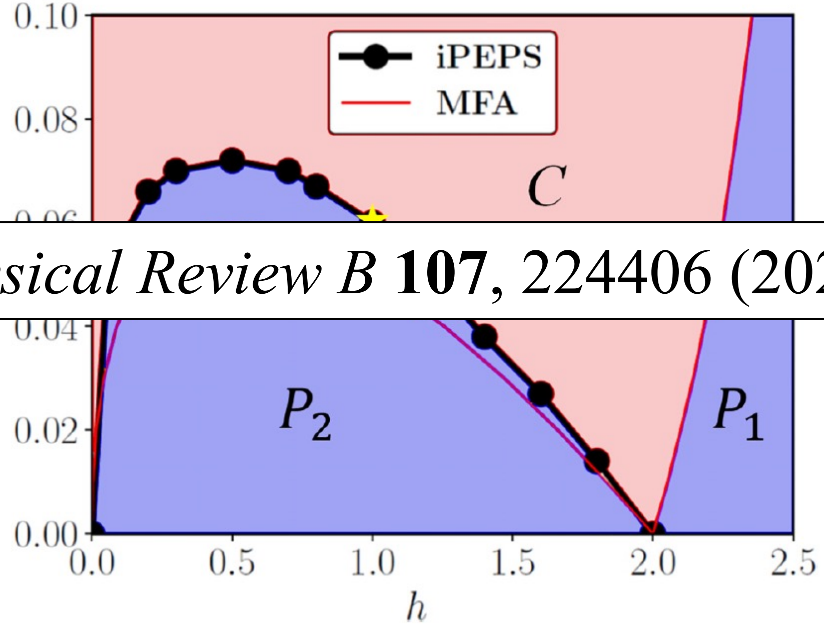


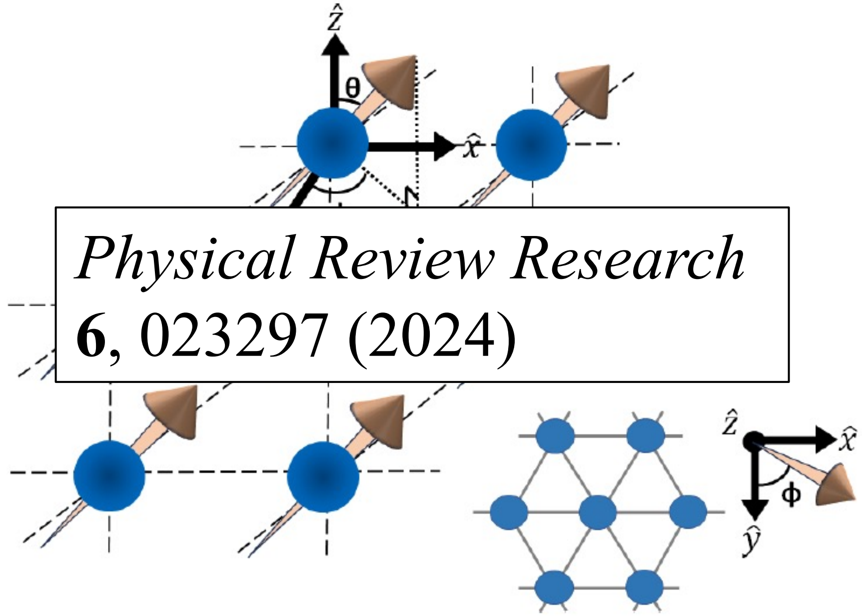
Journal of Physics: Condensed Matter **32**, 455401 (2020)



Communications Physics **5**, 130 (2022)



Physical Review B **107**, 224406 (2023)



Physical Review Research **6**, 023297 (2024)

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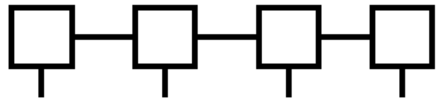

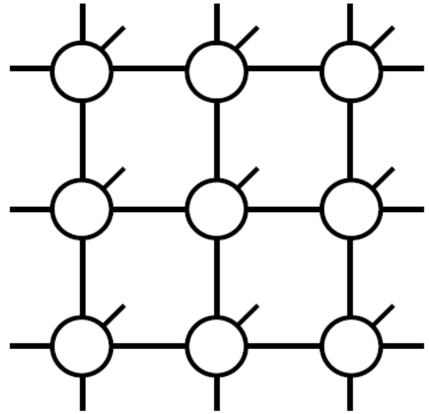

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- One way to bridge tensor networks to real experiments: excited state ⟵ How?

Courtesy of Prof. Ji-Yao Chen

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J. I. Cirac, D. Poilblanc, N. Schuch, and F. Verstraete, PRB (2011); R. Chi, Y. Liu, Y. Wan, H.-J. Liao, and T. Xiang, PRL (2022)

Excitation ansatz: MPS

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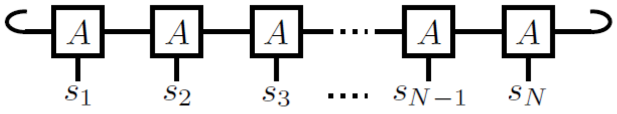
- One-particle excitation ansatz

  - Assume ground state can be approximated by a uniform MPS:

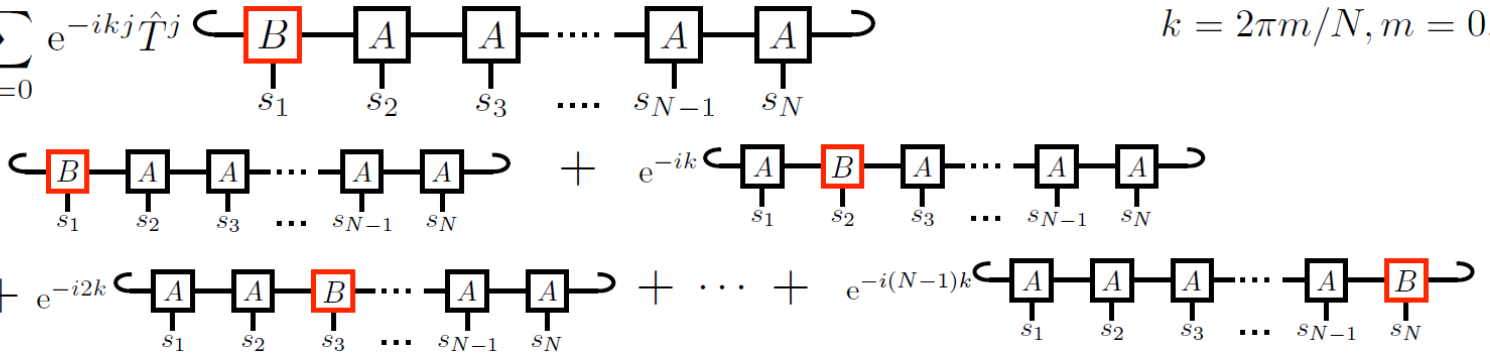
$|\Psi(A)\rangle =$



$$\hat{T}|\Psi(A)\rangle = |\Psi(A)\rangle$$

  - One-particle excited state takes the form (single mode approximation):

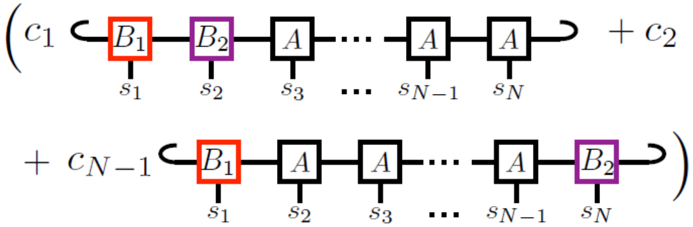
$|\Phi_k(B)\rangle = \sum_{j=0}^{N-1} e^{-ikj}\hat{T}^j$



$$k = 2\pi m/N, m = 0, 1, \ldots, N-1$$

- Two-particle excitation ansatz

$|\Phi_k(B_1, B_2)\rangle = \sum_{j=0}^{N-1} e^{-ikj}\hat{T}^j \Big(c_1 \ldots + c_2 \ldots + \cdots + c_{N-1} \ldots \Big)$



Physical Review B **85**, 035130 (2012)
Physical Review Letters **112**, 257202 (2014)

TN summation using generating function

Generating function (GF):

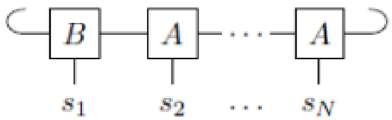
- In field theory, this function is often constructed and by taking the derivative, one can obtain the target values.
- Here, we are going to borrow the same idea and apply it for the tensor network ansatz.

Taking 1D system as an example
(with translational symmetry):

Corresponding GFs:

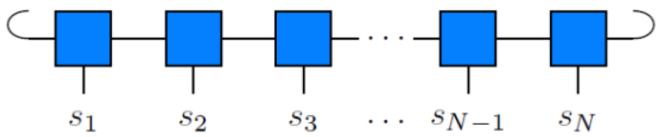
One-particle excitation:

$$|\Phi_k(B)\rangle = \sum_{j=0}^{N-1} e^{-ikj}\hat{T}^j$$



$$\frac{\partial |G_\Phi(\lambda)>}{\partial \lambda}|_{\lambda=0}$$

$$|G_\Phi(\lambda)\rangle =$$



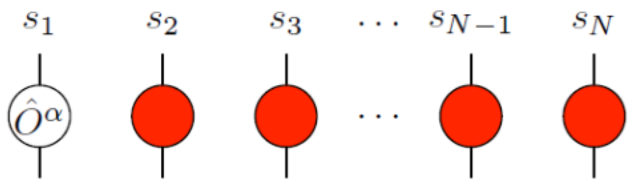
$$MPS_j(\lambda) = A + \lambda e^{-ikr_j} B$$

Static structural factor:

$$S^{\alpha,\beta}(k) = \sum_{j=1}^{N} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1 - \boldsymbol{r}_j)} \left\langle \hat{O}_1^\alpha \hat{O}_j^\beta \right\rangle$$

$$\left\langle \frac{\partial \hat{G}_{SF}(\lambda)}{\partial \lambda}|_{\lambda=0} \right\rangle$$

$$\hat{G}_{\mathrm{SF}}(\lambda) =$$

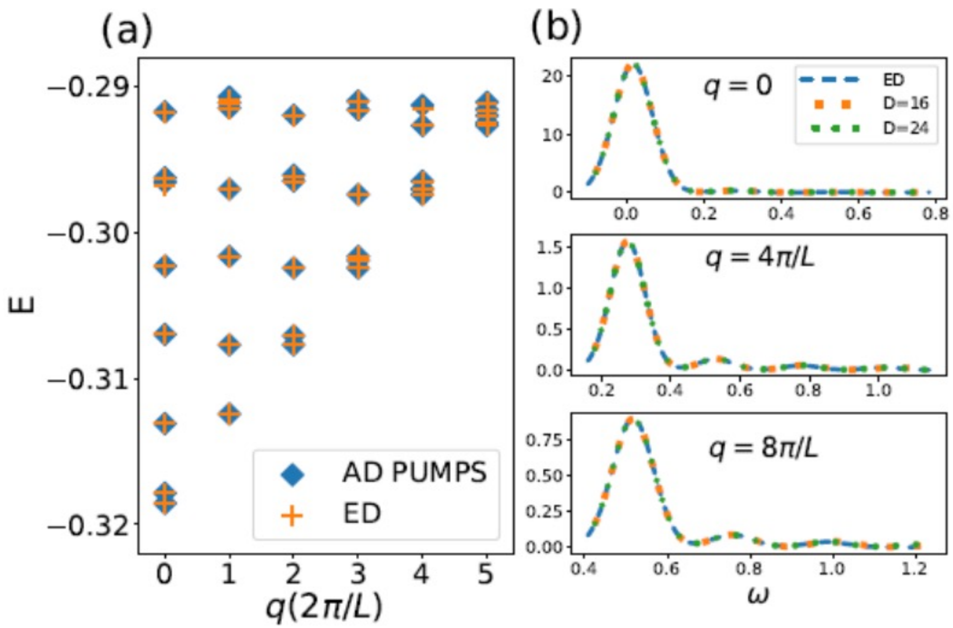


$$\hat{O}_j^\beta(\lambda) = I + \lambda e^{-ikr_j} \hat{O}^\beta$$

WLT, H.-K. Wu, N. Schuch, N. Kawashima, and J.-Y. Chen, *Physical Review B* **103**, 205155 (2021).

1D critical Ising chain

- With generating functions, now we only need to calculate one or a few tensor graphs.
- Moreover, the derivatives can be evaluated using automatic differentiation (AD), which is often utilized in neural networks.



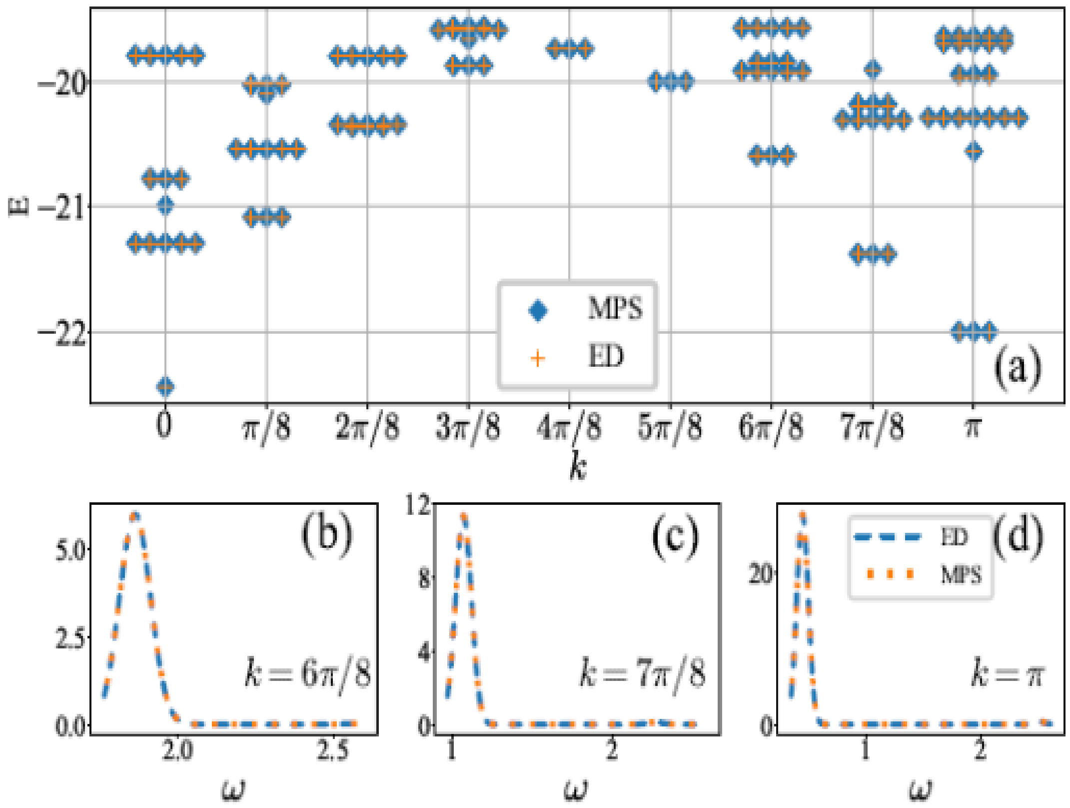
$$S^{\alpha}(k,\omega) = \sum_n |M_k^{\alpha}|^2 \delta\big(\omega - E_n^k + E_0\big),$$
$$M_k^{\alpha} = \langle \Phi_k(B_n)|S_k^{\alpha}|\psi(A)\rangle,$$
$$S_k^{\alpha} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{ikr_j} S_j^{\alpha}$$

- (a) low-energy spectrum by us and from exact diagonalization (ED).
- (b) spectrum weight (dynamical structural factor) with different bond dimension and ED

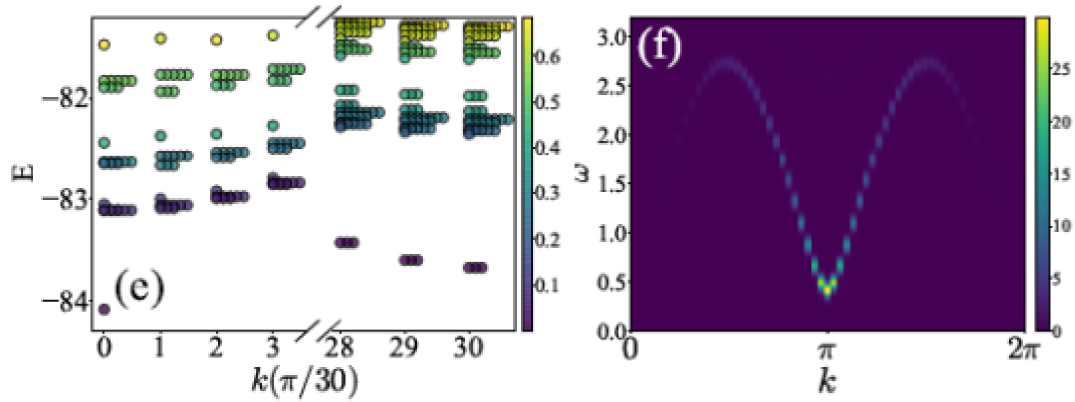
WLT, H.-K. Wu, N. Schuch, N. Kawashima, and J.-Y. Chen, *Physical Review B* **103**, 205155 (2021).

1D spin-1 Heisenberg chain

L=16:



L=60:

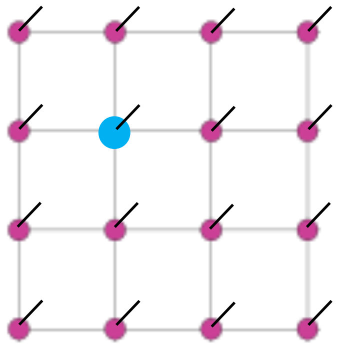


- Good benchmark accordance in smaller size with ED.
- Energy spectrum and dynamical structural factor can be obtained for larger system size.
- Haldane gap≈0.4105

WLT, H.-K. Wu, N. Schuch, N. Kawashima, and J.-Y. Chen, *Physical Review B* **103**, 205155 (2021).

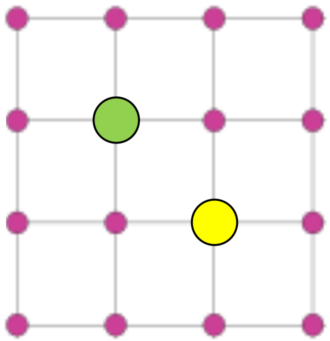
One-particle Bloch state in 2D

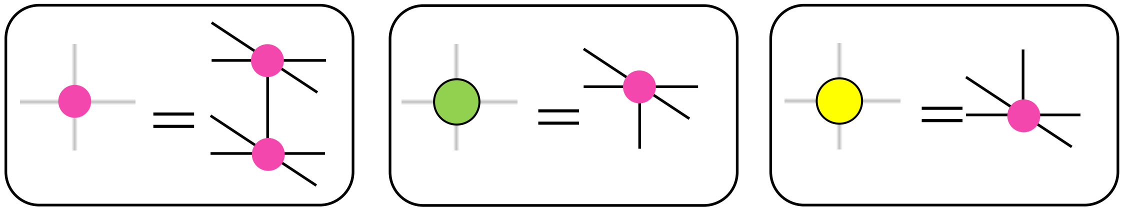
$$|\Phi_k(B)\rangle = \sum_{j=0}^{N-1} \mathrm{e}^{-ikj}\hat{T}^j$$



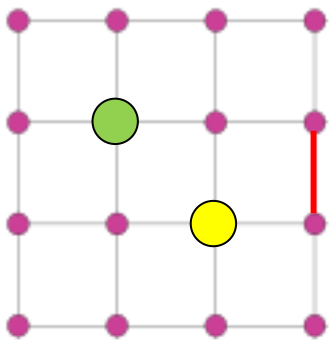
Goal: To find the corresponding impurity tensor so that the energy gives the lowest excited ones, second lowest excited ones, etc.

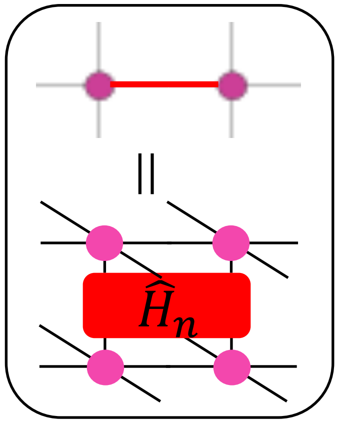
$$\mathbf{N}_{\mu\nu} = \sum_{x_1,x_2} e^{-ik(x_1-x_2))}$$





$$\mathbf{H}_{\mu\nu} = \sum_{x_1,x_2,n} e^{-ik(x_1-x_2)}$$

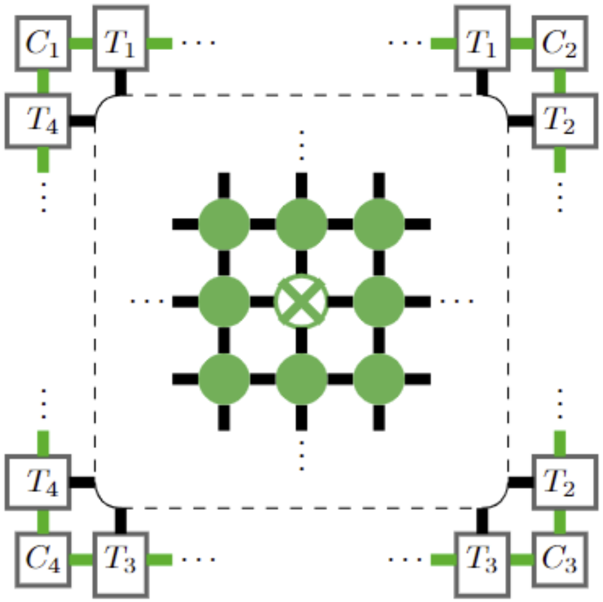




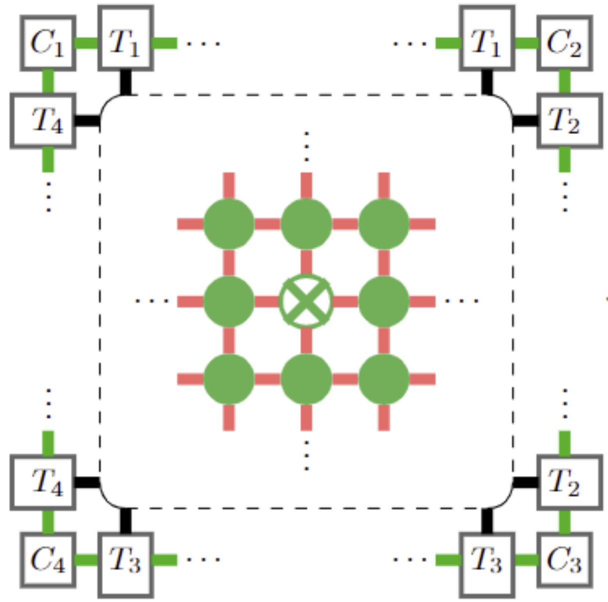
By solving $\mathbf{H}_{\mu\nu}\mathbf{B}^{\nu} = E\mathbf{N}_{\mu\nu}\mathbf{B}^{\nu}$, we can obtain a series of impurity tensors with corresponding energies.

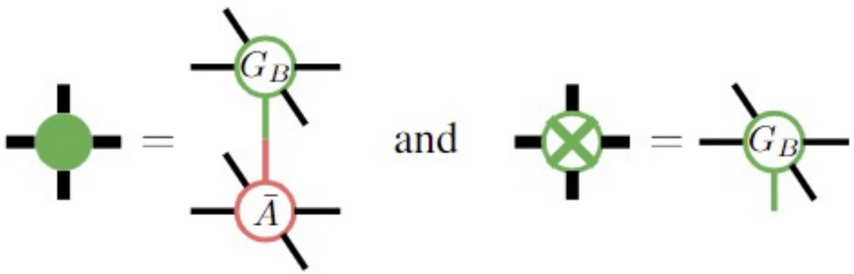
Generating function for iPEPS

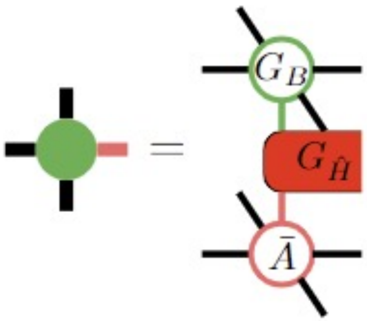
$G_{\mathbf{N}}(\lambda, B) =$



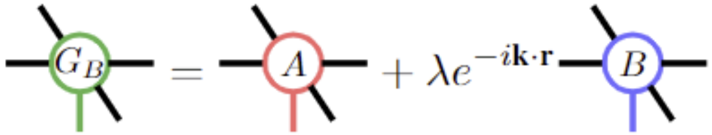
$G_{\mathbf{H}}(\lambda, \mu, B) =$







and $G_{\hat{H}} = \mathbb{I} + \mu \hat{H}_{\mathbf{r},\mathbf{r}+\hat{i}}$



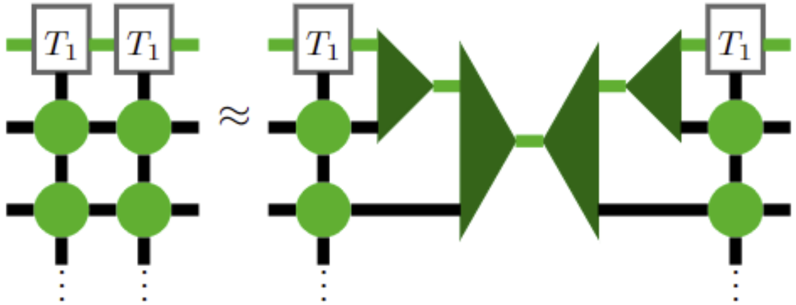
$$\mathbf{N} = \frac{\partial}{\partial B} G_{\mathbf{N}}(\lambda, B)\Big|_{\lambda=1, B=0}$$

$$\mathbf{H} = \frac{\partial^2}{\partial B \partial \mu} G_{\mathbf{H}}(\lambda, \mu, B)\Big|_{\lambda=1, \mu=0, B=0}$$

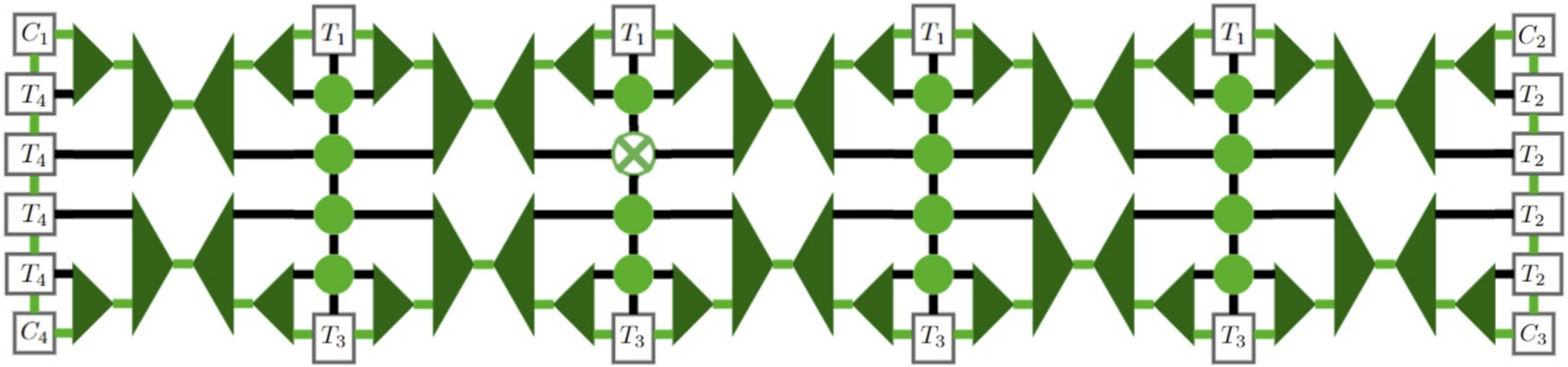
WLT, L. Vanderstraeten, N. Schuch, H.-Y. Lee, N. Kawashima, and J.-Y. Chen, *PRX Quantum* **5**, 010335 (2024)

Tensor compression

- In order to compress G_N and G_H, we insert the projectors.
- To include the projectors in both vertical and horizontal directions, we take the average.



Vertical compression for 4x4 bulk tensor:

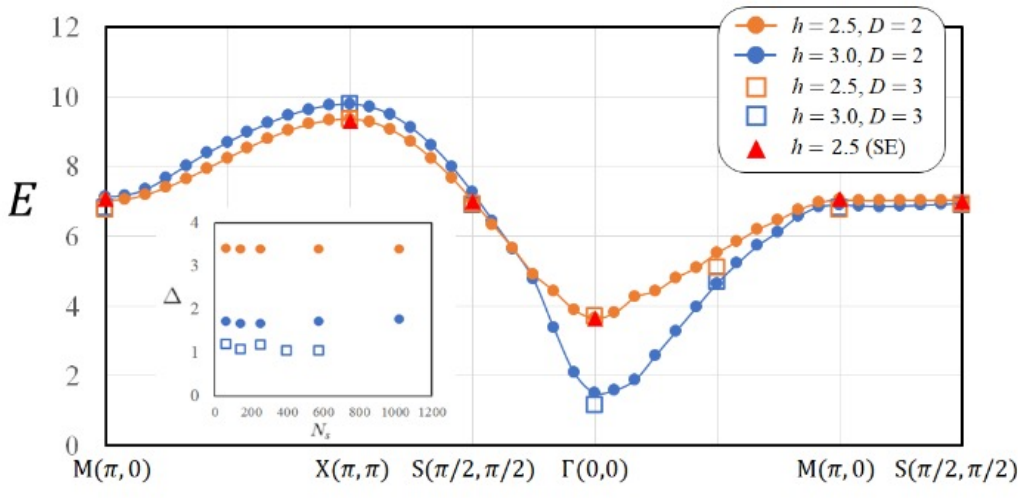


WLT, L. Vanderstraeten, N. Schuch, H.-Y. Lee, N. Kawashima, and J.-Y. Chen, *PRX Quantum* **5**, 010335 (2024)

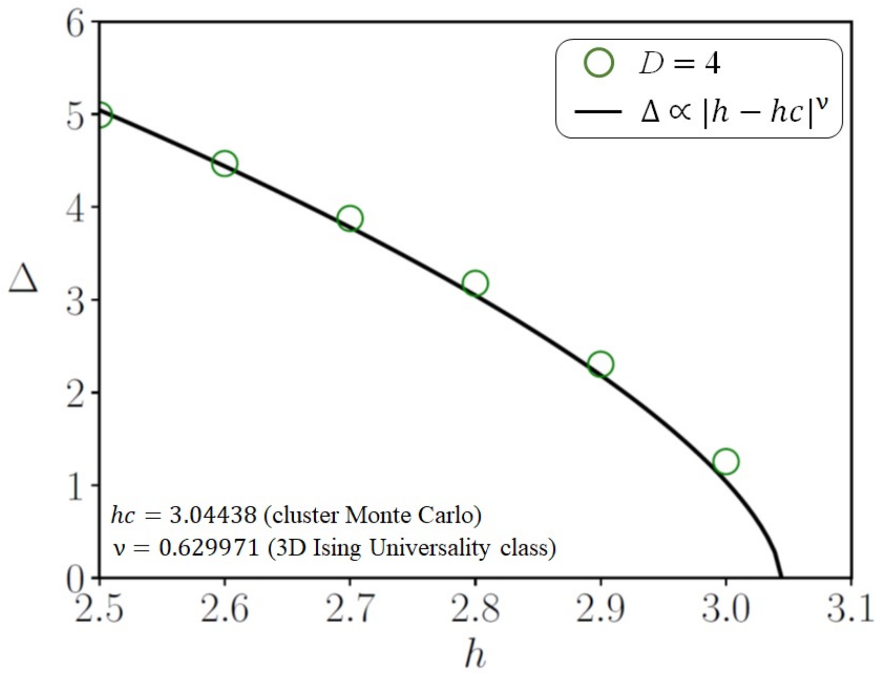
2D transverse-field Ising model

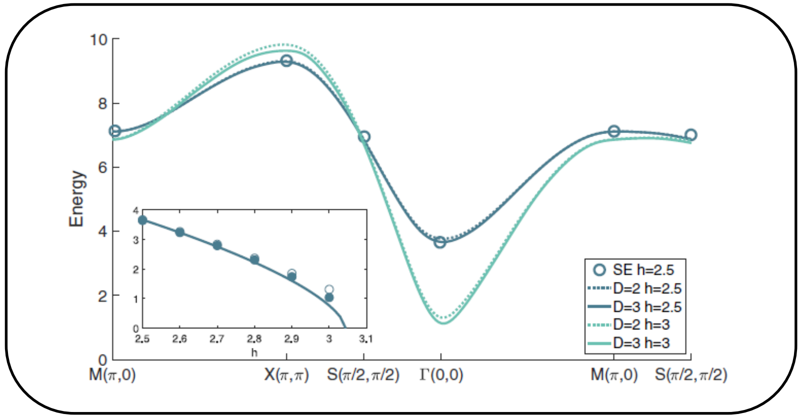
$$H = -J \sum_{\langle i,j \rangle} \sigma_i^x \sigma_j^x - h \sum_i \sigma_i^z$$

Dispersion (lowest excited state):



Energy gap:





- The energy dispersion looks well compared with previous results (cf. *Phys. Rev. B* **101**, 195109 (2020))
- The energy gap to transverse field function scales in accordance with the exponent of 3D Ising Universality class.

WLT, L. Vanderstraeten, N. Schuch, H.-Y. Lee, N. Kawashima, and J.-Y. Chen, *PRX Quantum* **5**, 010335 (2024)

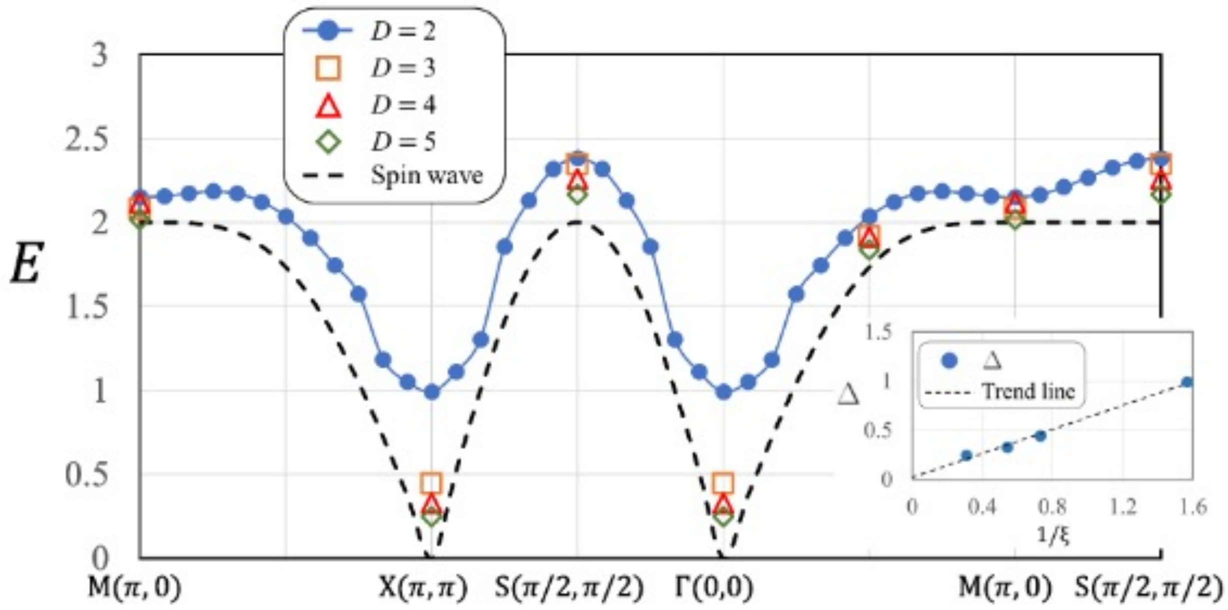
2D Heisenberg model

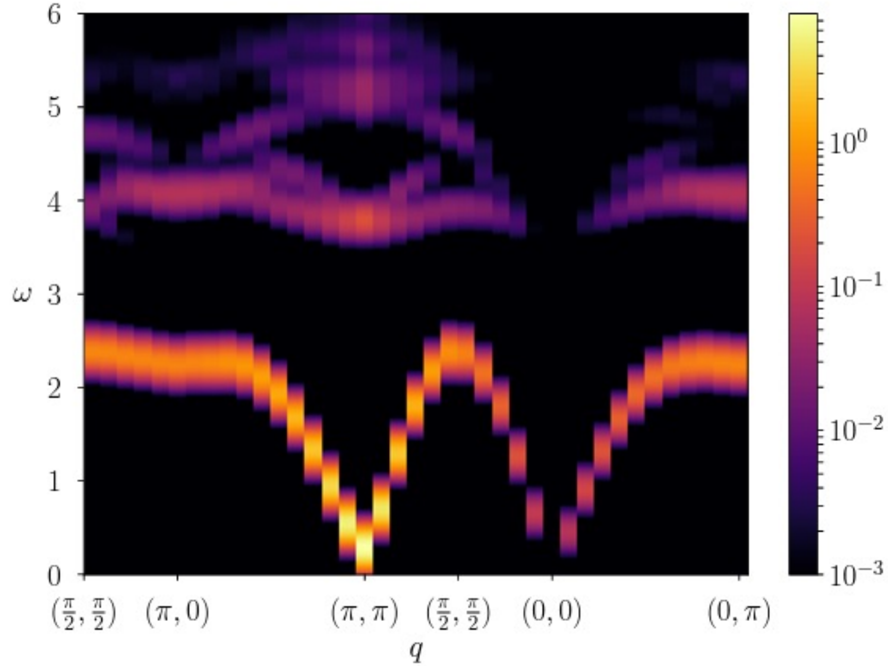
$$\mathrm{H} = J \sum_{\langle i,j \rangle} S_i^z S_j^z + \lambda \left(S_i^x S_j^x + S_i^y S_j^y \right)$$

with $J = 1$ and $\lambda = 1$

- Again, the dispersion of lowest excited energy benchmarks well (cf. *Phys. Rev. B* **98**, 100405(R) (2018)).
- Also, the gap scales to zero along with the inverse of bond dimension D, revealing the gapless nature of Heisenberg model.

Dispersion (lowest excited state):



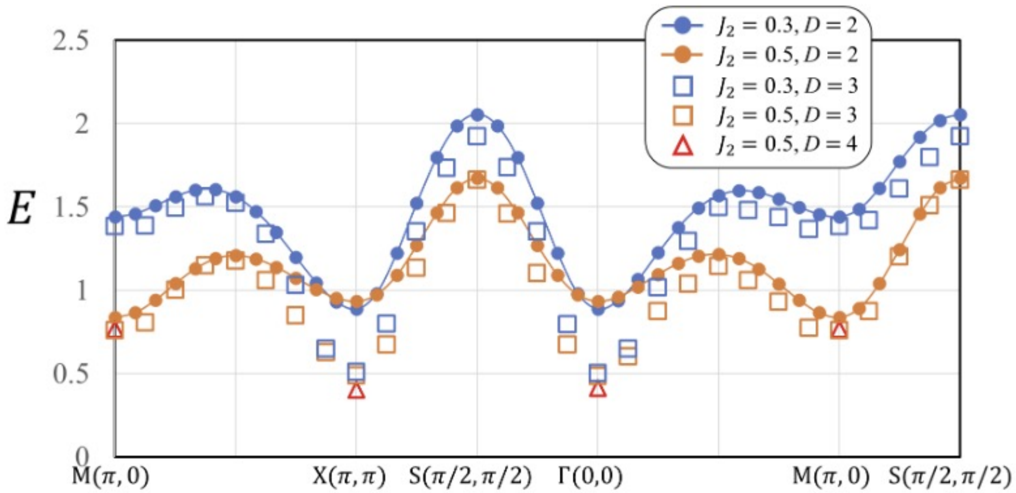


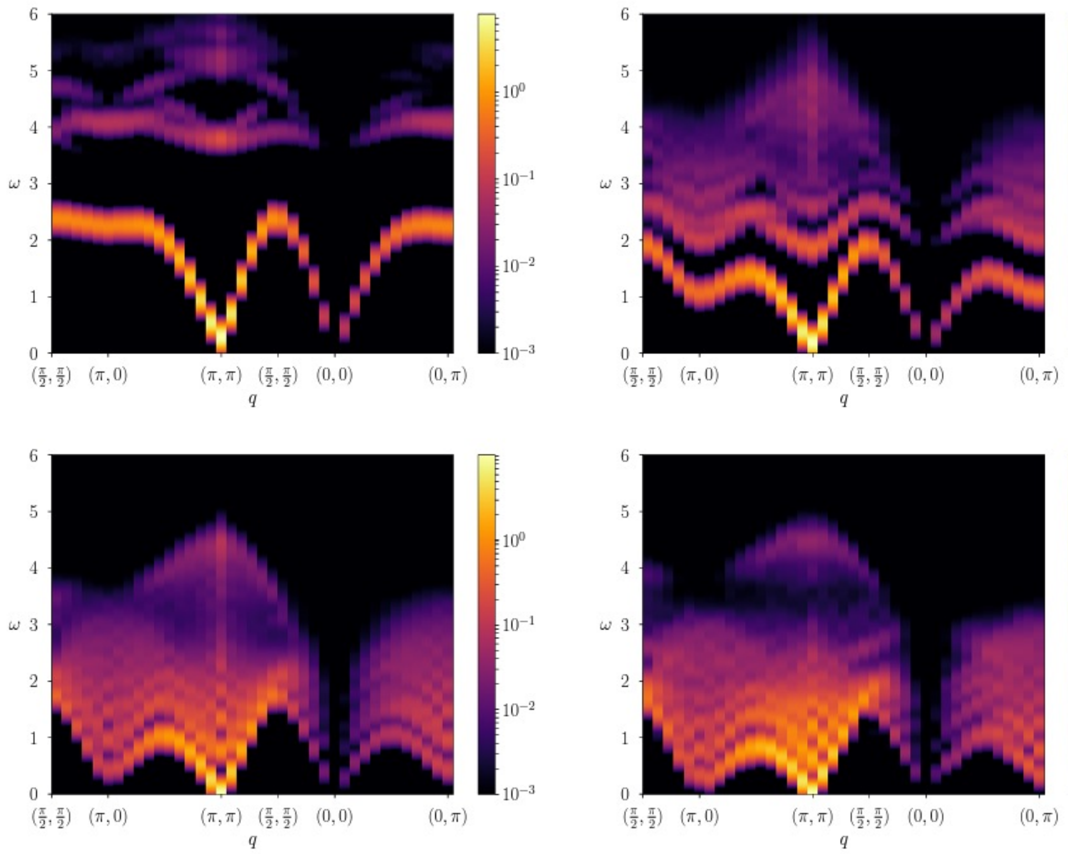
WLT, L. Vanderstraeten, N. Schuch, H.-Y. Lee, N. Kawashima, and J.-Y. Chen, *PRX Quantum* **5**, 010335 (2024)

$J_1 - J_2$ model

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Dispersion (lowest excited state):



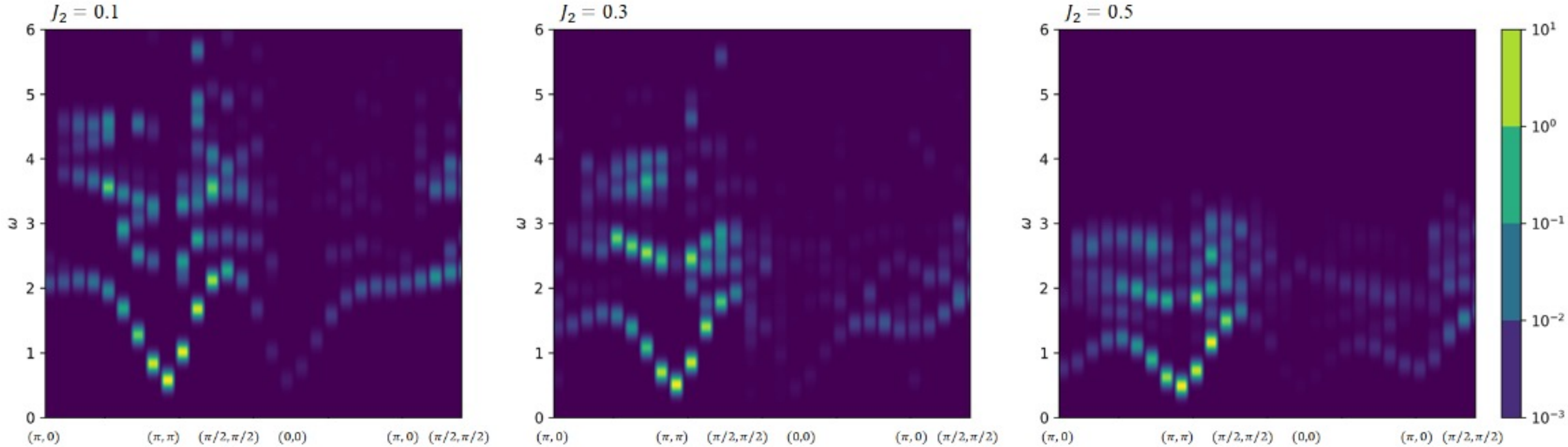


- The lowest excited states shares similar shape compared to VMC results (cf. *Phys. Rev. B* **98**, 100405(R) (2018)).

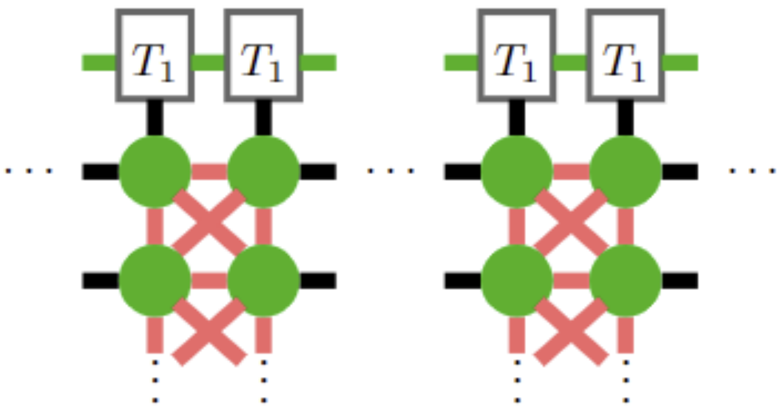
WLT, L. Vanderstraeten, N. Schuch, H.-Y. Lee, N. Kawashima, and J.-Y. Chen, *PRX Quantum* **5**, 010335 (2024)

$J_1 - J_2$ model

Dynamical structure factor:



- From the DSF we can see that the energy gap at M point gets softened and gradually becomes gapless.
- Also, spectral weights gather closer to the magnon branch, which might indicate a potential energy continuum.
- However, the computation with next nearest neighbor coupling is heavy…

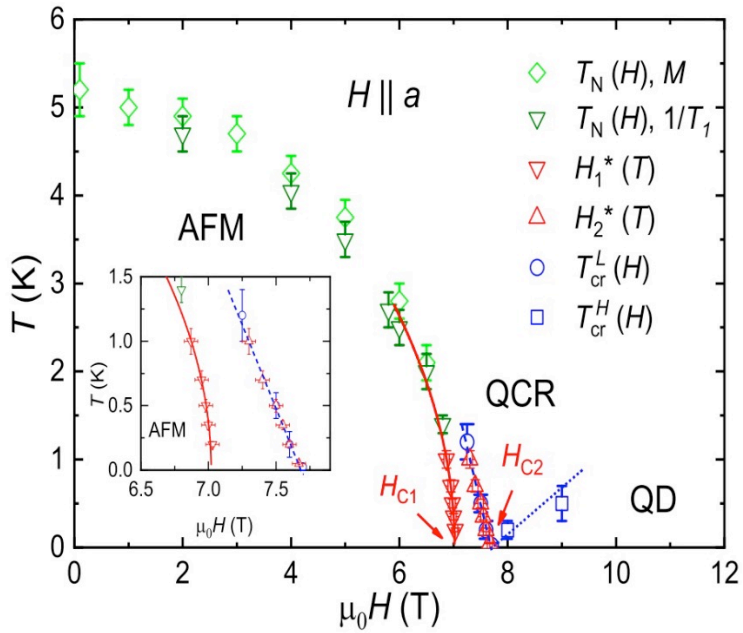


WLT, L. Vanderstraeten, N. Schuch, H.-Y. Lee, N. Kawashima, and J.-Y. Chen, *PRX Quantum* **5**, 010335 (2024)

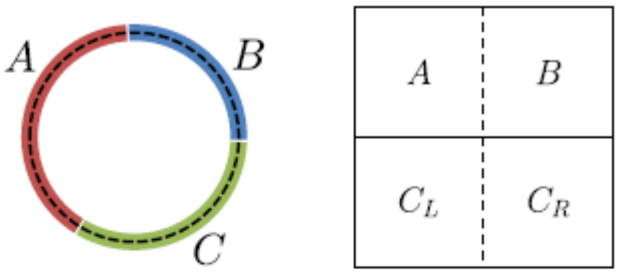
Future directions

- With the information of excited states, we can use them to construct the Gibbs state to probe the properties in the finite temperature.
- Unlike the purification, the information of low-energy excited states are believed to be better captured, leading to a potentially higher accuracy in the low temperature.

$$\mathcal{H} = \sum_{i=1}^{N} J(\Delta S_i^z S_{i+1}^z + S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) - B(S_i^x + B_y(-1)^i S_i^y)$$



Y. Cui et al., *Phys. Rev. Lett.* **123**, 067203 (2019)



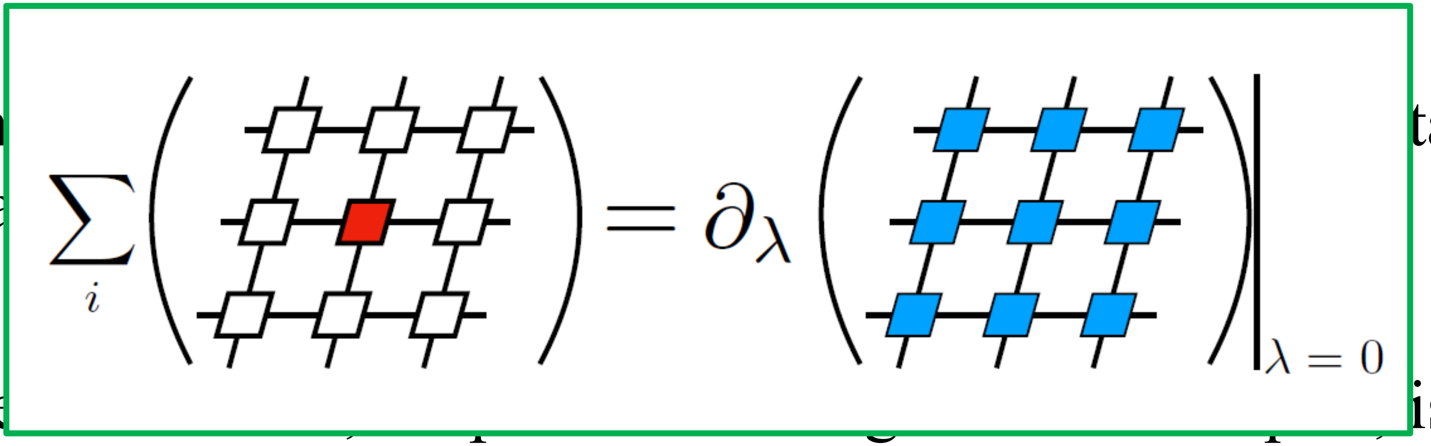
Y. Zou et al., *Phys. Rev. Lett.* **126**, 120501 (2021)

- Moreover, understanding the entanglement properties of many-body state has become very important.
- The tensor network construction for the excited states can be used to probe related properties.
- In sum, with the well constructed excited state ansatz, there are many potential usages.

Summary

- Tensor network algorithm is a powerful tool in representing the many-body wavefunctions.

- Con … tation
ansa



- Exte … is also
possible and applicable.

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- Studying more challenging issues, such as probing the finite temperature, is expected as one of the future goals.