PEPS for numerical studies of topological order

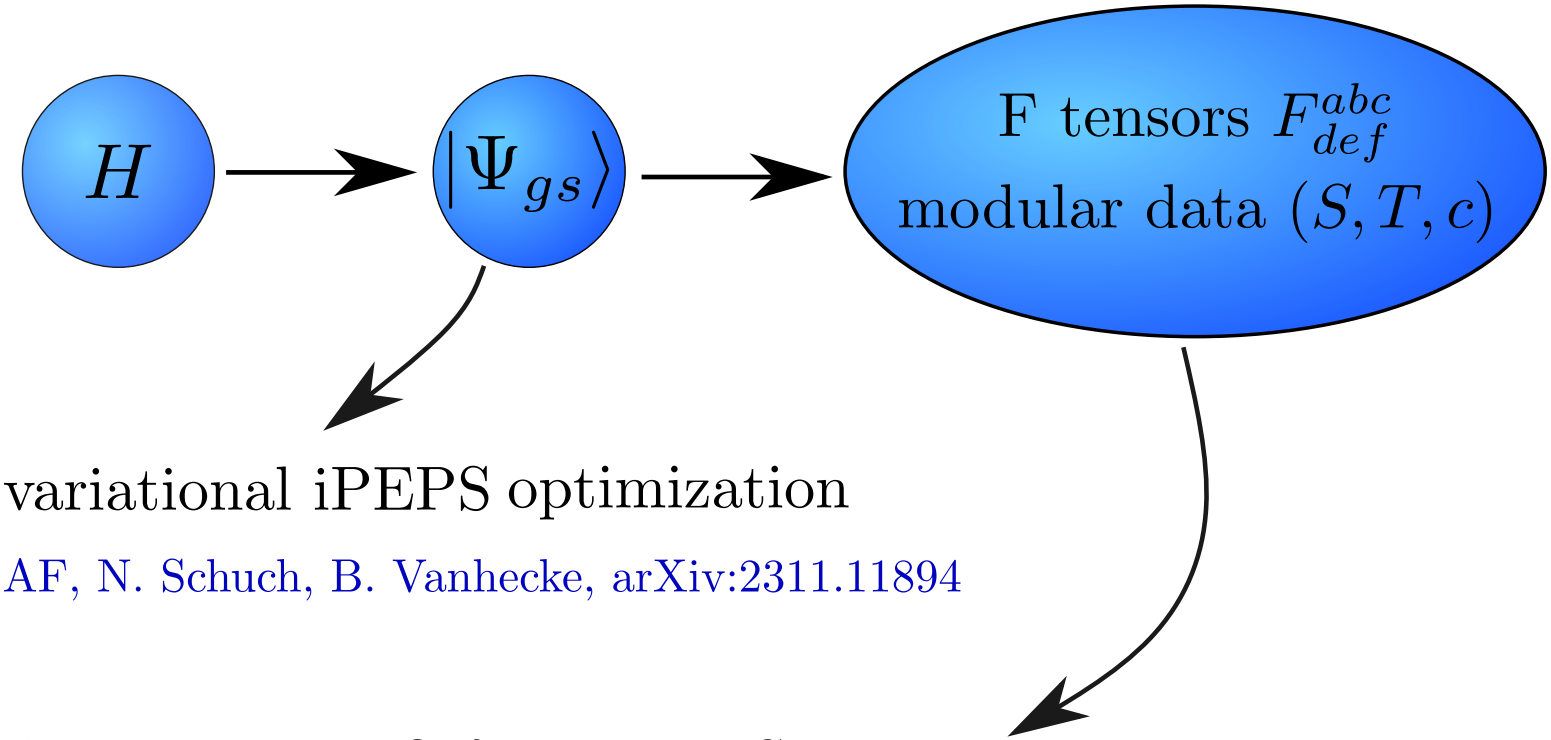
Anna Francuz

University of Vienna

30 Nov 2023

FWF Austrian Science Fund

Motivation & outlook



variational iPEPS optimization

AF, N. Schuch, B. Vanhecke, arXiv:2311.11894

determining TO from iPEPS

AF, J. Dziarmaga, G. Vidal, L. Cincio, PRB 101, 041108(R)

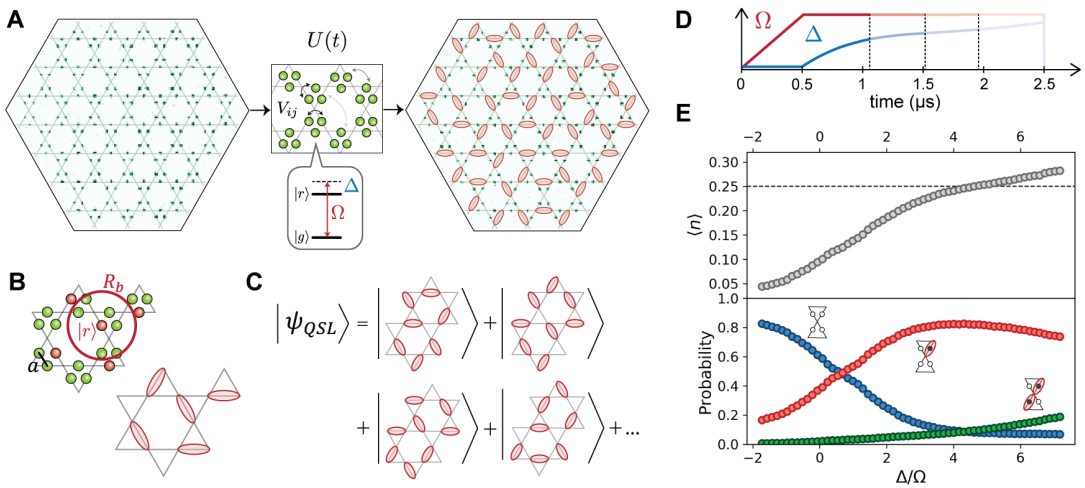
AF, J. Dziarmaga, PRB 102 (23), 235112

AF, L. Lootens, J. Dziarmaga, F. Verstraete, PRB 104 (19), 195152

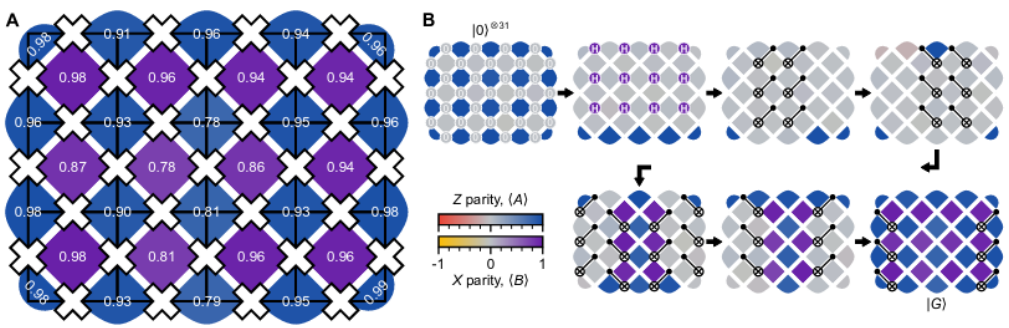
Experimental relevance

Quantum simulators

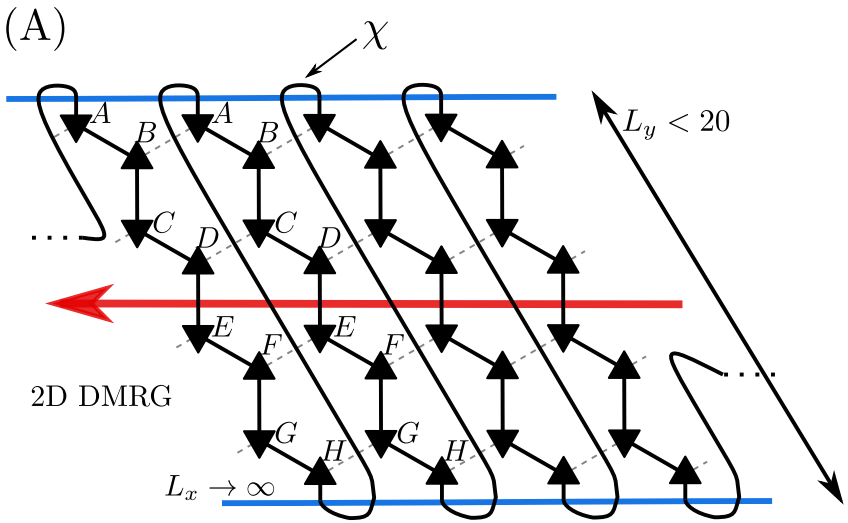
Probing Topological Spin Liquids on a Programmable Quantum Simulator, Science 374, 1242 (2021)

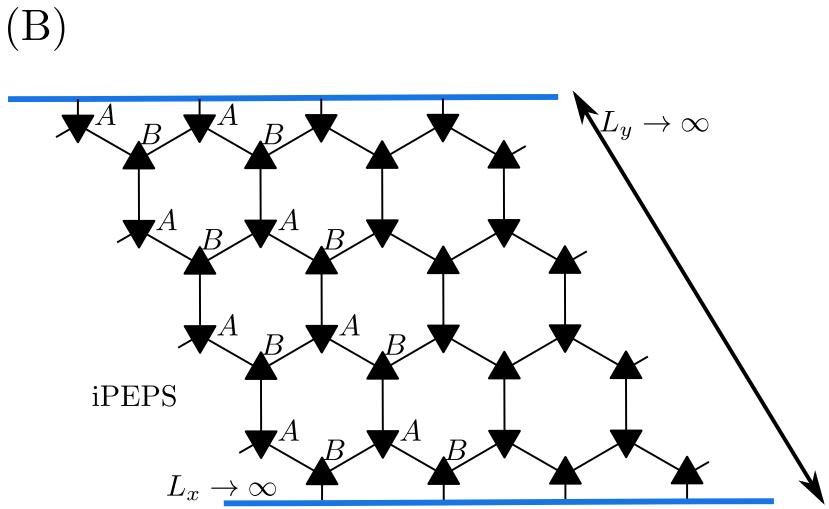


Realizing topologically ordered states on a quantum processor, Science 374, 1237-1241 (2021)



iPEPS vs 2D DMRG





- limited to cylinders of finite circumference L_y, $\xi \approx 1, 2$
- bond dimension χ grows exponentially with the circumference

- allows simulations in the thermodynamic limit, ξ is orders of magnitudes larger
- naturally incorporates 2D area law, bond dimension D limited by computational cost of algorithms

Gapped $\mathbb{Z}_2$ vs gapless $U(1)$ SL in S=1/2 Kagome AF? H.J.Liao et al. PRL 118 (2017)

Plan

1. Motivation

2. Setting the stage: gauge freedom, PEPS contraction
   - Gauge freedom
   - iPEPS contraction

3. Variational iPEPS optimization

4. Determining topological order
   - Characterization of topological order
   - Computational aspects

5. Conclusions

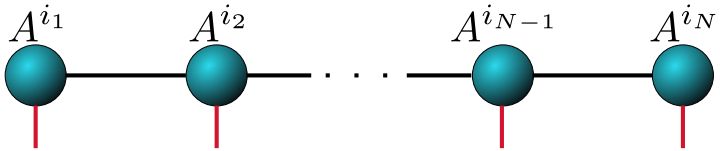
Setting the stage:

1. gauge freedom

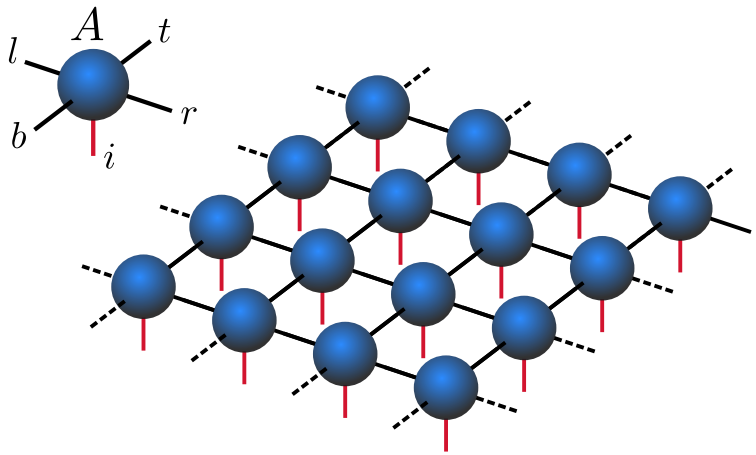
2. iPEPS contraction

Gauge transformations and symmetries

Matrix Product States

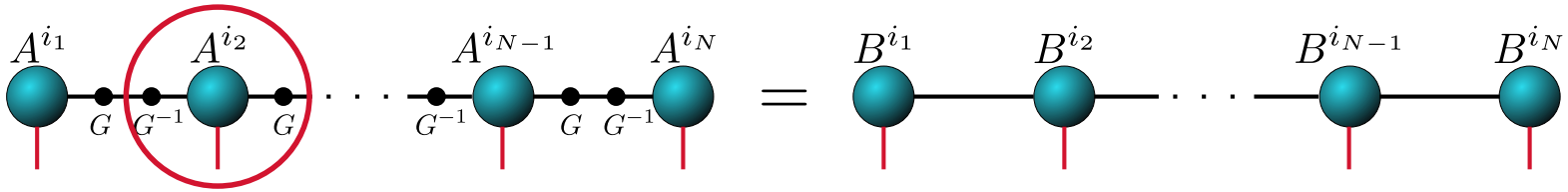


Projected Entangled Pair States

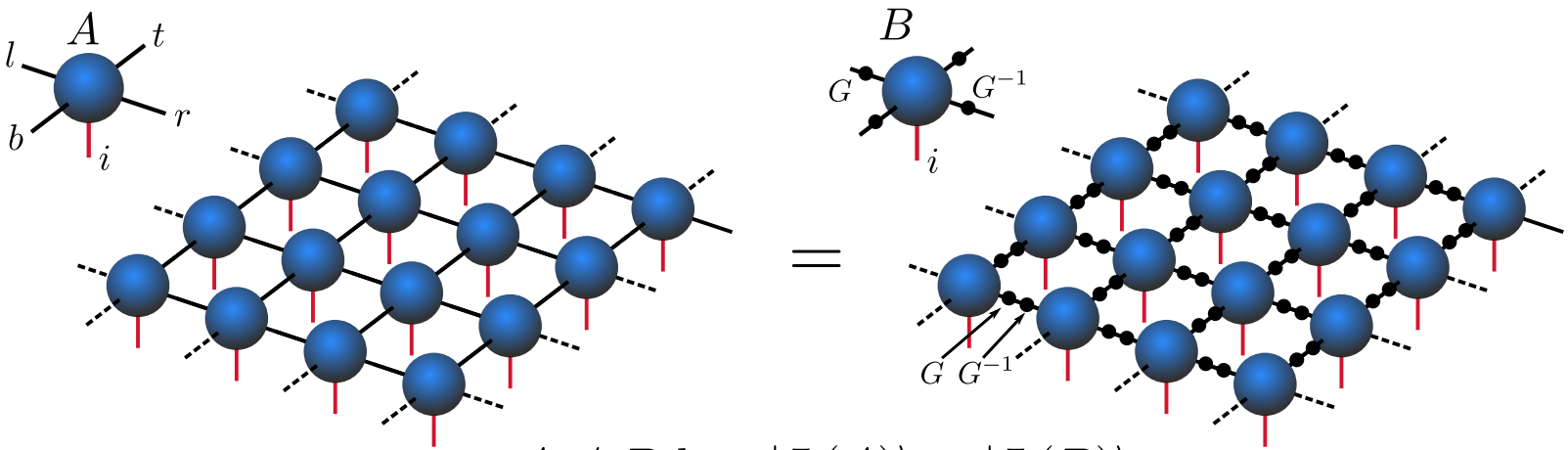


Gauge transformations and symmetries

Matrix Product States



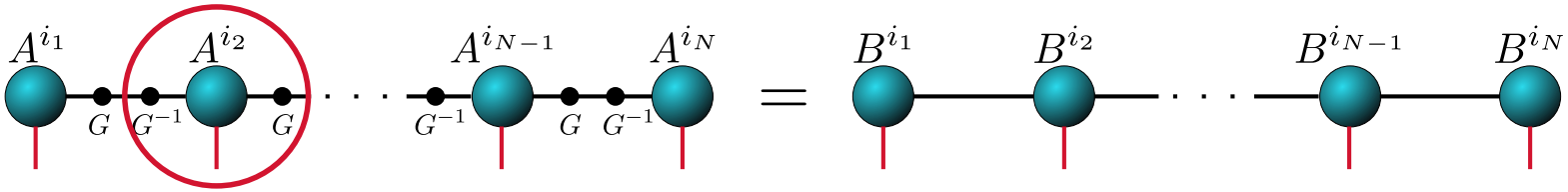
Projected Entangled Pair States



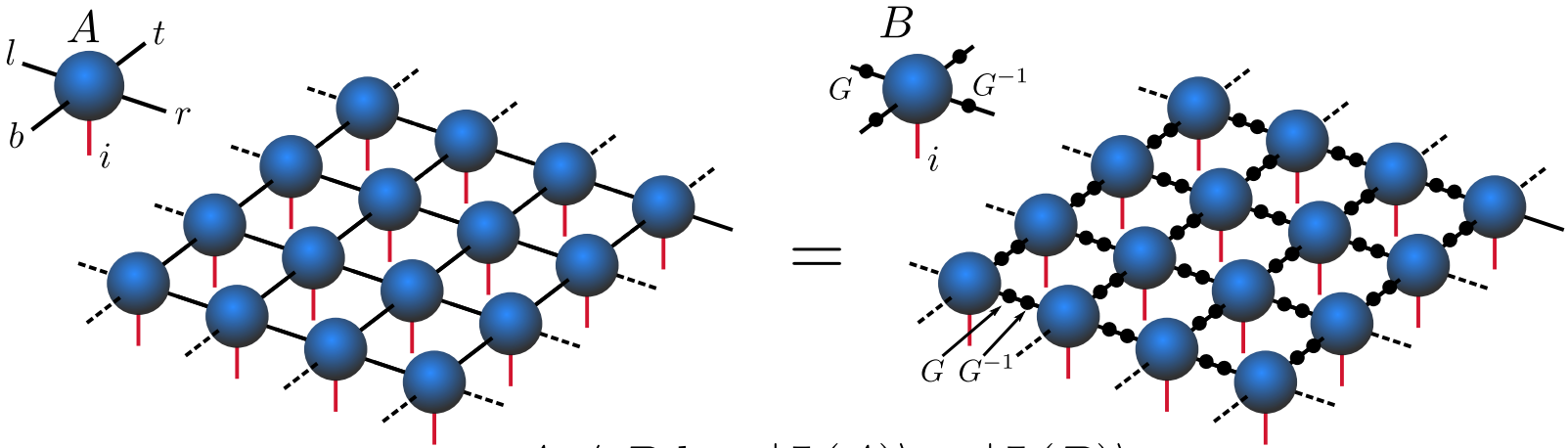
$A \neq B$ but $|\Psi(A)\rangle = |\Psi(B)\rangle$

Gauge transformations and symmetries

Matrix Product States

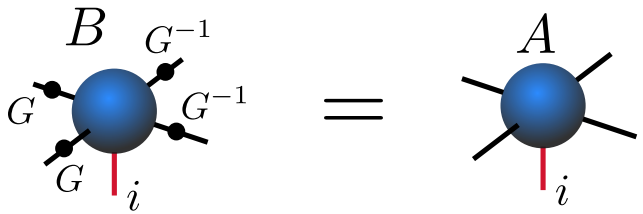


Projected Entangled Pair States



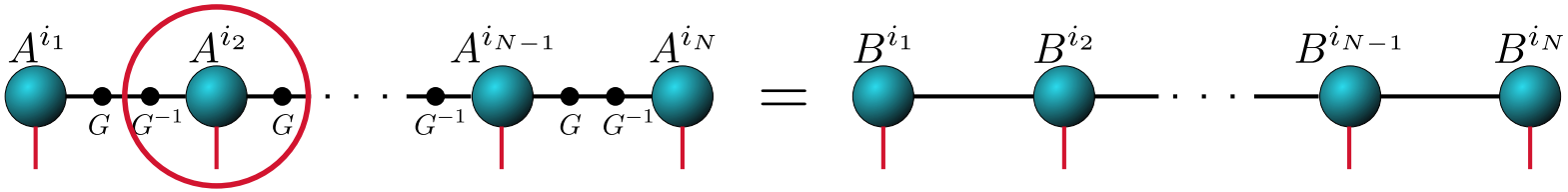
$A \neq B$ but $|\Psi(A)\rangle = |\Psi(B)\rangle$

MPO symmetry of PEPS

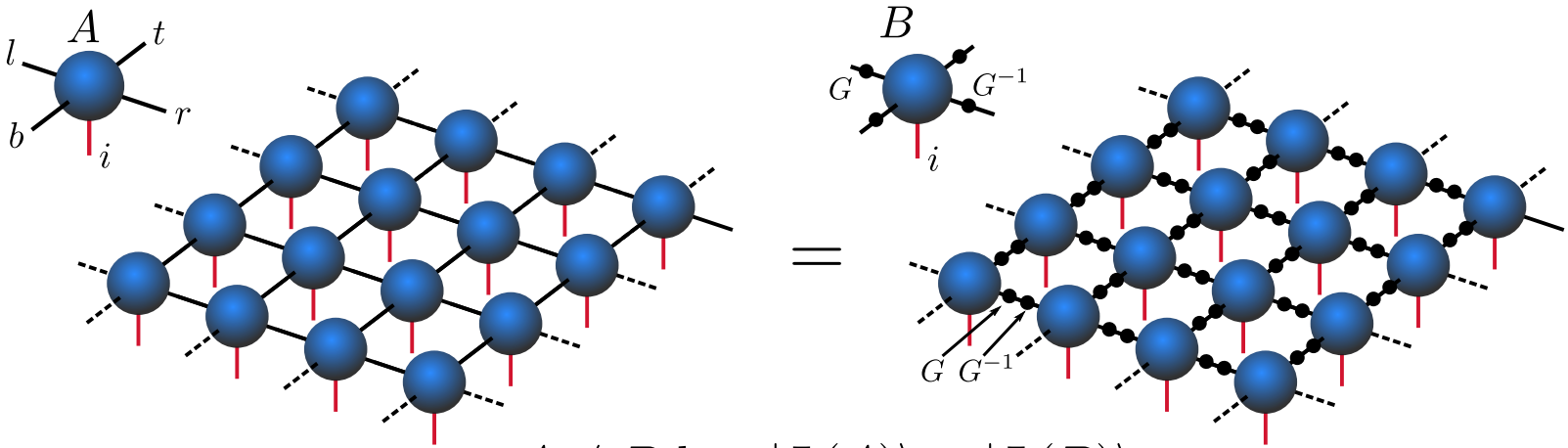


Gauge transformations and symmetries

Matrix Product States

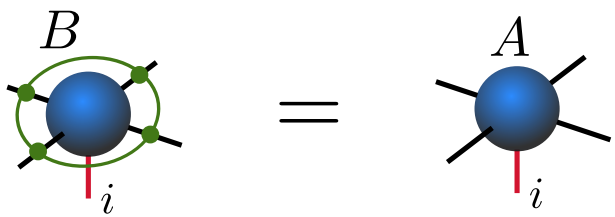


Projected Entangled Pair States



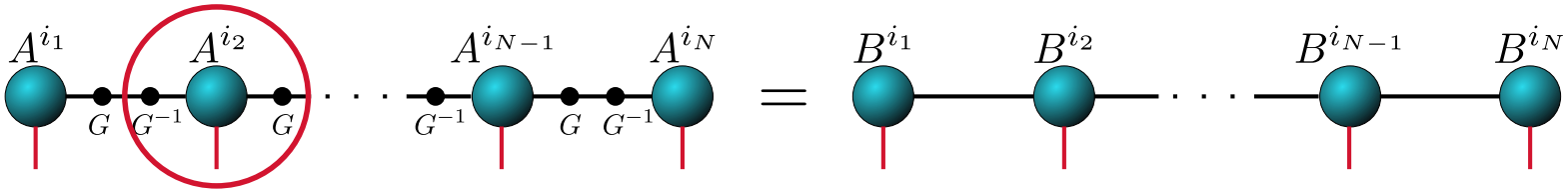
$A \neq B$ but $|\Psi(A)\rangle = |\Psi(B)\rangle$

MPO symmetry of PEPS

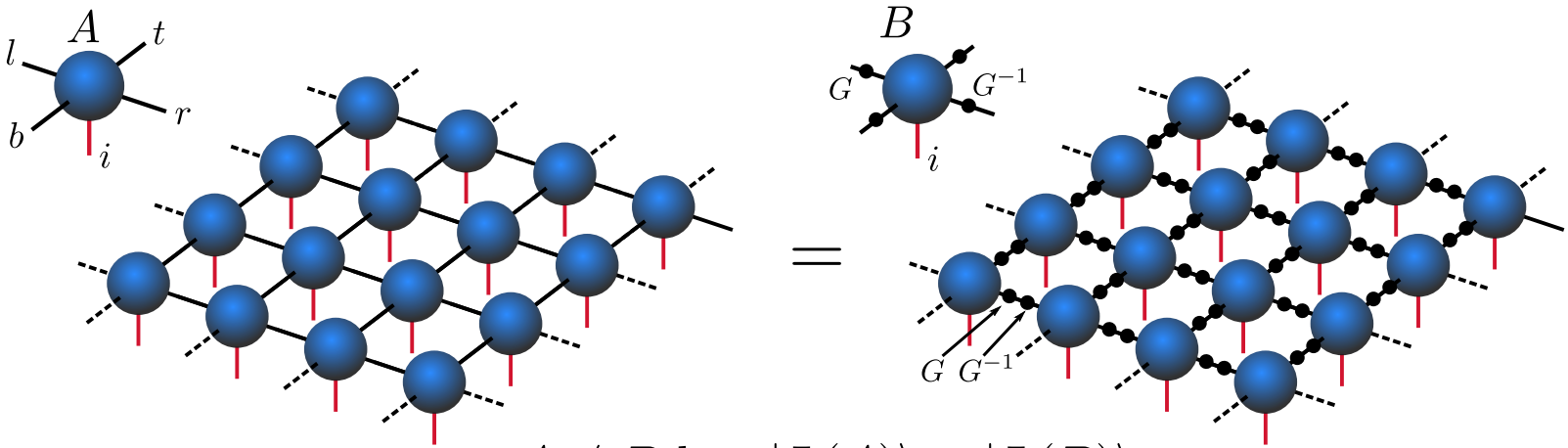


Gauge transformations and symmetries

Matrix Product States

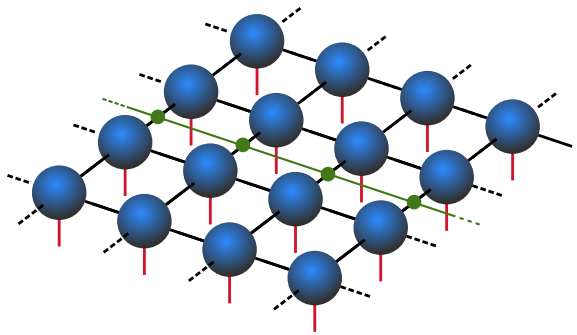


Projected Entangled Pair States

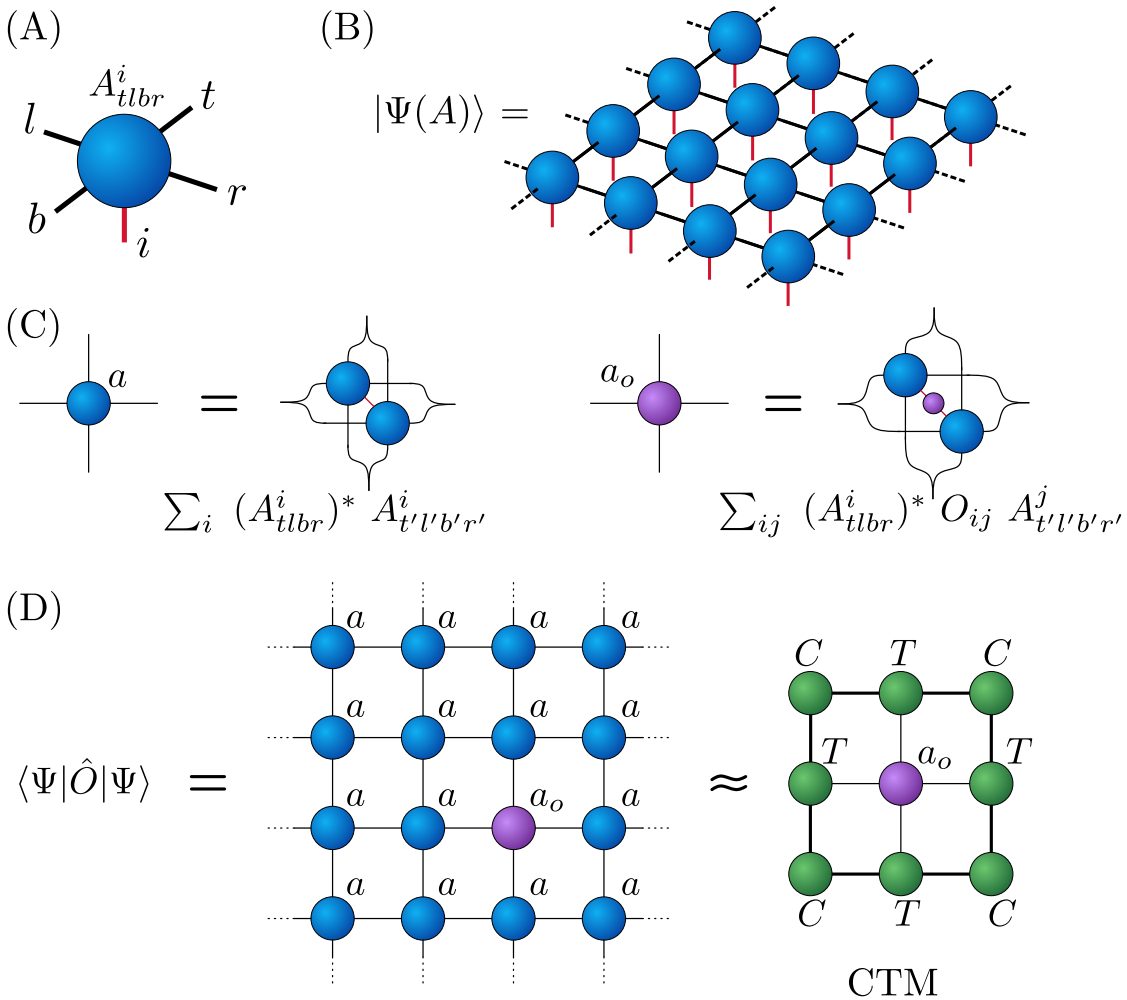


$$A \neq B \text{ but } |\Psi(A)\rangle = |\Psi(B)\rangle$$

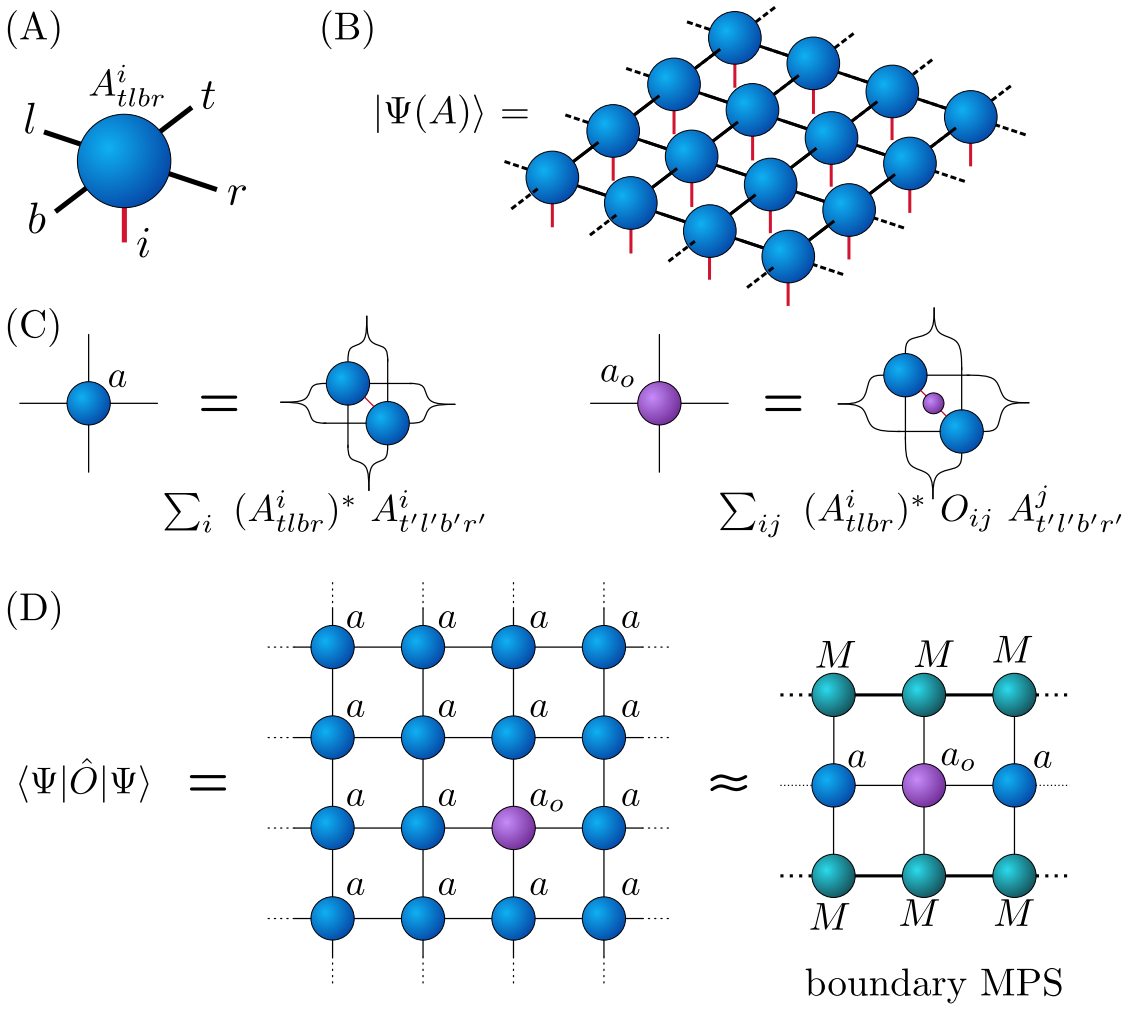
MPO symmetry of PEPS



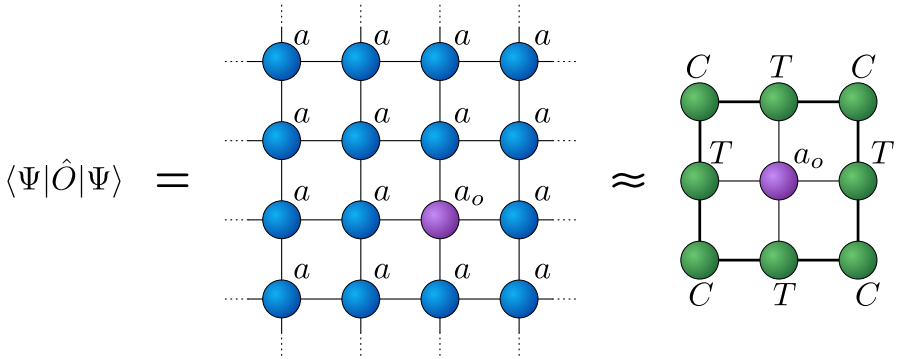
iPEPS contraction



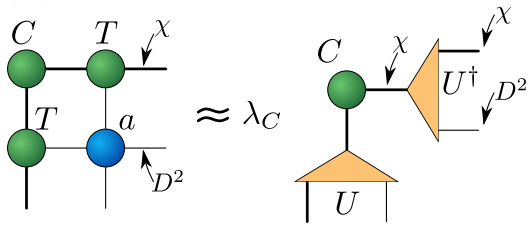
iPEPS contraction



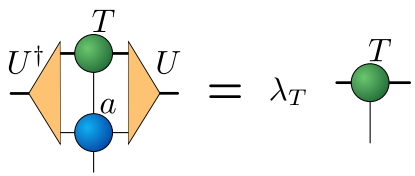
Corner Transfer Matrix



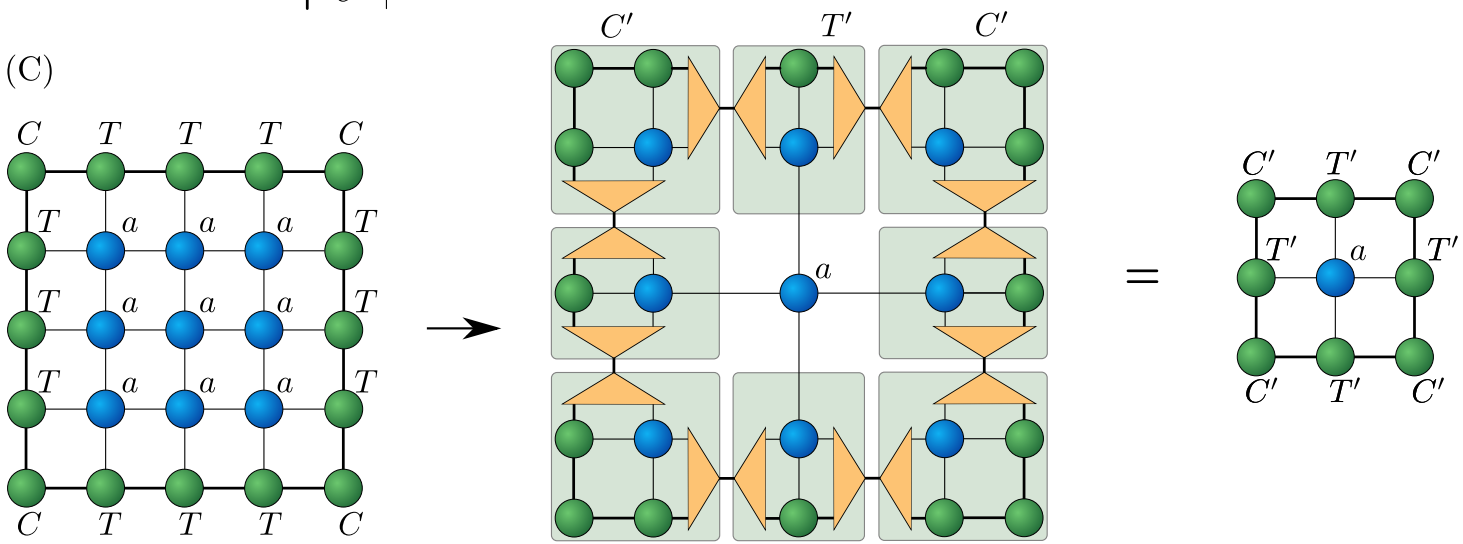
(A)



(B)



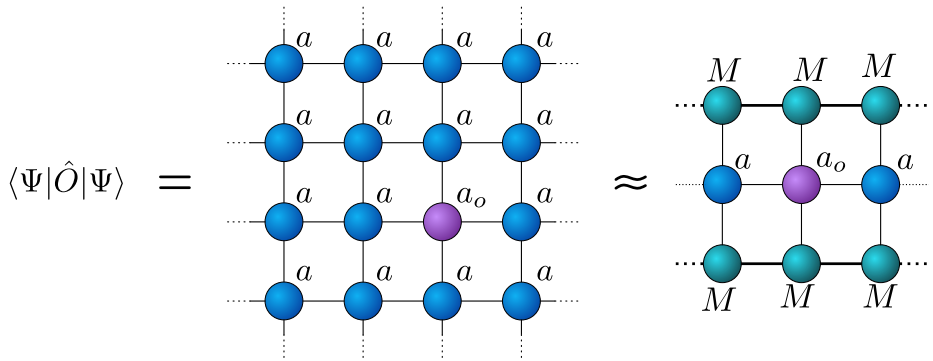
(C)

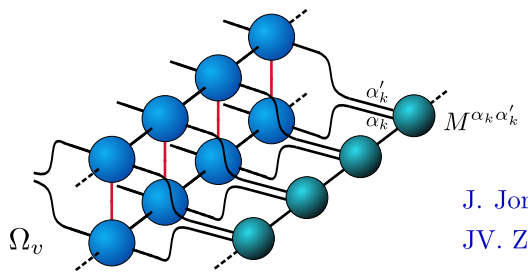


R. J. Baxter, Journal of Statistical Physics 19, 461 (1978)

T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. 65, 891 (1996)

Boundary MPS

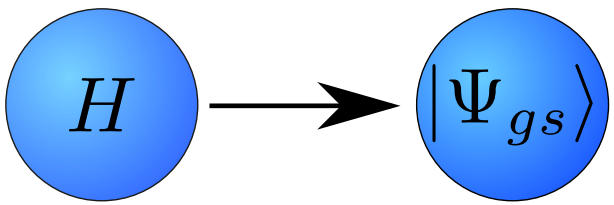




J. Jordan, R. Orús, G. Vidal, F. Verstraete, J. I.Cirac, PRL, 101, 250602 (2008)

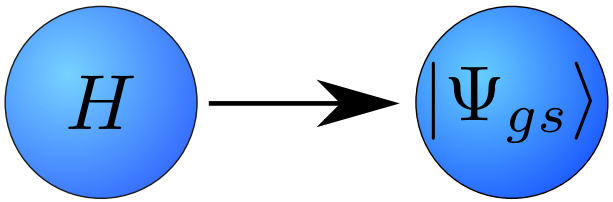
JV. Zauner-Stauber et al., Phys. Rev. B 97 (2018)

Variational iPEPS optimization



AF, N. Schuch, B. Vanhecke, arXiv:2311.11894

Variational iPEPS optimization



- Goal: optimize the ground state $|\Psi(A)\rangle$

$$E(A) = \frac{\langle\Psi(A)|\hat{H}|\Psi(A)\rangle}{\langle\Psi(A)|\Psi(A)\rangle} \quad \rightarrow \quad 0 = \frac{\partial}{\partial A}\frac{\langle\Psi(A)|\hat{H}|\Psi(A)\rangle}{\langle\Psi(A)|\Psi(A)\rangle} \Rightarrow |\Psi_{gs}(A^{\star})\rangle.$$

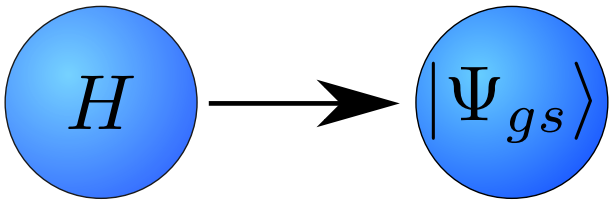
  algorithms: steepest descent, conjugate-gradient, L-BFGS

- Exact gradients within reach of AD:

  H-J. Liao, J-G. Liu, L. Wang, and T, Xiang, PRX 9, 031041 (2019)

  J. Hasik, D. Poilblanc, F. Becca, SciPost Phys. 10, 012 (2021)

Variational iPEPS optimization



- Goal: optimize the ground state $|\Psi(A)\rangle$

$$E(A) = \frac{\langle\Psi(A)|\hat{H}|\Psi(A)\rangle}{\langle\Psi(A)|\Psi(A)\rangle} \quad \rightarrow \quad 0 = \frac{\partial}{\partial A}\frac{\langle\Psi(A)|\hat{H}|\Psi(A)\rangle}{\langle\Psi(A)|\Psi(A)\rangle} \Rightarrow |\Psi_{gs}(A^{\star})\rangle.$$

  algorithms: steepest descent, conjugate-gradient, L-BFGS

- Exact gradients within reach of AD:

  H-J. Liao, J-G. Liu, L. Wang, and T, Xiang, PRX 9, 031041 (2019)

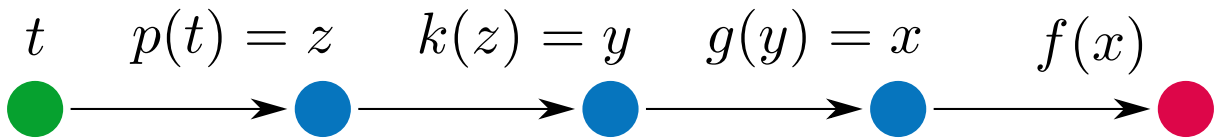
  J. Hasik, D. Poilblanc, F. Becca, SciPost Phys. 10, 012 (2021)

Can be problematic if treated as a black box: divergencies, inaccuracies

Automatic differentiation

Applies chain rule to the cost function automatically:

$$F(t) = f(g(k(p(t))))$$

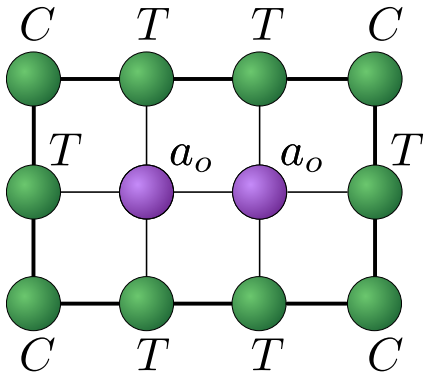


$$\frac{\partial F(t)}{\partial t_i} = \frac{\partial f(x)}{\partial x_j} \frac{\partial g(y)_j}{\partial y_n} \frac{\partial k(z)_n}{\partial z_m} \frac{\partial p(t)_m}{\partial t_i}$$

Energy gradient

Energy calculated approximately with CTM:

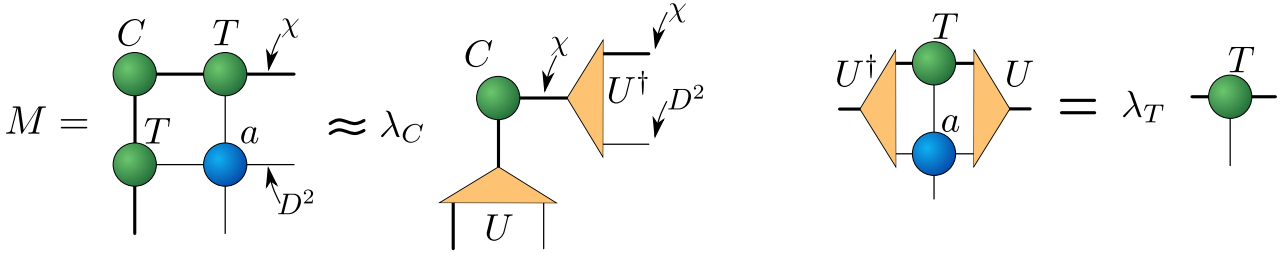
$$E \approx \tilde{E} = F(C, T, A, H) =$$



With $(C_k, T_k) \equiv x_k = f(x_{k-1}, A)$ its gradient is:

$$\begin{aligned} d\tilde{E} &= \frac{\partial F}{\partial A} dA + \frac{\partial F}{\partial x} dx, \\ dx &= \frac{\partial f}{\partial A} dA + \frac{\partial f}{\partial x_{n-1}} \left(\frac{\partial f}{\partial A} dA + \frac{\partial f}{\partial x_{n-2}} (...) \right) \end{aligned}$$

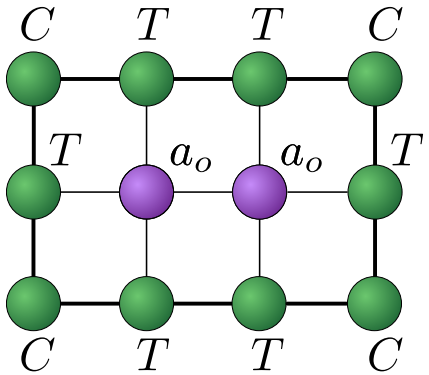
CTM:



Energy gradient

Energy calculated approximately with CTM:

$$E \approx \tilde{E} = F(C, T, A, H) =$$

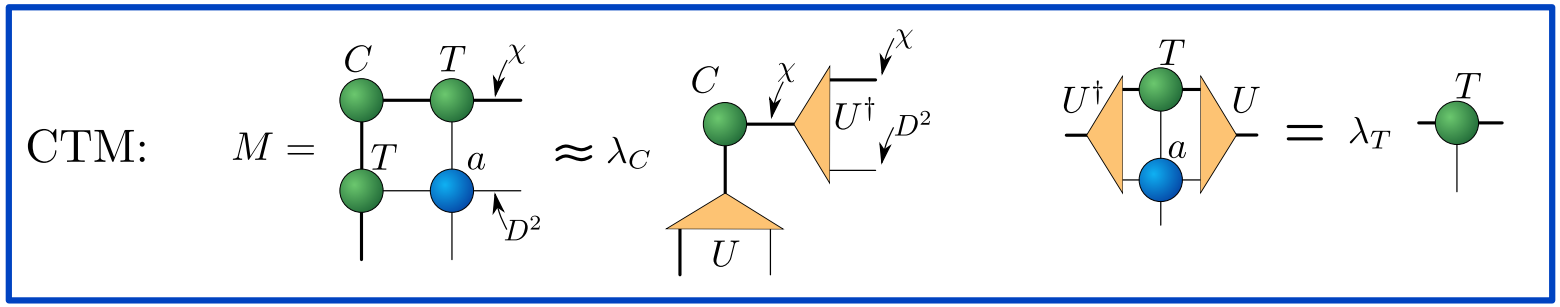


With $(C_k, T_k) \equiv x_k = f(x_{k-1}, A)$ its gradient is:

$$\begin{aligned} d\tilde{E} &= \frac{\partial F}{\partial A} dA + \frac{\partial F}{\partial x} dx, \\ dx &= \frac{\partial f}{\partial A} dA + \frac{\partial f}{\partial x_{n-1}} \left(\frac{\partial f}{\partial A} dA + \frac{\partial f}{\partial x_{n-2}} (...) \right) \end{aligned}$$

Problems:

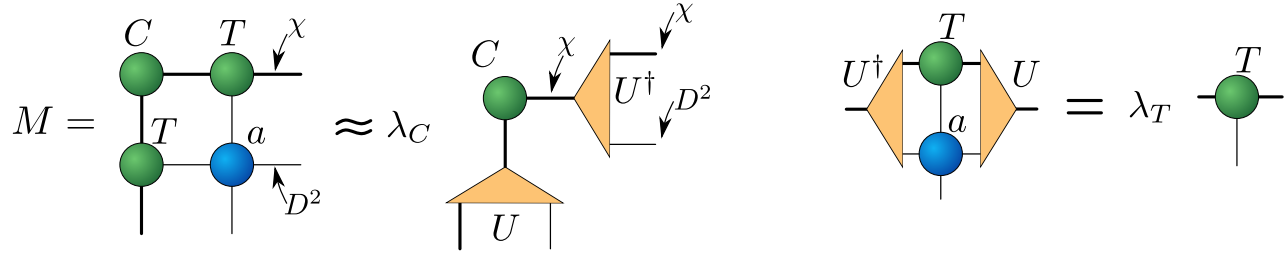
1. costly in memory, need for many iterations
2. gradient of EIG (SVD) poorly conditioned in case of degenerate spectra
3. currently only approximate!



Problem 1: memory intensive, many iterations

Solution: fixed point differentiation

$$dx = \sum_{k=0}^{\infty} \left(\frac{\partial f}{\partial x}\right)^k \frac{\partial f}{\partial A} dA = \left(1 - \frac{\partial f}{\partial x}\right)^{-1} \frac{\partial f}{\partial A} dA.$$

CTM: 

Problem 1: memory intensive, many iterations

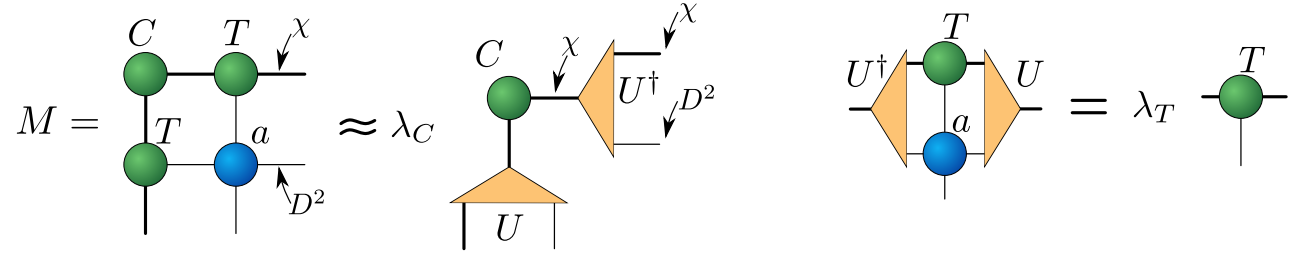
Solution: fixed point differentiation

$$dx = \sum_{k=0}^{\infty} \left(\frac{\partial f}{\partial x}\right)^k \frac{\partial f}{\partial A} dA = \left(1 - \frac{\partial f}{\partial x}\right)^{-1} \frac{\partial f}{\partial A} dA.$$

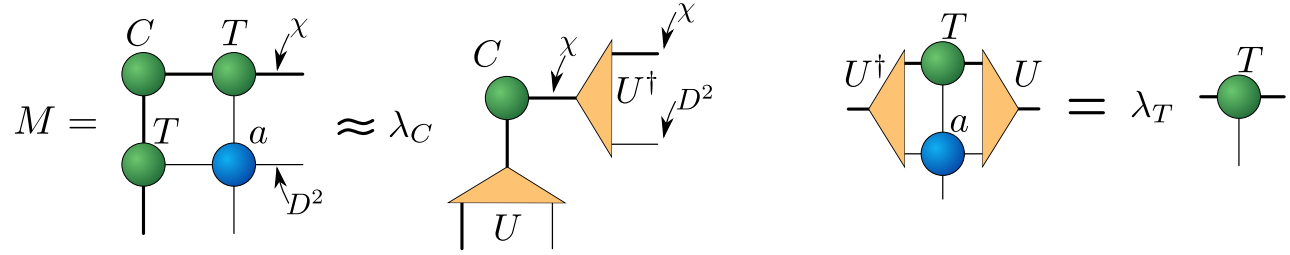
But: requires element-wise convergence $x = f(x, A)$

$$UCU^\dagger = (U\sigma)\, C\, (\sigma^\dagger U^\dagger) \;\Rightarrow\; \hat{T} \xrightarrow{\mathsf{f}} \sigma^\dagger \hat{T} \sigma = T.$$

with σ satisfying additionally $[C, \sigma] = 0,\ \sigma\sigma^\dagger = \mathbb{I}$

CTM: 

Problem 2&3: gradient of EIG(SVD): divergent, approximate

CTM: 

Problem 2&3: gradient of EIG(SVD): divergent, approximate

Solution: Q-deformed CTM with $Q = \mathbb{I}$ and full M eigedecomposition

regular CTM

$$M \approx UsU^\dagger$$

Q-deformed CTM with full M decomposition

$$M = PCP^\dagger + P_\perp C_\perp P_\perp^\dagger$$

$\longrightarrow$

$$ds = \mathbb{I} \circ (U^\dagger dM U)$$
$$dU = Ud\omega + U_\perp dX$$
$$d\omega = F \circ (U^\dagger dM U)$$
$$F_{ij} = \frac{1}{s_j - s_i},\ i \neq j$$
$$(\mathbb{I} - UU^\dagger) dM U = U_\perp dX s$$

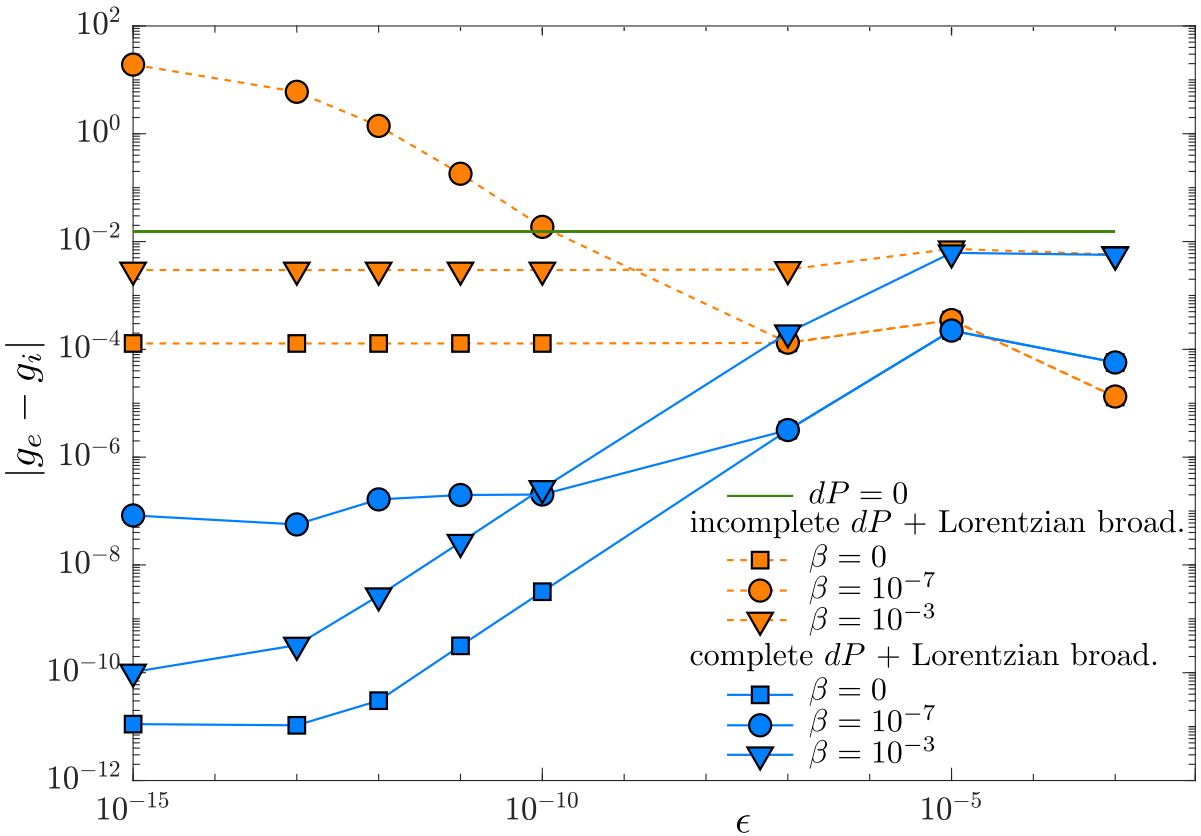
$$dC = P^\dagger dM P$$
$$dP = Pd\omega + P_\perp dX$$
$$d\omega = 0$$
$$(\mathbb{I} - PP^\dagger) dM P = dPC - \underline{(\mathbb{I} - PP^\dagger) M dP}$$

Comparison of gradients

State: $|\Psi(A)\rangle$: $A = \mathcal{A}_{RVB}^{SU(2)} + \beta \mathcal{A}^{SB}$, with $D = 3, \chi = 160$

Hamiltonian: $H = J_1 \sum_{i,j \in NN, \alpha} f(\alpha) S_i^\alpha S_j^\alpha + J_2 \sum_{i,j \in NNN} \vec{S}_i \cdot \vec{S}_j$

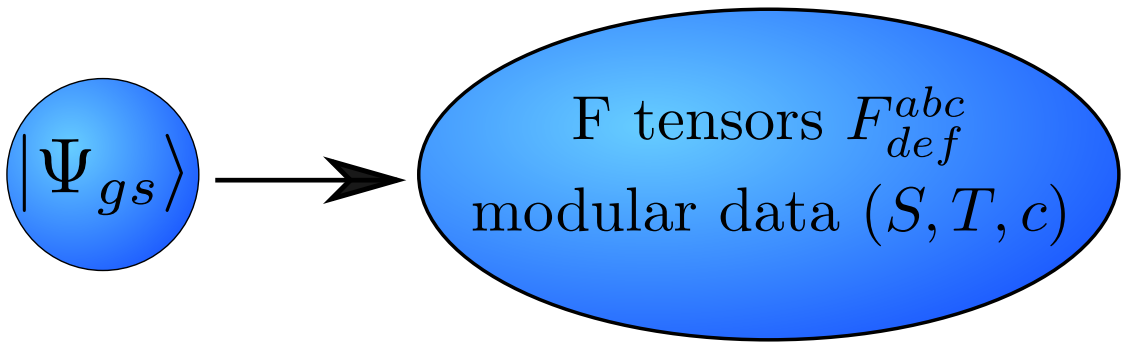
with $SU(2)$ symmetry breaking anisotropy $f([x, y, z]) = [-1, 1 + \beta, -1 + \beta]$



- our gradient g_e
- Green: $dP = 0$*
- Orange: current AD
- Blue: using Sylvester equation for dP

*SPG Crone, P Corboz PRB 101 (11), 115143 (2020)

Determining Topological order



AF, J. Dziarmaga, G. Vidal, L. Cincio, PRB 101, 041108(R)

AF, J. Dziarmaga, PRB 102 (23), 235112

AF, L. Lootens, J. Dziarmaga, F. Verstraete, PRB 104 (19), 195152

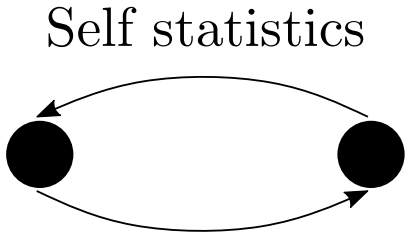
Characterization of topological order

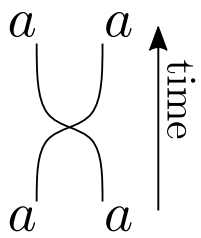
1. Mutual and self statistics – modular data (S, T, c)

2. Fusion categories – F symbols F^{abc}_{def}

Characterization of topological order

1. Mutual and self statistics – modular data (S, T, c)
   - Topological T matrix – self statistics

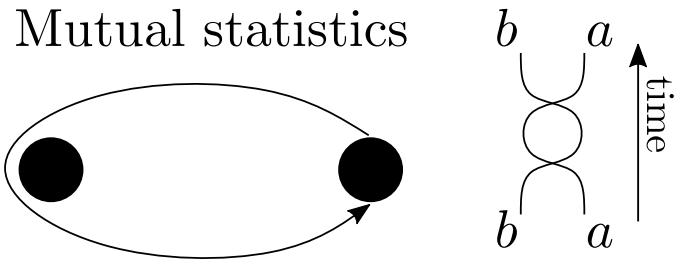




2. Fusion categories – F symbols F^{abc}_{def}

Characterization of topological order

1. Mutual and self statistics – modular data (S, T, c)
   - Topological T matrix – self statistics
   - Topological S matrix – mutual statistics

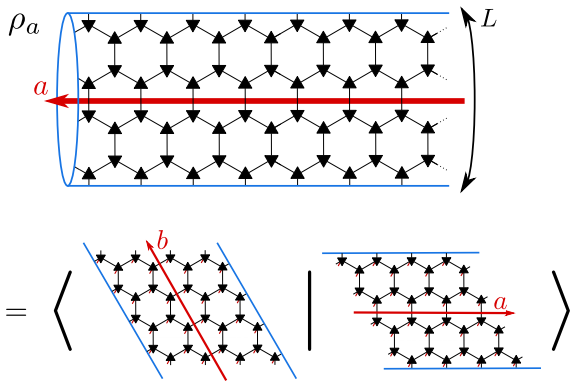


2. Fusion categories – F symbols F^{abc}_{def}

Characterization of topological order

1. Mutual and self statistics – modular data (S, T, c)
   - Topological T matrix – self statistics
   - Topological S matrix – mutual statistics
   - Can be extracted from ground states:

$$(S \cdot T)_{ab} = \langle \Psi_b^{\mathfrak{st}} | \Psi_a \rangle$$



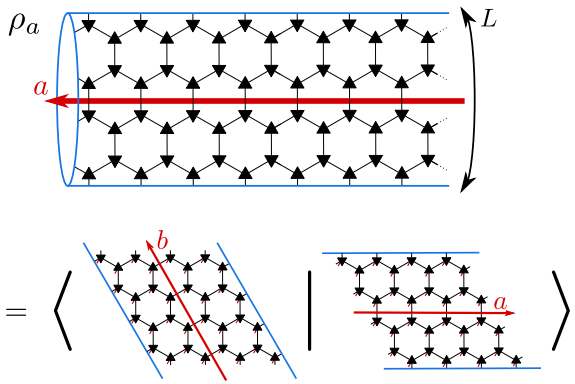
Y. Zhang, T. Grover, A. Turner, M. Oshikawa, A. Vishwanath, PRB (2012)

2. Fusion categories – F symbols F^{abc}_{def}

Characterization of topological order

1. Mutual and self statistics – modular data (S, T, c)
   - Topological T matrix – self statistics
   - Topological S matrix – mutual statistics
   - Can be extracted from ground states:

$$(S \cdot T)_{ab} = \langle \Psi_b^{\mathfrak{st}} | \Psi_a \rangle$$

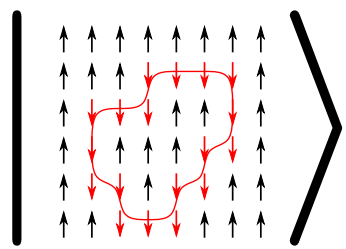


Y. Zhang, T. Grover, A. Turner, M. Oshikawa, A. Vishwanath, PRB (2012)

2. Fusion categories – F symbols F_{def}^{abc}

$$|\Phi_{Z_2}\rangle = \sum_{all\ closed\ strings}$$

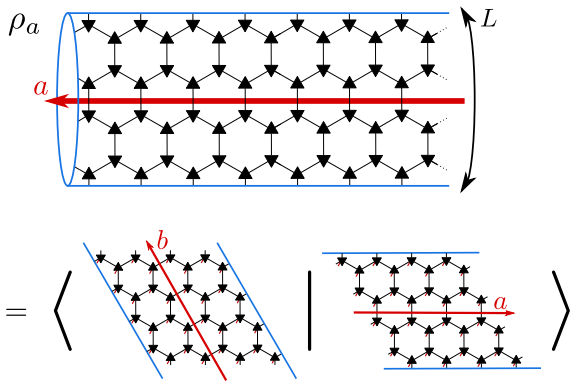
$$|\Phi_{ds}\rangle = \sum_{all\ closed\ strings} (-1)^{N_{loops}}$$



Characterization of topological order

1. Mutual and self statistics – modular data (S, T, c)
   - Topological T matrix – self statistics
   - Topological S matrix – mutual statistics
   - Can be extracted from ground states:

$$(S \cdot T)_{ab} = \langle \Psi_b^{\mathfrak{st}} | \Psi_a \rangle$$

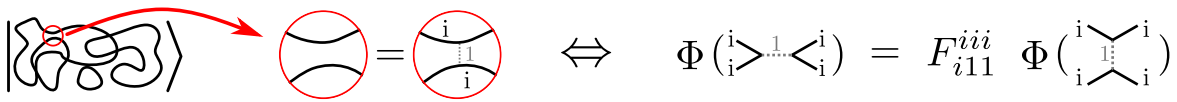


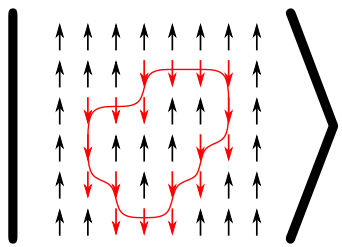
Y. Zhang, T. Grover, A. Turner, M. Oshikawa, A. Vishwanath, PRB (2012)

2. Fusion categories – F symbols F_{def}^{abc}

$$|\Phi_{Z_2}\rangle = \sum_{all\ closed\ strings}$$

$$|\Phi_{ds}\rangle = \sum_{all\ closed\ strings} (-1)^{N_{loops}}$$

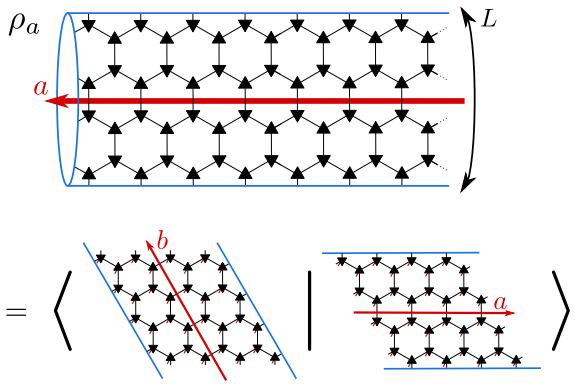




Characterization of topological order

1. Mutual and self statistics – modular data (S, T, c)
   - Topological T matrix – self statistics
   - Topological S matrix – mutual statistics
   - Can be extracted from ground states:

$$(S \cdot T)_{ab} = \langle \Psi_b^{\mathfrak{st}} | \Psi_a \rangle$$



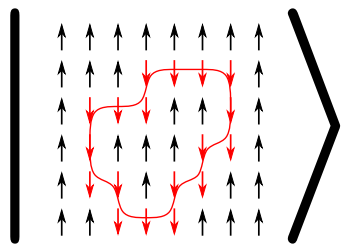
Y. Zhang, T. Grover, A. Turner, M. Oshikawa, A. Vishwanath, PRB (2012)

2. Fusion categories – F symbols F^{abc}_{def}

$$|\Phi_{Z_2}\rangle = \sum_{all\ closed\ strings}$$

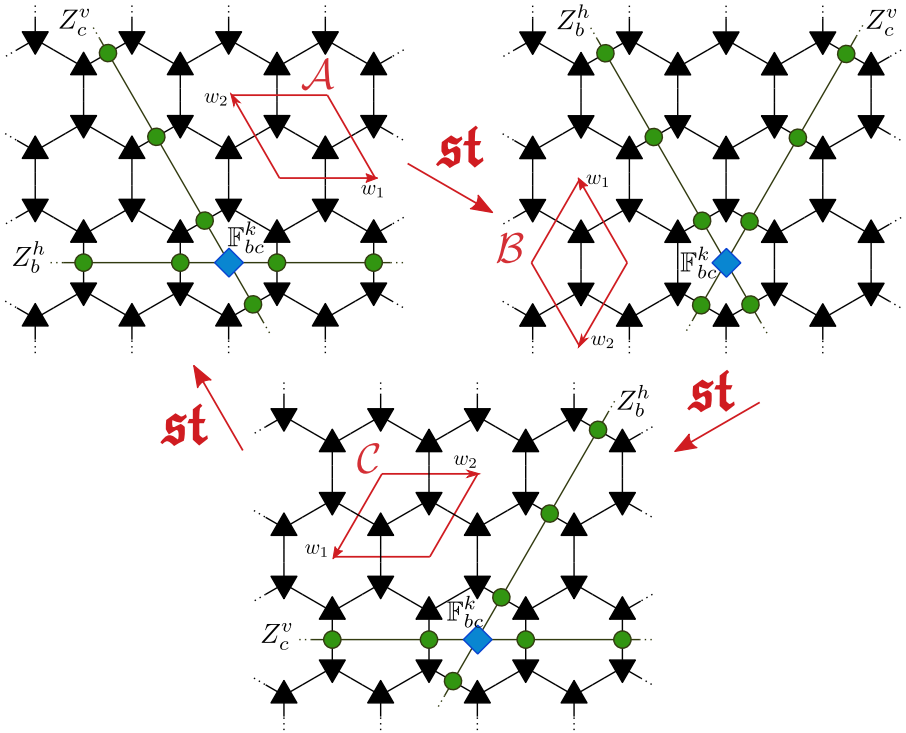
$$|\Phi_{ds}\rangle = \sum_{all\ closed\ strings} (-1)^{N_{loops}}$$

$$\Phi\left(\begin{smallmatrix} \mathrm{i} & & \mathrm{l} \\ & \mathrm{m} & \\ \mathrm{j} & & \mathrm{k} \end{smallmatrix}\right) = \sum_n F^{ijk}_{lmn}\ \Phi\left(\begin{smallmatrix} \mathrm{i} & & \mathrm{l} \\ & \mathrm{n} & \\ \mathrm{j} & & \mathrm{k} \end{smallmatrix}\right)$$



M. A. Levin, X. G. Wen, PRB (2012)

1. Extracting topological S and T matrices:

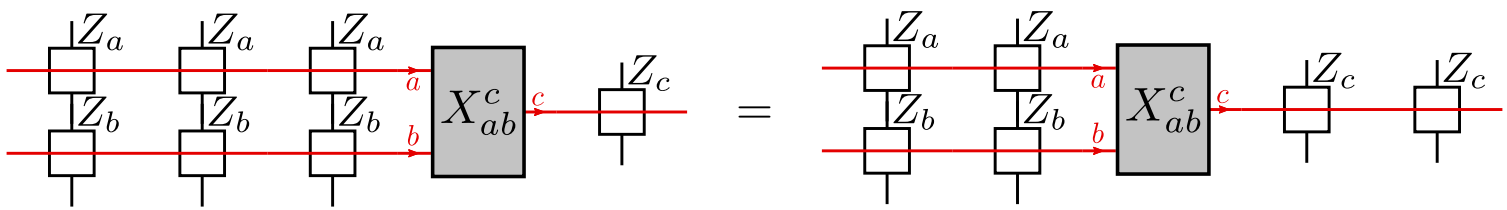


Crucial step:

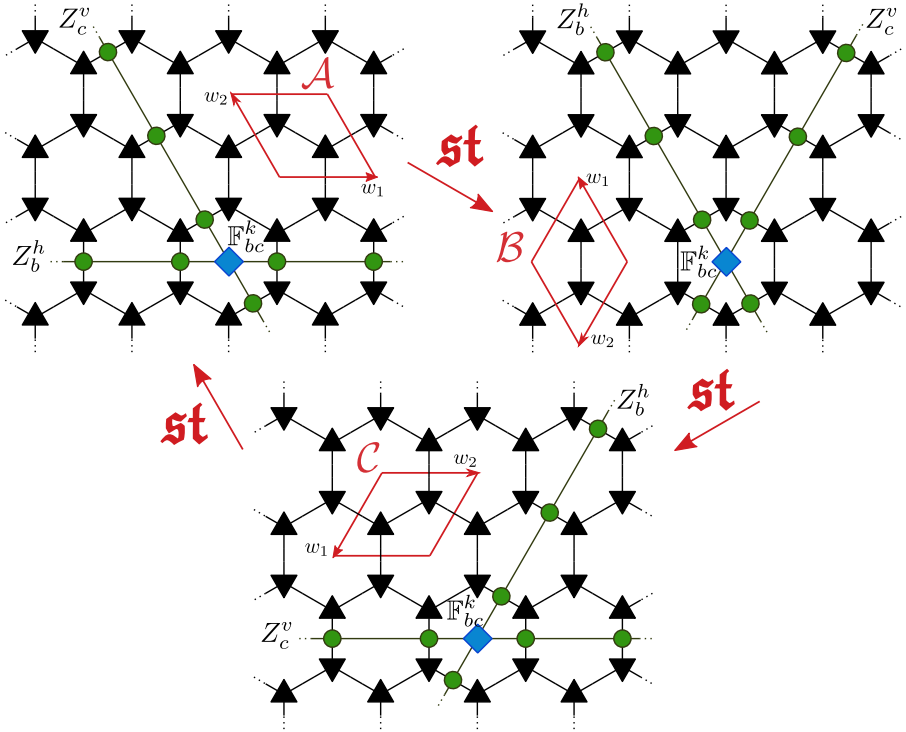
numerical optimization of iMPO symmetries of iPEPS, obeying fusion ring:

$$Z_a \cdot Z_b = \sum_c N_{ab}^c Z_c$$

2. Calculating F symbols



1. Extracting topological S and T matrices:

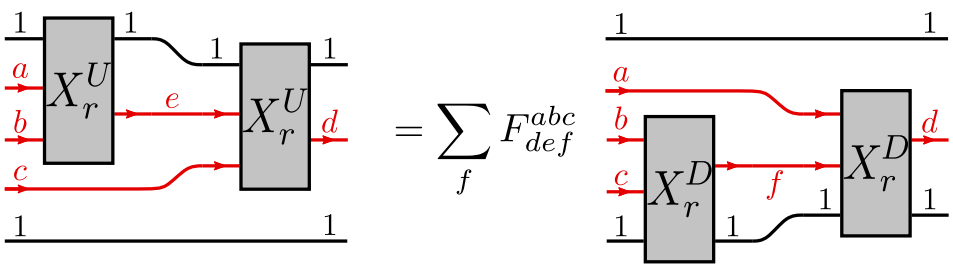


Crucial step:

numerical optimization of iMPO symmetries of iPEPS, obeying fusion ring:

$$Z_a \cdot Z_b = \sum_c N_{ab}^c Z_c$$

2. Calculating F symbols



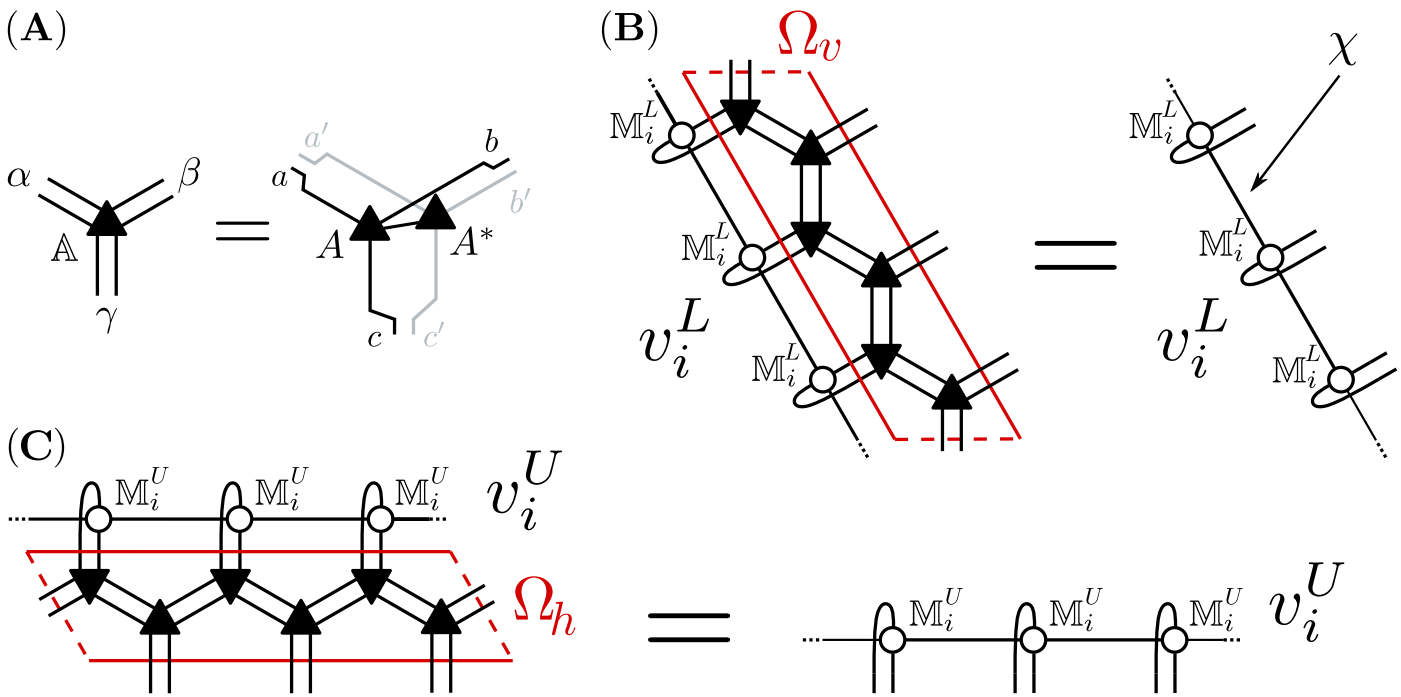
Fundamental theorem of MPS:
Gauge transf. X_{ab}^c, $(X_{ab}^c)^{-1}$

J.I.Cirac, D.Pérez-García, N.Schuch, F.Verstraete, Annals of Physics (2017)

Computational aspects

Obtaining iMPO symmetries of iPEPS

- Find all boundary iMPO fixed points V_i (V. Zauner-Stauber et al, PRB 97, 045145)



Obtaining iMPO symmetries of iPEPS

- Find all boundary iMPO fixed points V_i (V. Zauner-Stauber et al, PRB 97, 045145)
- Find all iMPO symmetries and their fusion rules: $Z_a Z_b = \sum_c N_{ab}^c Z_c$

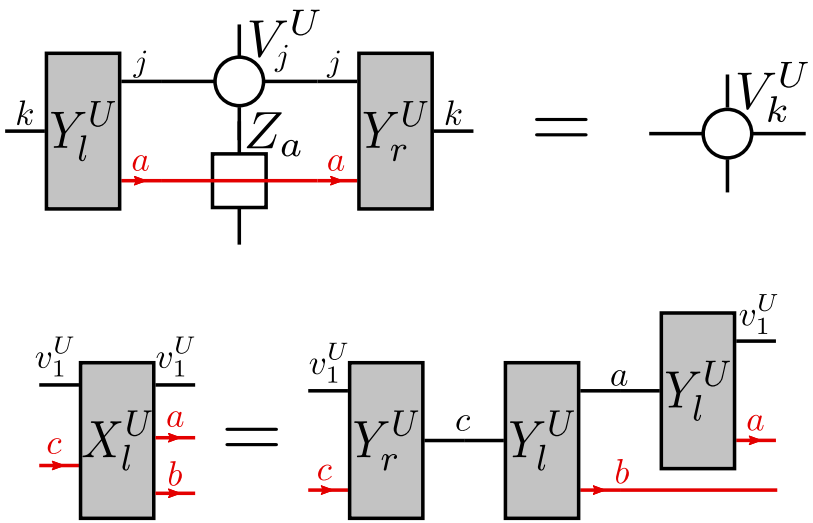
$$\min_{Z_a} |V_i \cdot Z_a - V_j|^2$$

F-symbols

Symmetry Z with minimal bond dimension obtained from:

$$\min_{Z_a} \; |v_1^U \cdot Z_a - v_a^U|^2 + |v_1^D \cdot Z_a^T - v_{\bar{a}}^D|^2$$

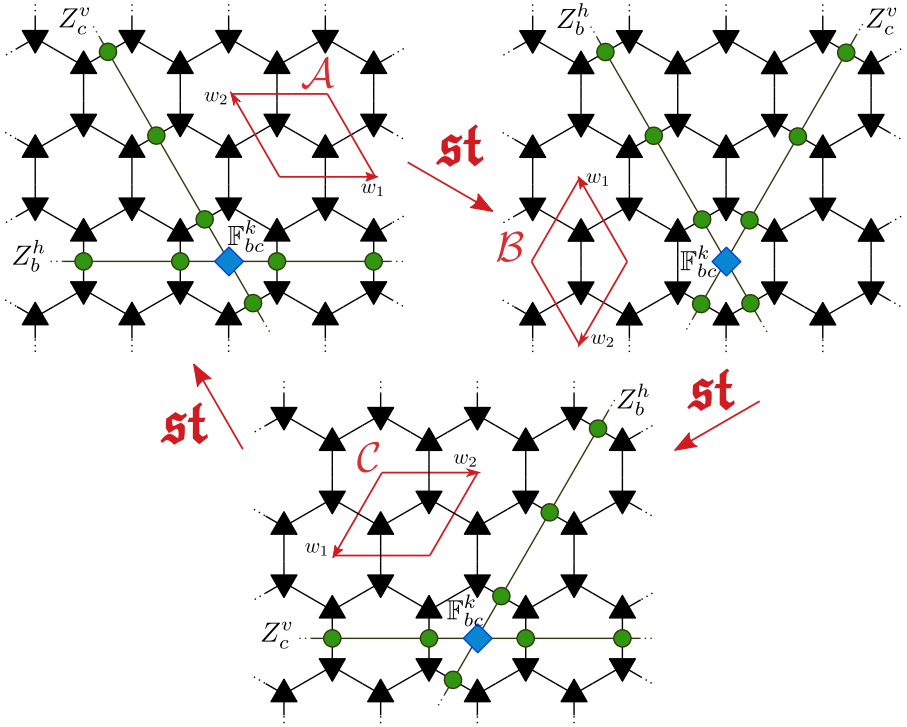
X zipper obtained from Y zippers:



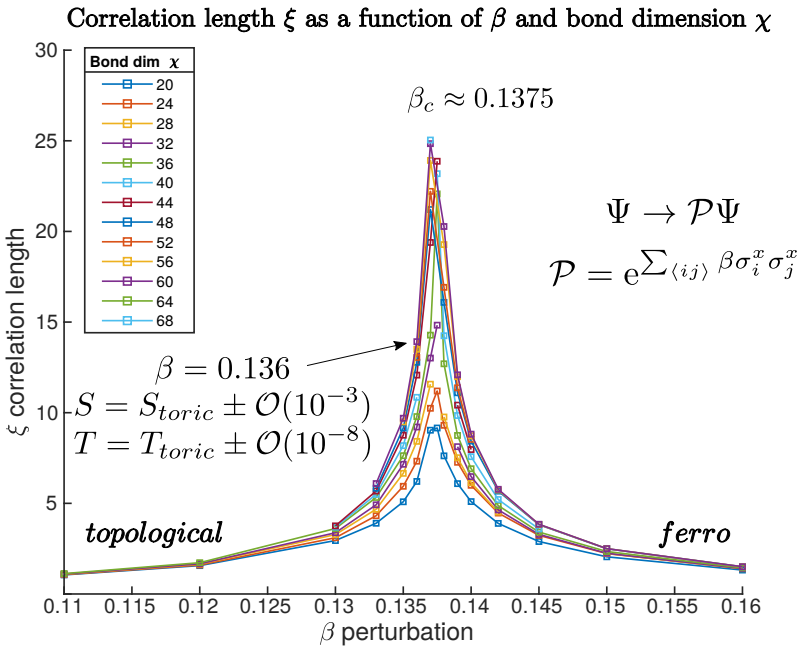
Results

AF, J. Dziarmaga, G. Vidal, L. Cincio, PRB 101, 041108(R)
AF, J. Dziarmaga, PRB 102 (23), 235112
AF, L. Lootens, J. Dziarmaga, F. Verstraete, PRB 104 (19), 195152

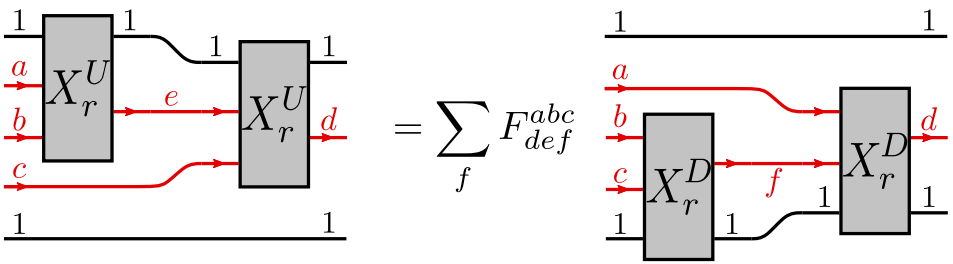
1. Extracting topological S and T matrices:



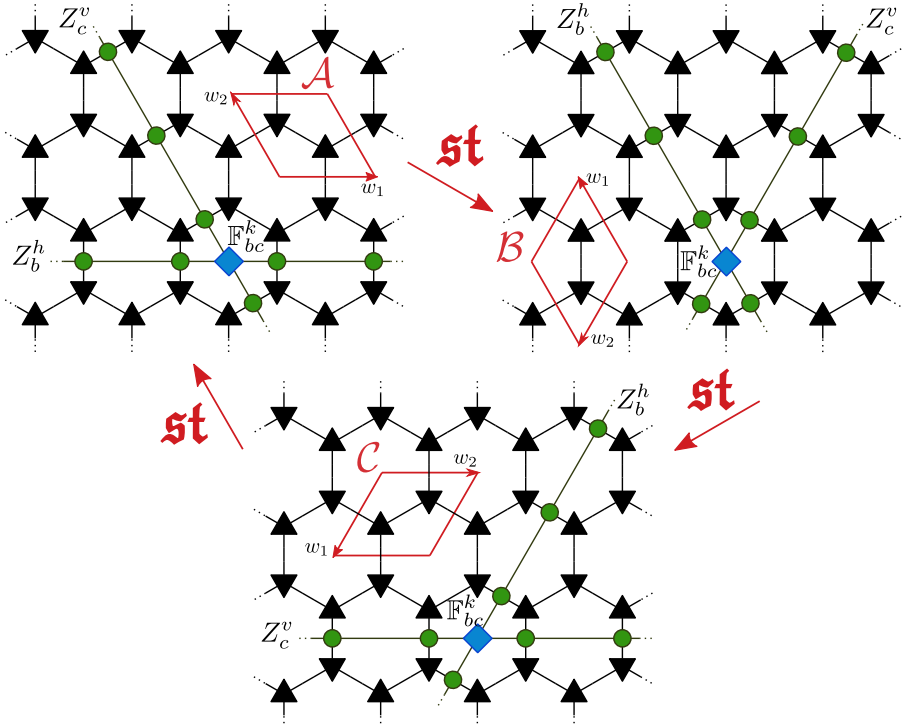
Ferromagnetic perturbation of the toric code:



2. Calculating F symbols

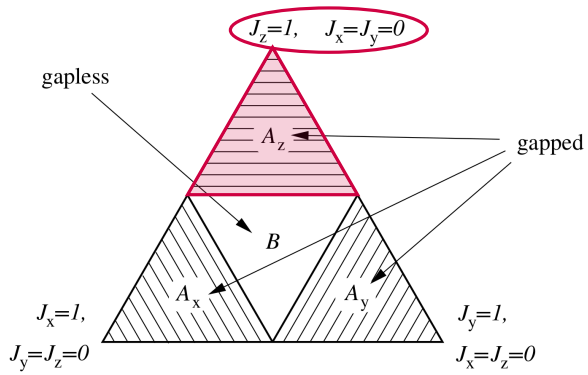


1. Extracting topological S and T matrices:



Kitaev model in Abelian phase:

$$H = -\sum_{\gamma-link} J_\gamma \sigma_j^\gamma \sigma_k^\gamma$$

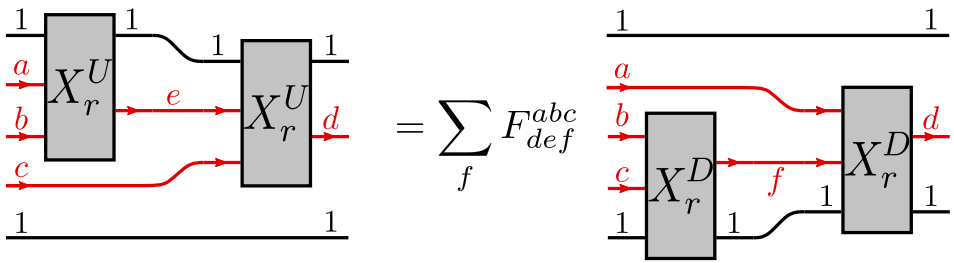


$$S = S_{\text{tc}} + \epsilon_S, \quad T = T_{\text{tc}} + \epsilon_T \,,$$

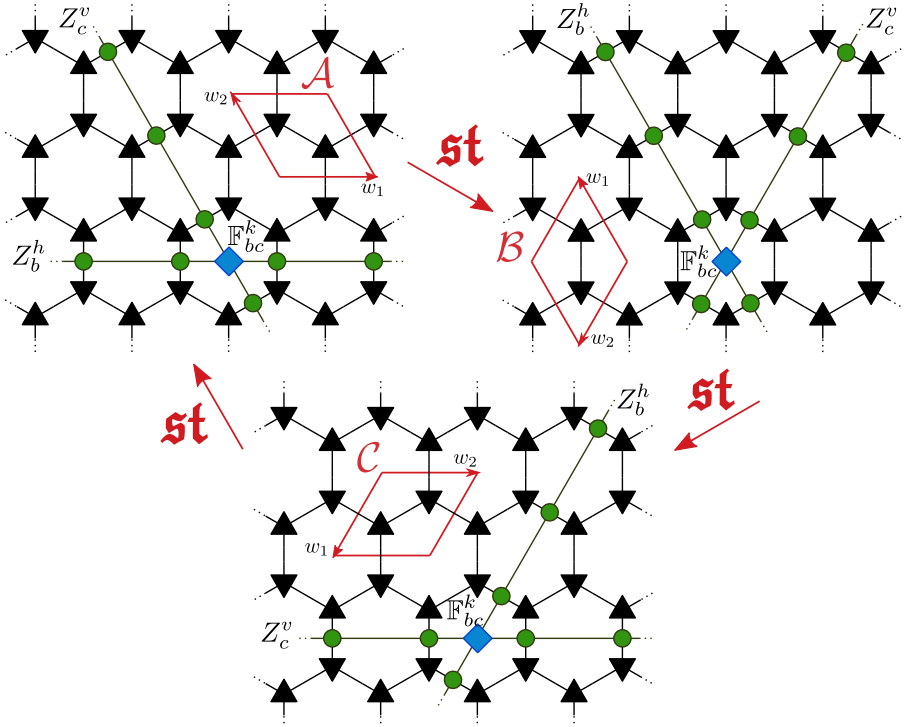
$$|\epsilon_S|_{max}, |\epsilon_T|_{max} \sim \mathcal{O}(10^{-3})$$

A.Kitaev, Annals of Physics (2006)

2. Calculating F symbols

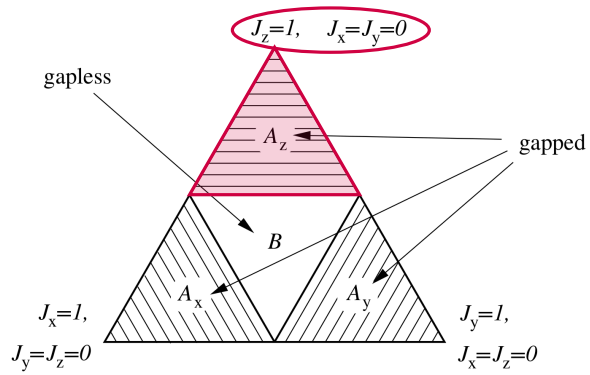


1. Extracting topological S and T matrices:



Kitaev model in Abelian phase:

$$H = -\sum_{\gamma-link} J_\gamma \sigma_j^\gamma \sigma_k^\gamma$$

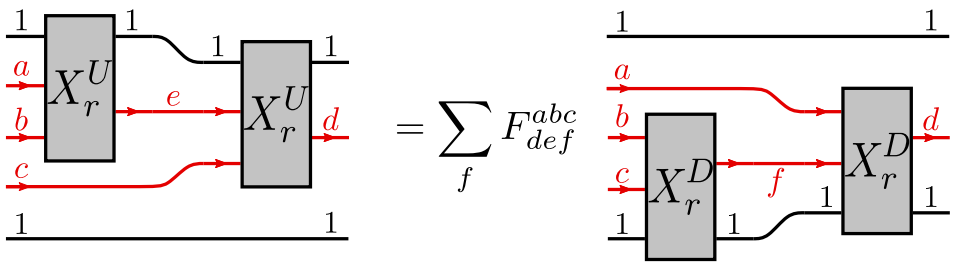


$$S = S_{\text{tc}} + \epsilon_S, \quad T = T_{\text{tc}} + \epsilon_T \,,$$

$$|\epsilon_S|_{max}, |\epsilon_T|_{max} \sim \mathcal{O}(10^{-3})$$

A.Kitaev, Annals of Physics (2006)

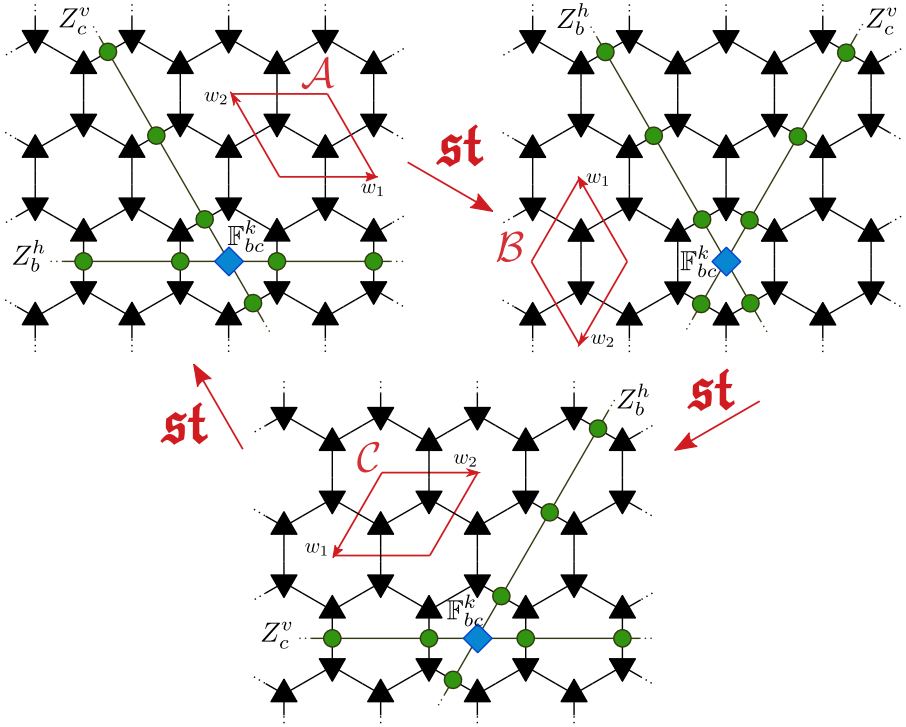
2. Calculating F symbols



For $J = 0.44$, $|\epsilon_F| \sim \mathcal{O}(10^{-4})$

$$|\epsilon_S|_{max}, |\epsilon_T|_{max} \sim \mathcal{O}(10^{-4})$$

1. Extracting topological S and T matrices:



Longer correlation lengths, $\xi > 1$:

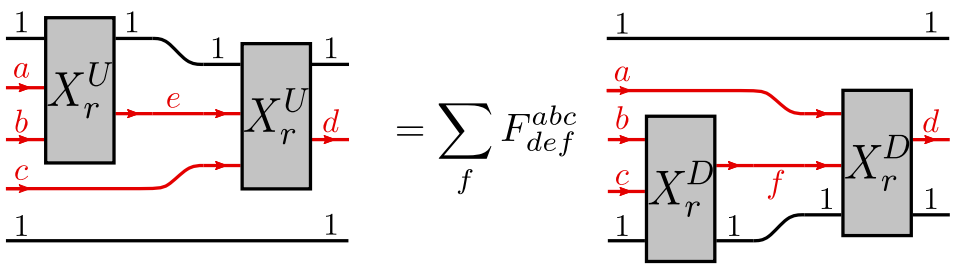
Apply local filtering to *dFib*:

$$|\Psi\rangle = \prod_i e^{\beta\sigma_i^z} |\Psi_{dFib}\rangle$$

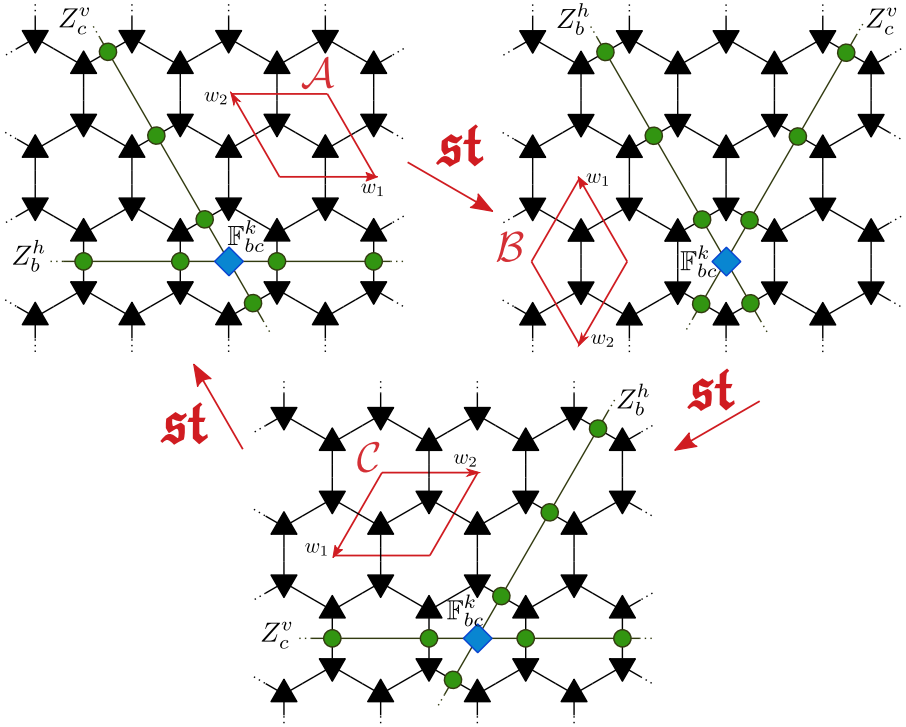
$\xi = 2.3$:

$$|\epsilon_S|_{max} \sim \mathcal{O}(10^{-3}),$$
$$|\epsilon_T|_{max} \sim \mathcal{O}(10^{-7})$$

2. Calculating F symbols



1. Extracting topological S and T matrices:



Longer correlation lengths, $\xi > 1$:

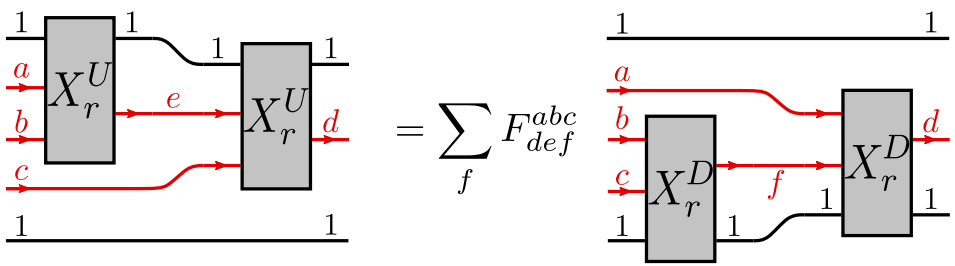
Apply local filtering to *dFib*:

$$|\Psi\rangle = \prod_i e^{\beta\sigma_i^z} |\Psi_{dFib}\rangle$$

$\xi = 2.3$:

$$|\epsilon_S|_{max} \sim \mathcal{O}(10^{-3}),$$
$$|\epsilon_T|_{max} \sim \mathcal{O}(10^{-7})$$

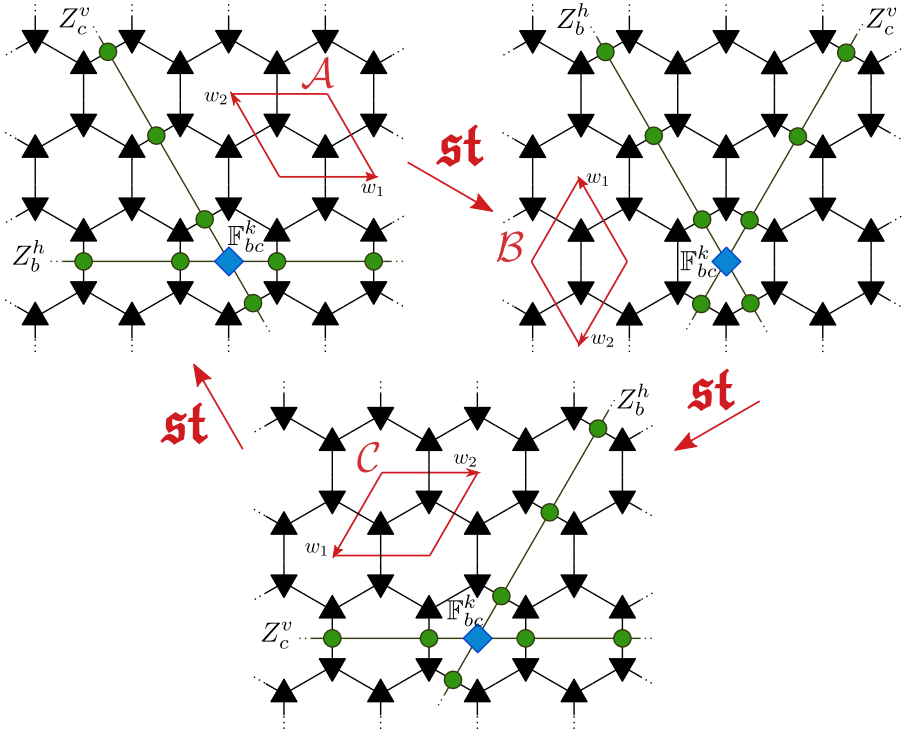
2. Calculating F symbols



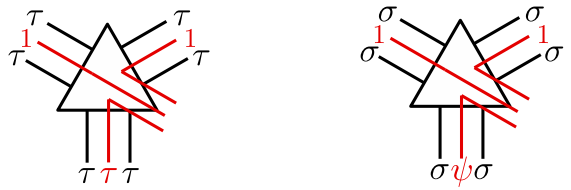
$$\xi = 2.3 : \ |\epsilon_F| \sim \mathcal{O}(10^{-2})$$

$$|\epsilon_S|_{max} \sim \mathcal{O}(10^{-3}),$$
$$|\epsilon_T|_{max} \sim \mathcal{O}(10^{-6})$$

1. Extracting topological S and T matrices:



Perturbation of tensor symmetry:



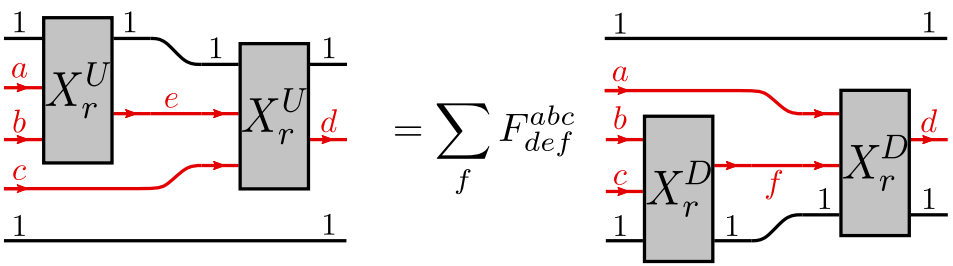
Vertex violating term:

$$T \rightarrow T + \epsilon\ T_p$$

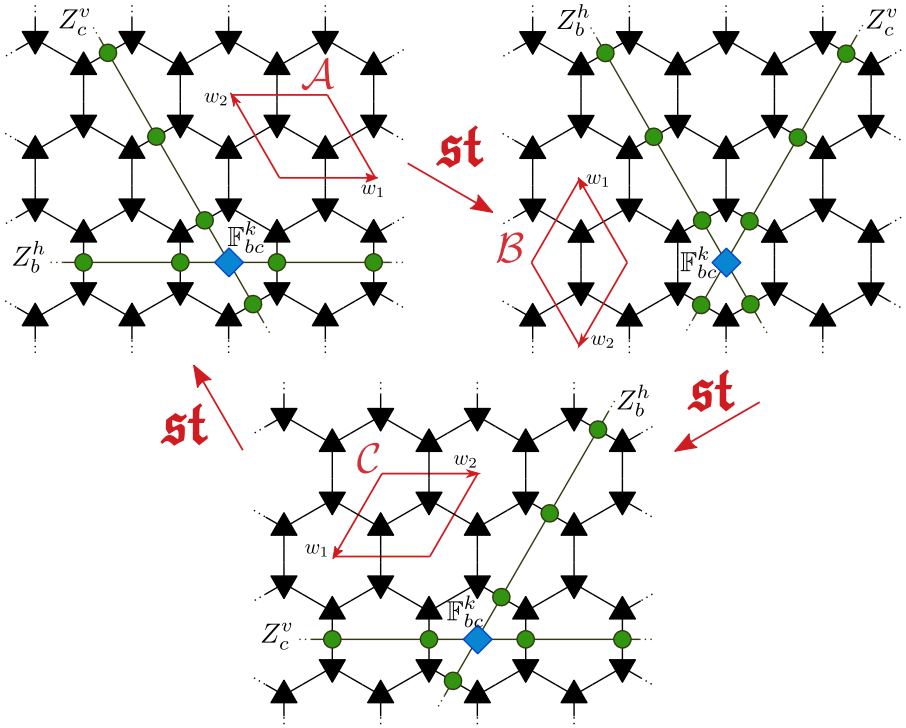
- Fibonacci:
  $\epsilon = 0.1,\ \epsilon_T \sim \epsilon_S \sim \mathcal{O}(10^{-3})$
- Ising:
  $\epsilon = 0.5,\ \epsilon_T \sim \epsilon_S \sim \mathcal{O}(10^{-6})$

S. K. Shukla, M. B. Şahinoğlu, F. Pollmann, X. Chen, PRB (2018)

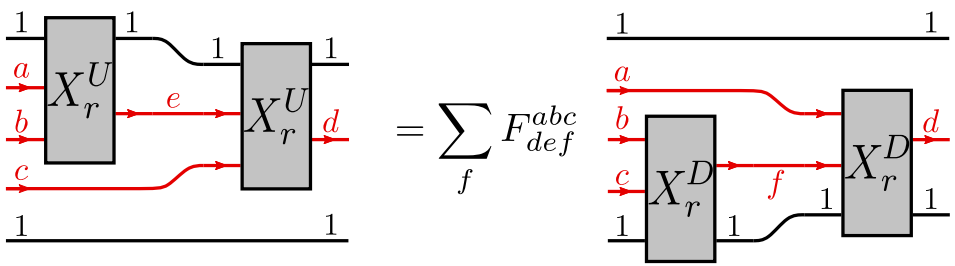
2. Calculating F symbols



1. Extracting topological S and T matrices:



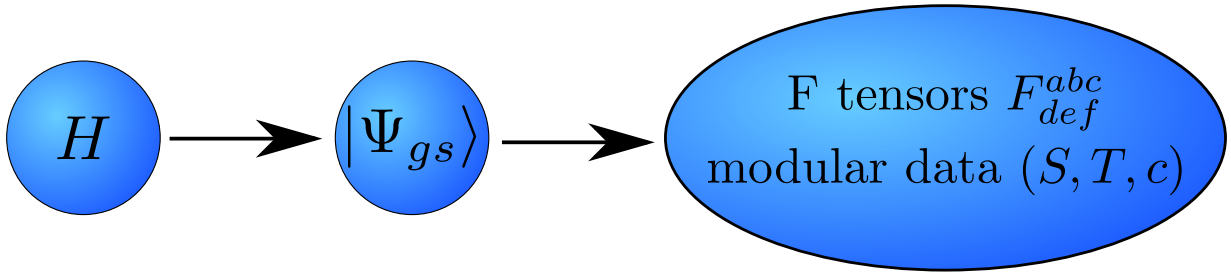
2. Calculating F symbols



$D(S_3)$ and $\mathrm{Rep}(S_3)$ string nets:

$$\mathcal{C}_1 = \mathrm{Rep}(S_3): \ Z_1, Z_\pi, Z_\psi$$
$$\mathcal{C}_2 = \mathrm{Vec}_{S_3}: \ Z_{1,2,3,4,5,6}$$
$$Z(\mathrm{Rep}(S3)) = Z(\mathrm{Vec}_{S_3})$$

Conclusions & outlook

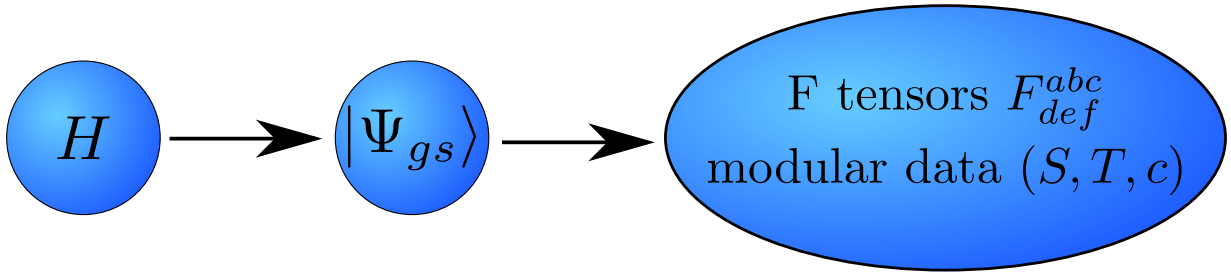


- Unbiased iPEPS optimization: change in just few lines of the code

$$
\begin{aligned}
dC &= \mathbb{I} \circ (P^\dagger dMP) \\
dP &= Pd\omega + P_\perp dX \\
d\omega &= F \circ (P^\dagger dMP) \\
P_\perp dX &= (1 - PP^\dagger) dMPC^{-1}
\end{aligned}
\quad \longrightarrow \quad
\begin{aligned}
dC &= P^\dagger dMP \\
dP &= Pd\omega + P_\perp dX \\
d\omega &= 0 \\
(\mathbb{I} - PP^\dagger) dMP &= dPC - \underline{(\mathbb{I} - PP^\dagger) MdP}
\end{aligned}
$$

- Characterization of phases with iPEPS:
  – non-local topological S and T matrices
  – unitary fusion category – fusion rules F^{abc}_{def}
- Apply directly to lattice Hamiltonians (e.g. Kitaev model):
  – thermodynamic limit
  – no symmetries assumed
- Simulation of experimental setup, realistic Hamiltonians

Conclusions & outlook



- Unbiased iPEPS optimization: change in just few lines of the code

$$\begin{aligned} dC &= \mathbb{I} \circ (P^\dagger dMP) \\ dP &= Pd\omega + P_\perp dX \\ d\omega &= F \circ (P^\dagger dMP) \\ P_\perp dX &= (1 - PP^\dagger) dMPC^{-1} \end{aligned} \longrightarrow \begin{aligned} dC &= P^\dagger dMP \\ dP &= Pd\omega + P_\perp dX \\ d\omega &= 0 \\ (\mathbb{I} - PP^\dagger) dMP &= dPC - \underline{(\mathbb{I} - PP^\dagger) MdP} \end{aligned}$$

- Characterization of phases with iPEPS:
  – non-local topological S and T matrices
  – unitary fusion category – fusion rules F^{abc}_{def}
- Apply directly to lattice Hamiltonians (e.g. Kitaev model):
  – thermodynamic limit
  – no symmetries assumed
- Simulation of experimental setup, realistic Hamiltonians

Thank you!