PEPS - Variational perspective & algos

Juraj Hasik
University of Amsterdam
j.hasik@uva.nl
(14.09.2023)

The many-body problem

Many-body electron problem …

$$\hat{H} = \sum_{I=1}^{N_a} \frac{\hat{P}_I}{2M_I} + \sum_{i=1}^{N_e} \frac{\hat{p}_I}{2m_e} - \sum_{I,i} \frac{Z_I e^2}{|\hat{r}_i - \hat{R}_I|} + \sum_{i>j} \frac{e^2}{|\hat{r}_i - \hat{r}_j|} + \sum_{I>J} \frac{Z_I Z_J e^2}{|\hat{R}_i - \hat{R}_j|}$$

? Ground states – phases & transitions, excitations – dynamics

Classically – state of the system given by O(**N**) data
Quantum mechanics – instead O(**exp(N)**) is required

"The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved. …"

— Paul A. M. Dirac 'Quantum Mechanics of Many-Electron Systems', Proceedings of the Royal Society (1929), A, 123, 714-733.

The many-body problem

"(cont.) It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation."

— Paul A. M. Dirac 'Quantum Mechanics of Many-Electron Systems', Proceedings of the Royal Society (1929), A, 123, 714-733.

Simplify the problem: Electrons moving in an effective potential generated by static nuclei. [Adiabatic approx.]

$$\hat{H}_{eff} = \sum_{i=1}^{N_e} \frac{\hat{p}_I}{2m_e} + \sum_{i>j} \frac{e^2}{|\hat{r}_i - \hat{r}_j|} + \sum_{i=1}^{N_e} V(\hat{r}_i)$$

Nuclei in plethora of materials arrange in a **lattice**
⇒ periodic potential.

The many-body problem

Still O(**exp(N)**) problem – Hilbert space of $\Psi(r_1,\ldots,r_N)$ is $\mathbb{C}^{3N}$. How to proceed ?

- Ignore interactions: **band theory**

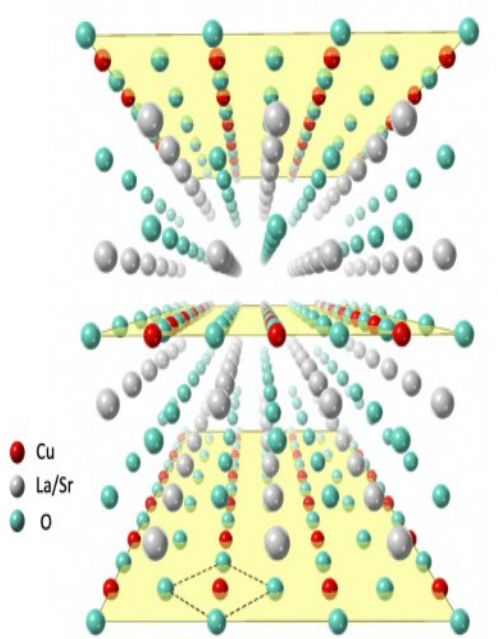
That's too drastic. **Antiferromagnetism**, **superconductivity**, **FQHE,** … ?

- **Truncate both interactions and Hilbert space**
  - Consider only few electrons and few atomic orbitals ϕ per lattice site
  - Interactions decay fast with distance

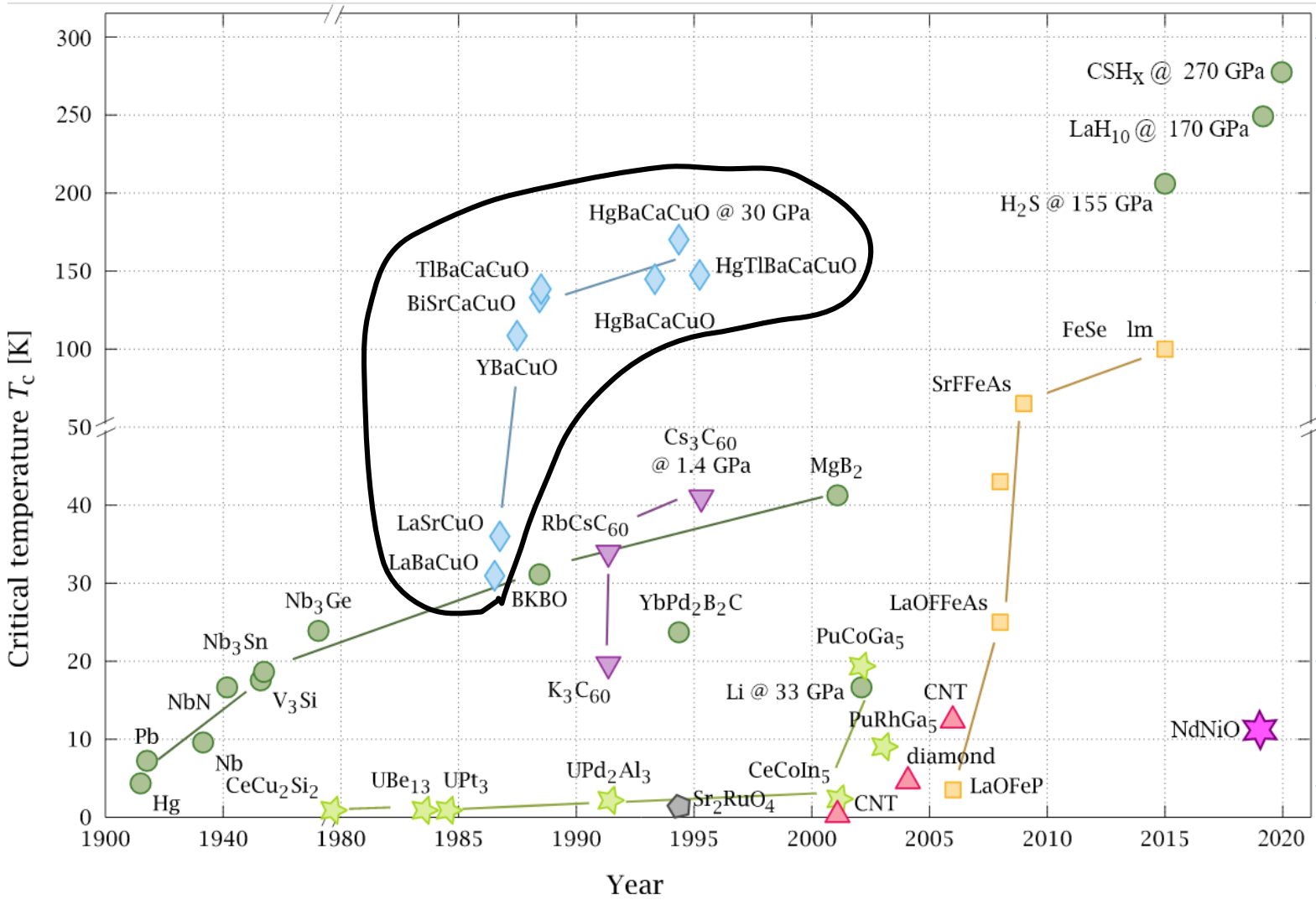
$$\langle \phi_m(i)|V_{ee}|\phi_n(j)\rangle \approx \exp\left(-|i-j|\right)$$

Motivations: High-T_c superconductivity

Believed to be driven by **2D physics** of copper-populated layers



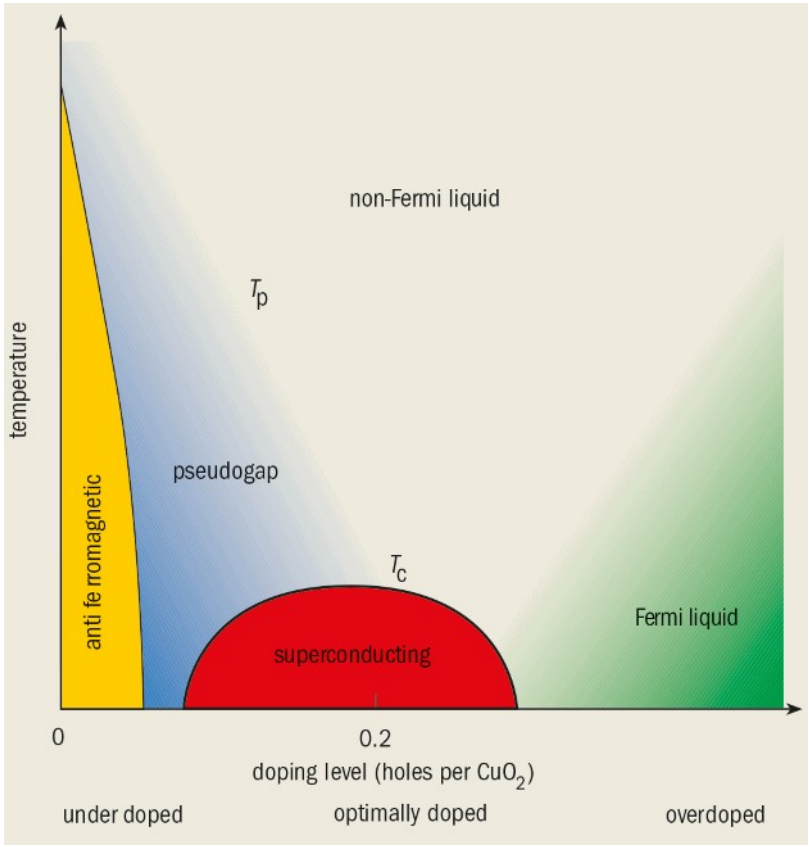
Singh et al, PRB (2022)



Wikipedia.org

Motivations: High-T_c superconductivity

Motivation for the Resonating Valence Bond (**RVB**) theory (Anderson)



Physicsworld.org

Single-band **Hubbard model**

$$H = -t \sum_{\langle i,j \rangle,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

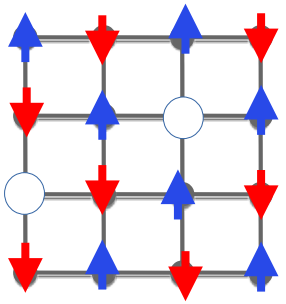
(Some of the) puzzles: Pseudogap,
T-linear resistivity

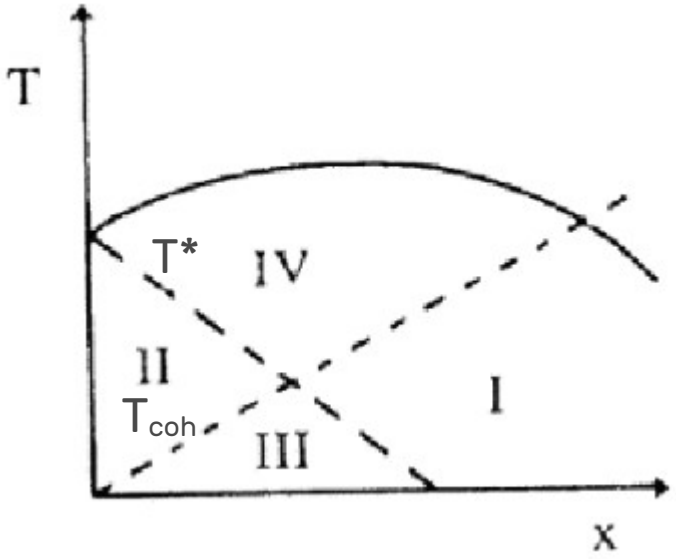
Consider **large-*U*** limit (and t' ...)

$$H = J \sum_{\langle i,j \rangle} S_i . S_j + J' \sum_{\langle\langle i,j \rangle\rangle} S_i . S_j + \dots$$

Motivations: High-T_c superconductivity

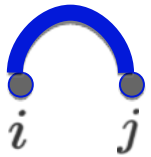
Motivation for the Resonating Valence Bond (**RVB**) theory (Anderson): hole **frustrates** AFM state





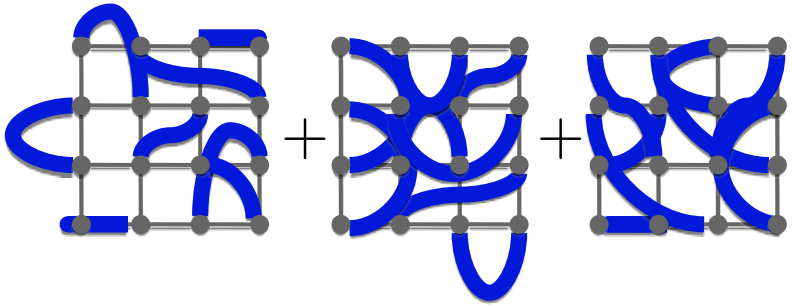
P. Lee (2007)

Valence bond (spin singlet) is favourable

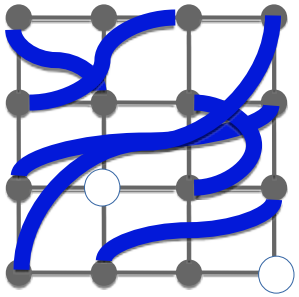


$$\frac{1}{\sqrt{2}}(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle) \qquad e(\mathrm{VB}) = -\frac{3}{4}J$$

RVB - macroscopic superposition



$$+\ldots = \sum_c \phi_c|c\rangle$$



- VB formation T*
- coherence T_{coh}
- **Spin liquid**: lattice symmetries, SU(2), topo-order

Motivations: FQHE

Quantum matter beyond Landau-Ginzburg paradigm

Discovery: D. C. Tsui, H. L. Stormer, & A. C. Gossard, PRL (1982)

First theory: R. B. Laughlin PRL (1983)

Topological order

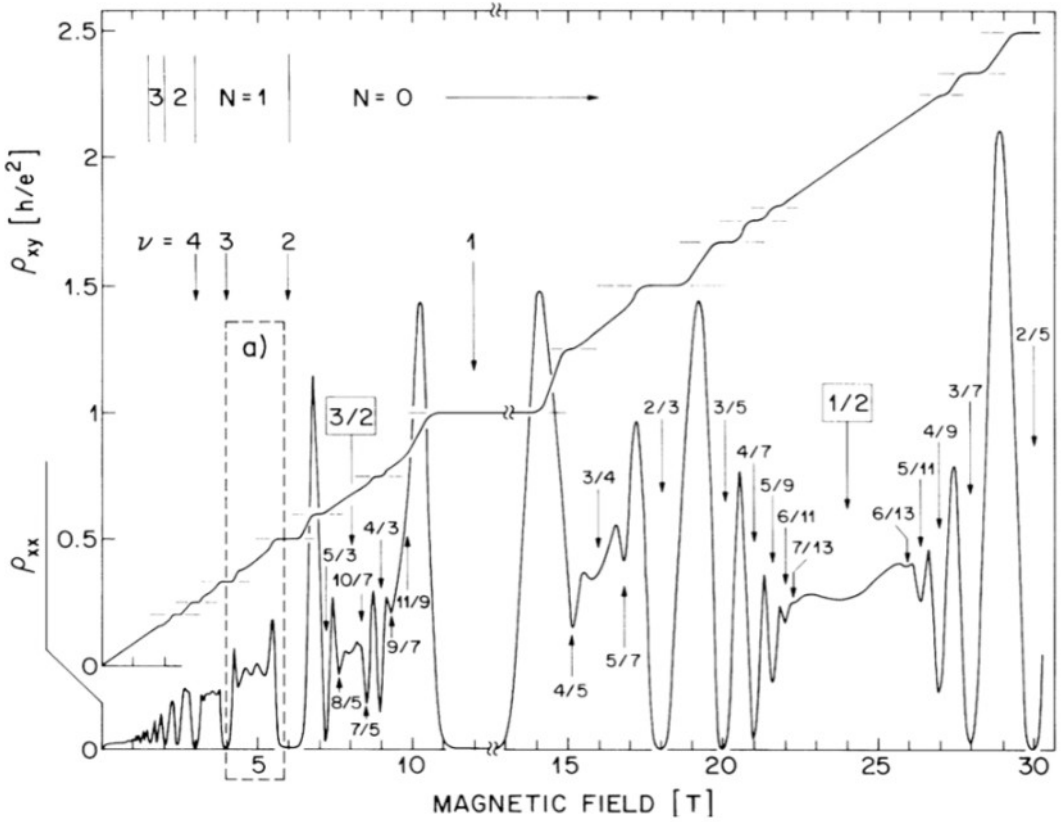
- Fractionally charged quasiparticles

Goldman, Su, Science (1995)
Saminadayar, Glattli, Jin, and Etienne, PRL (1997)
de-Picciotto et al, Nature (1997)
Martin et al, Science (2004)

- Anyonic exchange statistics

Nobel Prize 1998

Laughlin, Störmer, Tsui



R. Willett, J. P. Eisenstein, H. L. Stormer, D. C. Tsui, A. C. Gossard and H. English, PRL (1987)

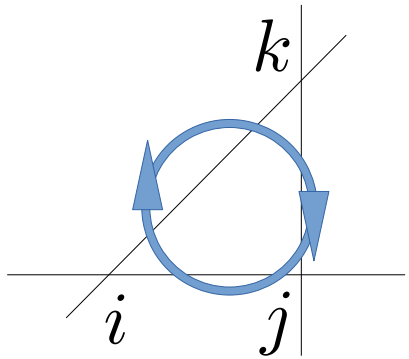
Motivations: FQHE

Fractional statistics ⇔violation of **P** and **T** symmetry

Chiral spin states: (spontaneously) violate **P** and **T** but preserve **PT**

$$\langle \mathbf{S_i} \cdot (\mathbf{S_j} \times \mathbf{S_k}) \rangle \neq 0$$

$$\Leftrightarrow P_{ijk} - P_{ijk}^{-1} \neq 0$$



$$P|ijk\rangle = |jki\rangle$$

Chiral spin liquids (CSL) –

lattice analogues of FQH states Wen, Wilczek, Zee, PRL (1989)

- **Occurence in (2D) materials in Nature ?**

Motivations: FQHE

Prime candidate: Triangular lattice Hubbard model

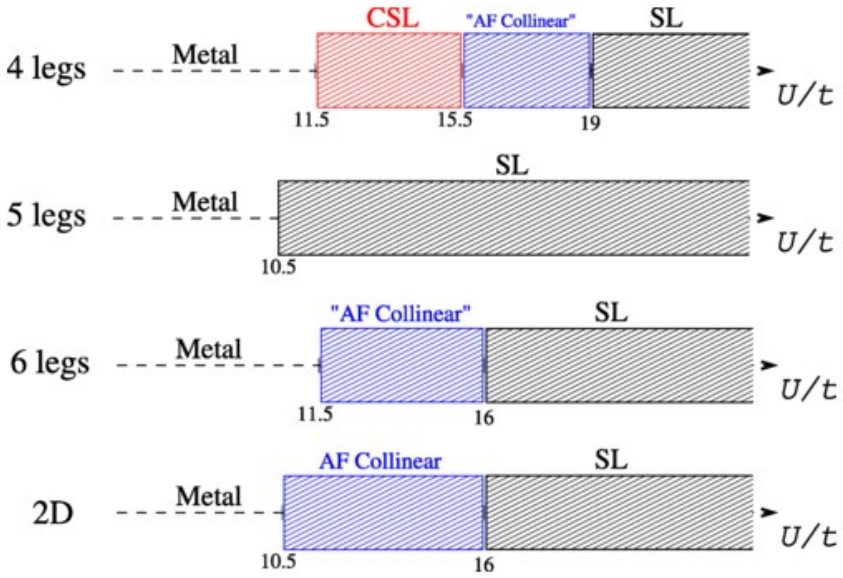
A. Szasz, J. Motruk, M. P. Zaletel, and J. E. Moore, PRX (2020); Chen et al, arXiv:2102.05560 (2021)
T. Cookmeyer, J, Motruk, J. E. Moore, PRL (2021); L. Tocchio, A. Montorsi, F. Becca, PRR (2021)
*SU(3) Boos et al, Phys. Rev. Research 2, 023098 (2020)

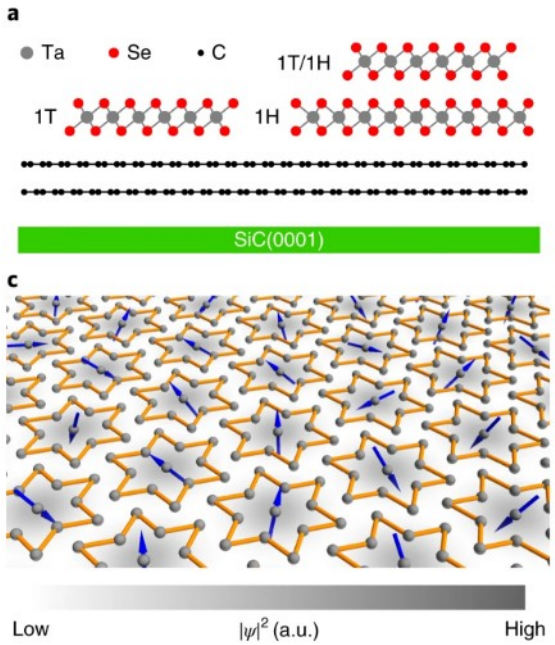
- transition metal dichalcogenide 1T-TaS_2

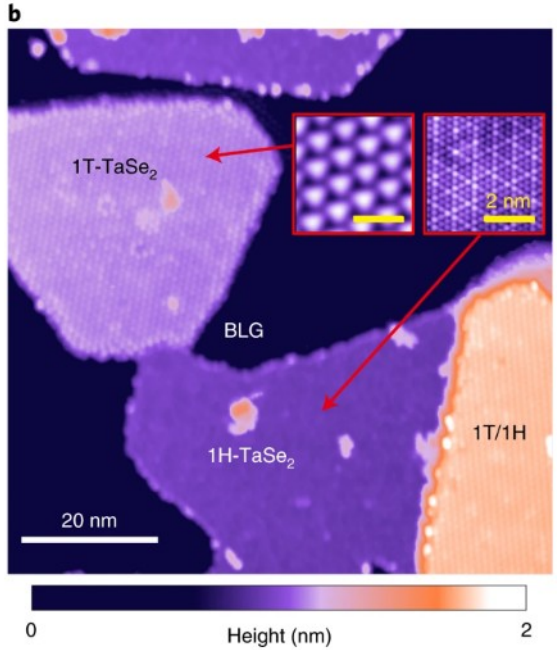
Ruan et al, Nature Physics 17, 1154 (2021)

- Organic salts κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$

Miksch et al, Science 372, 276 (2021)







iPEPS

Variational approach
with tensor networks

1) **Parametrize**: cleverly parametrize many-body wavefunction

2) **Optimize**: find parameter values which minimize the energy

3) **Analyze**: read off physics from the optimal *ansatz*

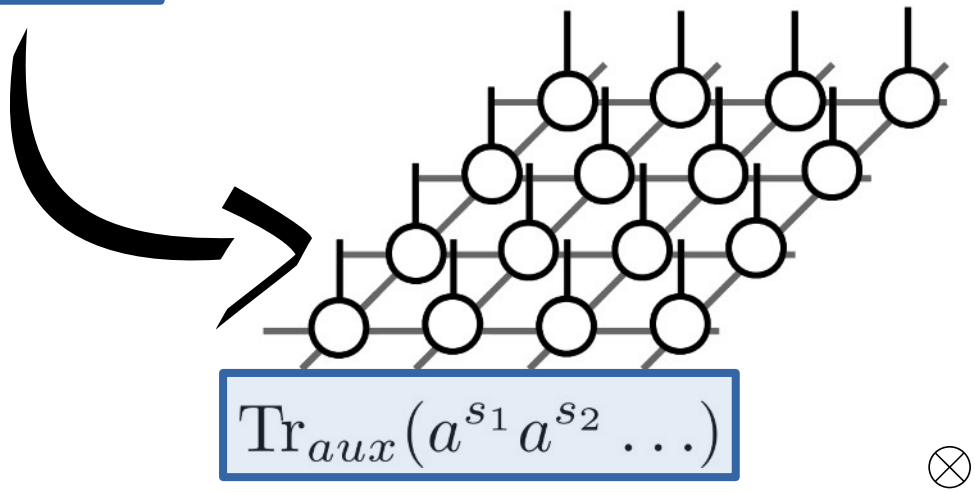
iPEPS as variational ansatz

Variational states targeting GS of lattice models

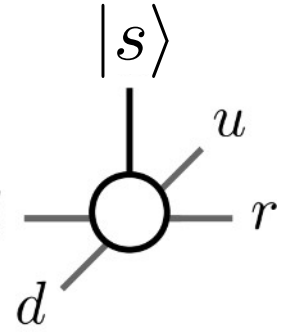
F. Verstraete and J. I. Cirac, arXiv:cond-mat/0407066, (2004)
Jordan et al., Phys. Rev. Lett. 101, 250602, (2008)

$$|\psi\rangle = \sum_{s_1 s_2 \ldots} c_{s_1 s_2 \ldots} |s_1 s_2 \ldots\rangle$$

iPEPS



$$a^s_{ulrd} :=$$



$$\otimes_4 \mathcal{H}^{aux} \rightarrow \mathcal{H}(S = 1/2)$$

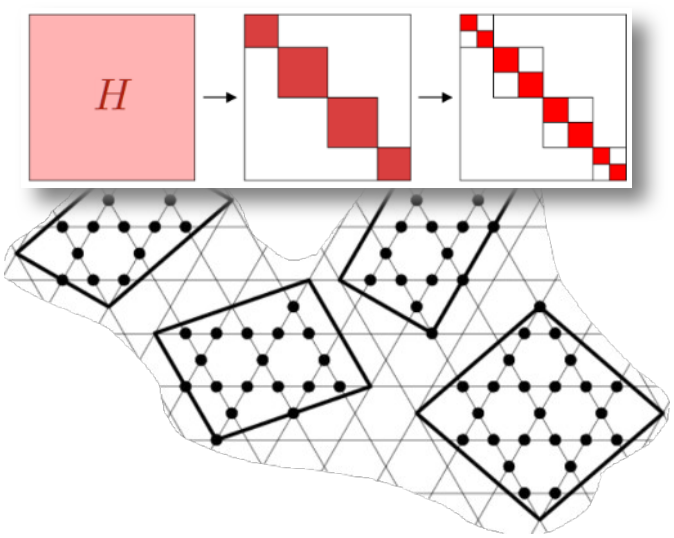
- Obey **area law of entanglement entropy** – virtue (and an issue)
- Observables have to be **approximated**
- Systematically improved through **bond dimension D** = dim(H^{aux})

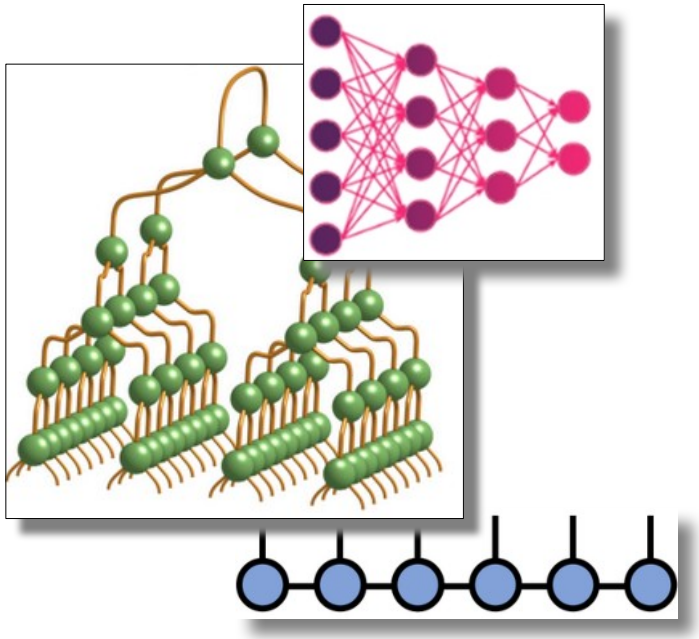
iPEPS as variational ansatz

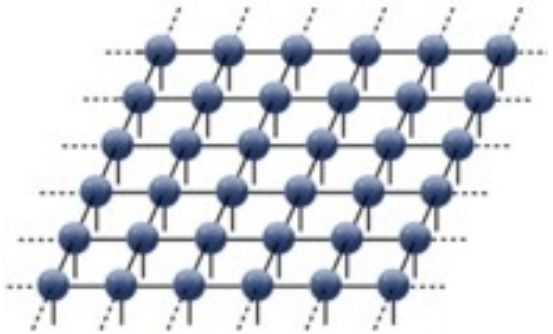
Exact diagonalization

VMC/NN, MPS/TTN

iPEPS







$O(10)$ $O(100)$ $O(\infty)^*$ N

Full $\mathcal{H}$ $S \propto |\partial A|$ / $S \propto |A|$ $S \propto |\partial A|$

Entanglement entropy

Exact diagonalization studies, Sandvik; Seman et al., arXiv:1508.01523; Montangero, Rico, Silvi, Phil. Trans. R. Soc. A. (2014); TN.org, APS.org

IPEPS - Observables

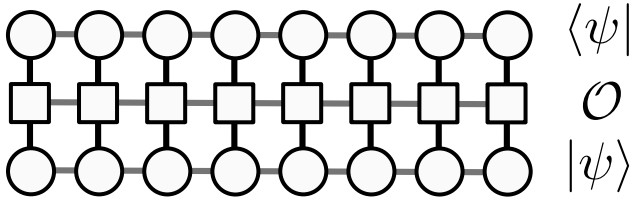
Evaluating observables

iPEPS Observables: MPS recap

Recall (infinite) **Matrix Product states** in 1D

- finite

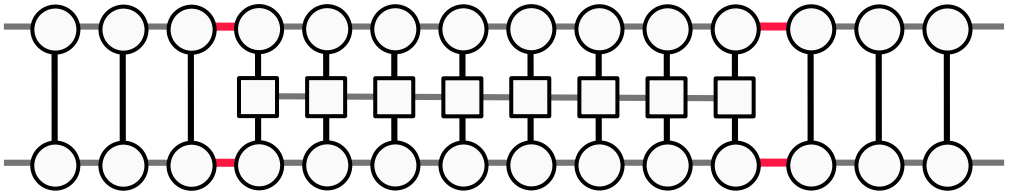
$$\langle\psi|\mathcal{O}|\psi\rangle =$$



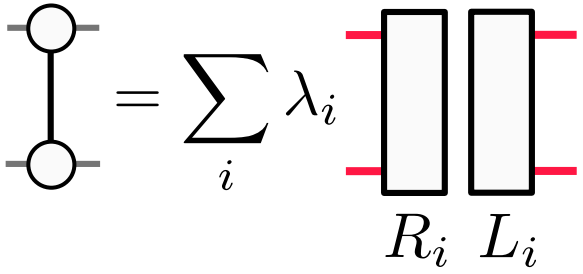
complexity: $\mathcal{O}(ND^3)$

- Infinite translationary invariant state

$$\langle\psi|\mathcal{O}|\psi\rangle \propto \cdots$$

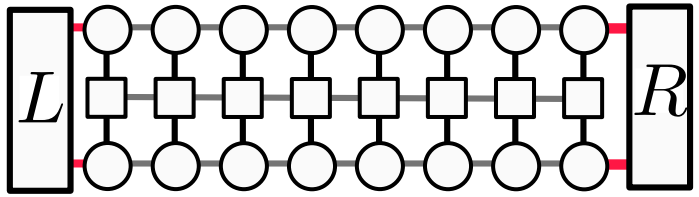


$\cdots$



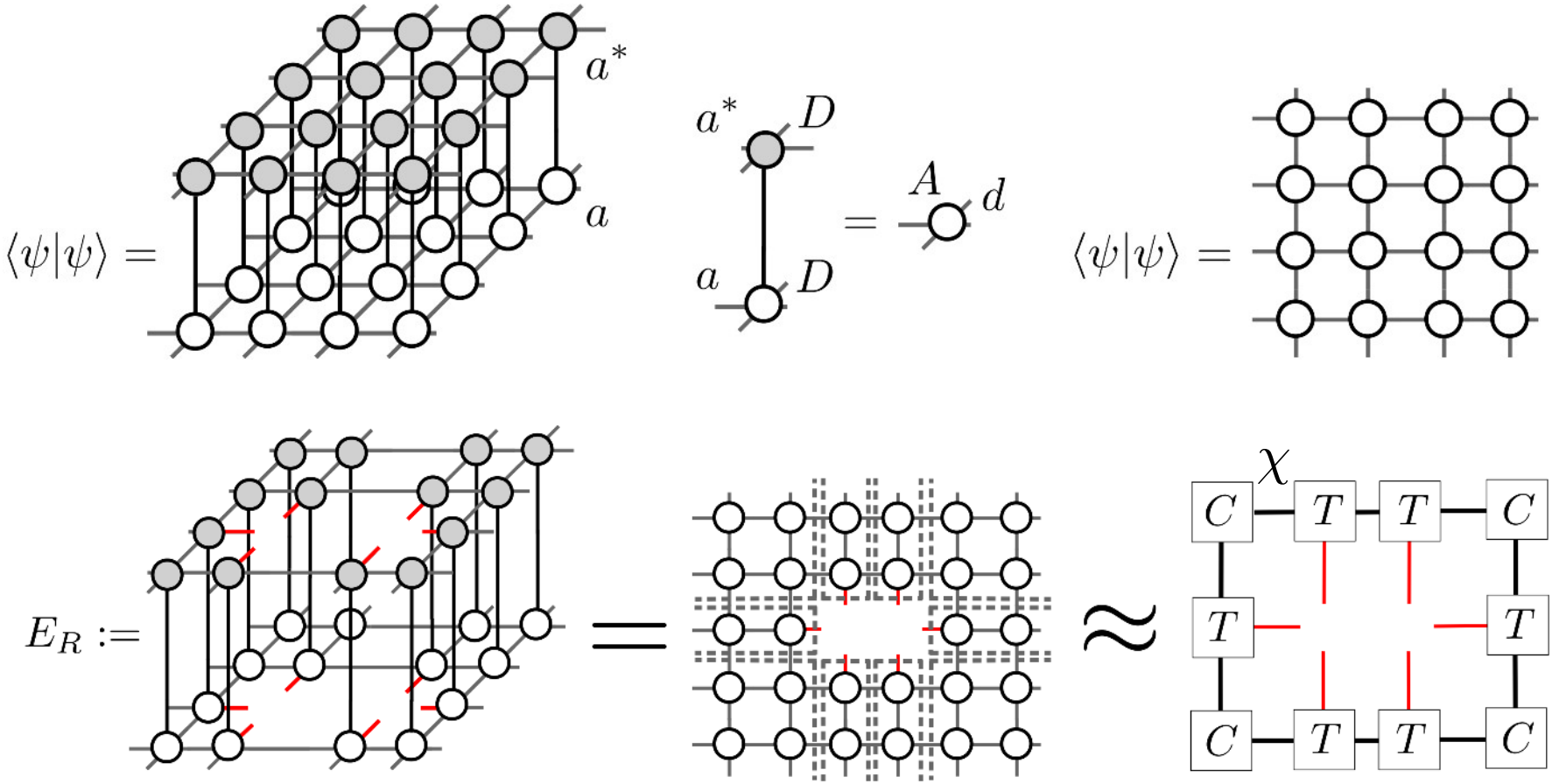
$E_R :=$

$$\langle\psi|\mathcal{O}|\psi\rangle \propto$$



iPEPS Observables: CTMRG

Consider **reduced environments** (E_R) of region R …



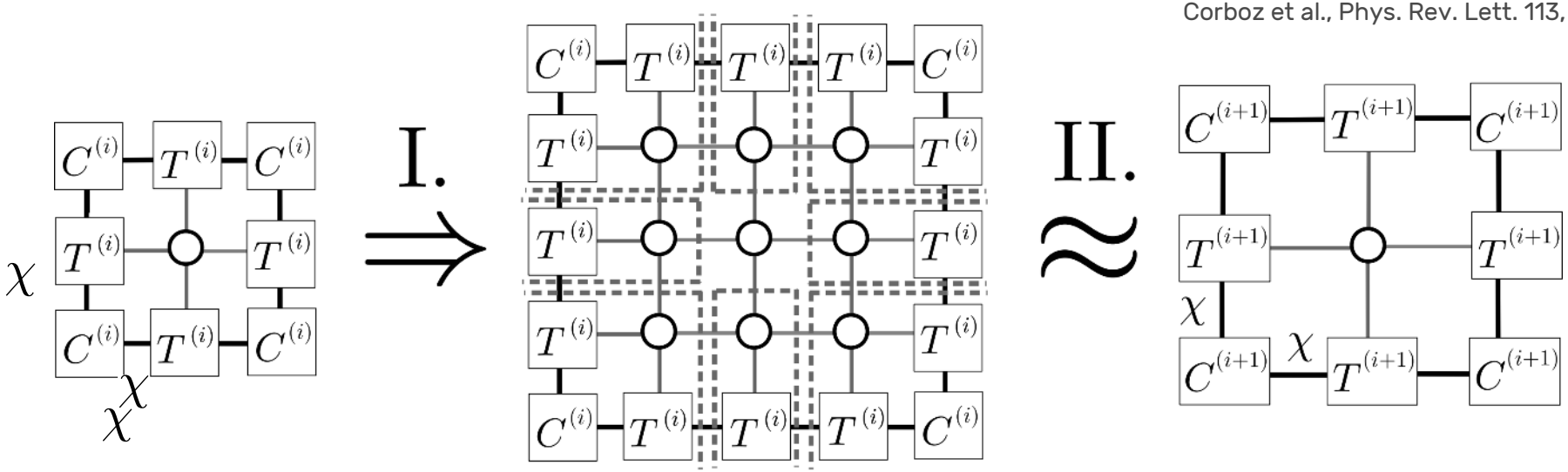
Approximate infinite parts of TNs by finite tensors C,T of dimensions **χ** x **χ** and **χ** x **χ** x **D²**

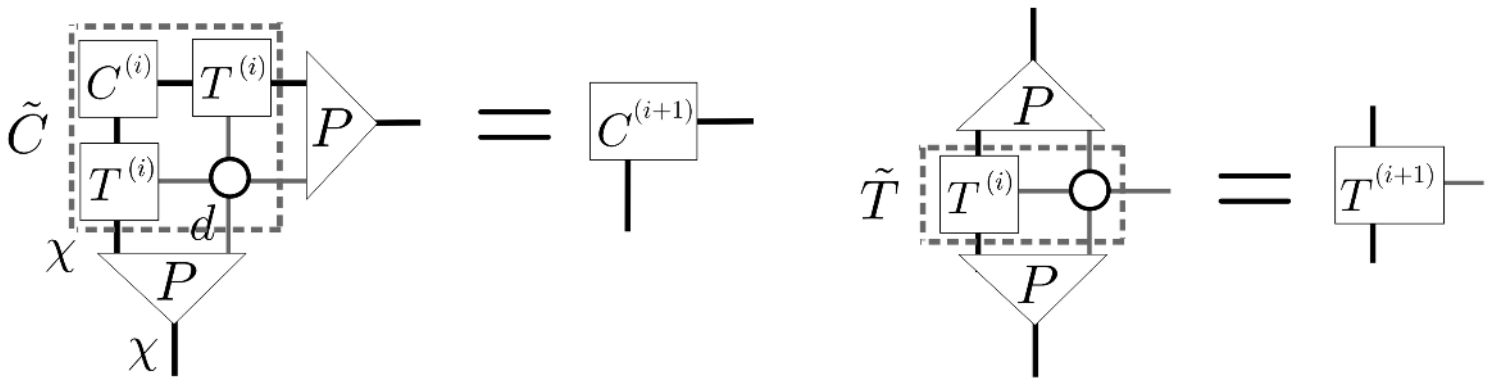
iPEPS Observables: CTMRG

How to find C, T ? Use corner transfer matrix renormalization group (**CTMRG**) – Complexity **$O(\chi^3 D^6)$**

T. Nishino and K. Okunishi, JPSJ 65, 891 (1996), R. Orús and G. Vidal, Phys. Rev. B 78, 155117 (2008)

Corboz et al., Phys. Rev. Lett. 113, 046402, (2014)



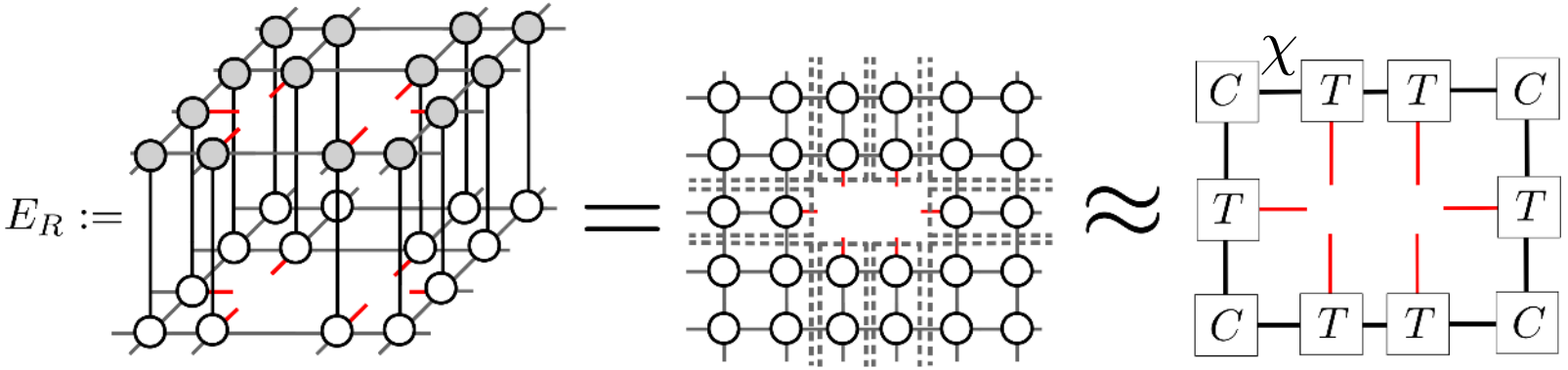


... iterate until **fixed point** C,T

iPEPS Observables: Environments

From **reduced environments** (E_R) of region R …

… build **reduced density matrices** (ρ_R) of region R



Construct **environments**

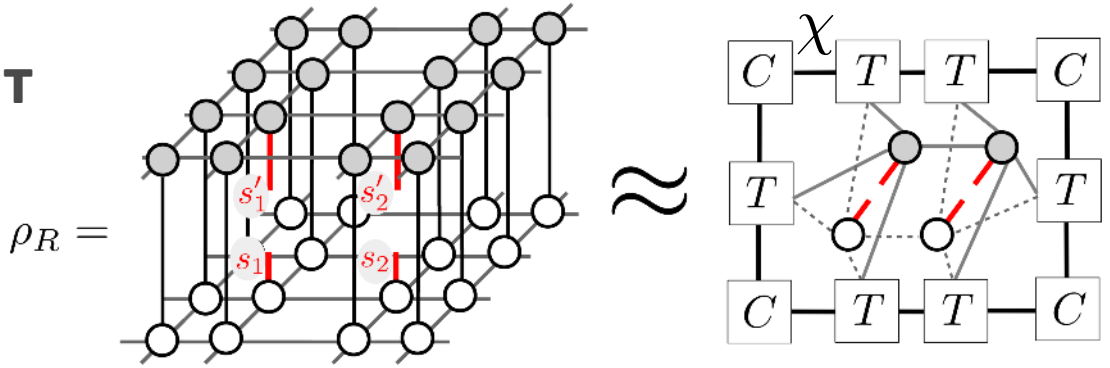
- corners **C,** half-row/-columns **T**

Baxter, J. Stat. Phys. 17, 1 (1977);

Nishino, Okanishi (90's)

- Alternative: **Channels**

Vanderstraeten et al. (2015, 2016)



New control parameter:

env. dimension χ

Any observable inside the region R is:

$$\langle \mathcal{O} \rangle_\chi \approx \mathrm{Tr}(\rho_R(\chi)\mathcal{O})$$

IPEPS - Optimization

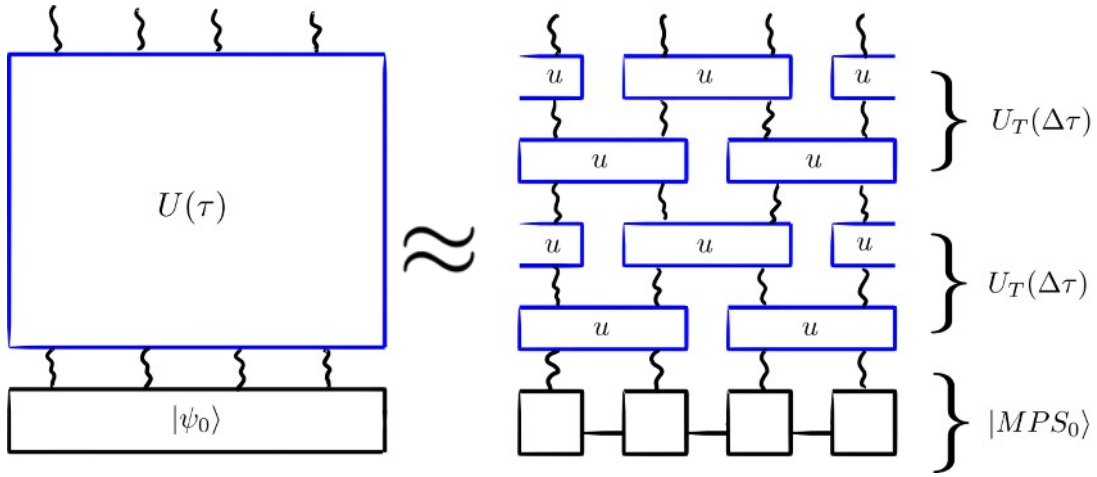
Optimizing tensors

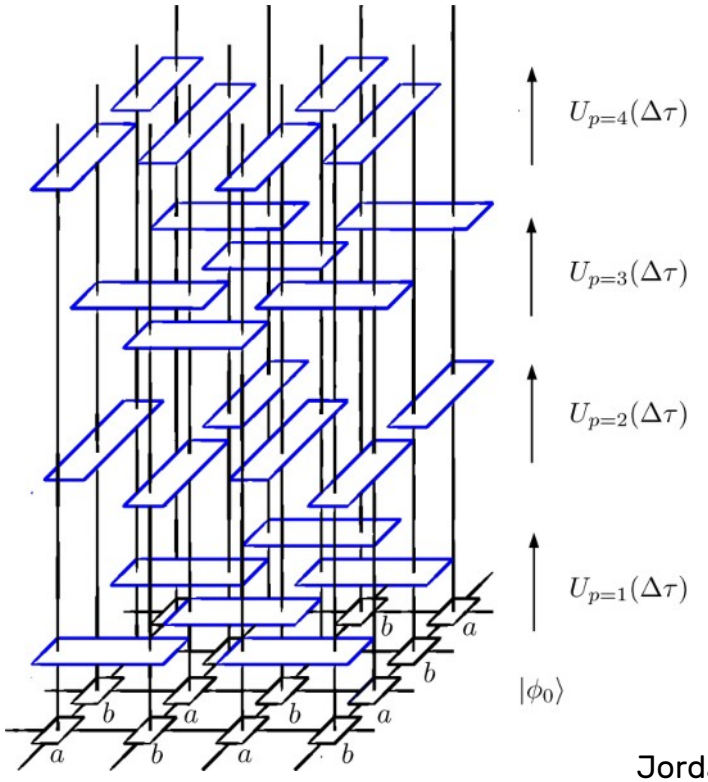
iPEPS Optimization

Warning: **Optimization is hard !**

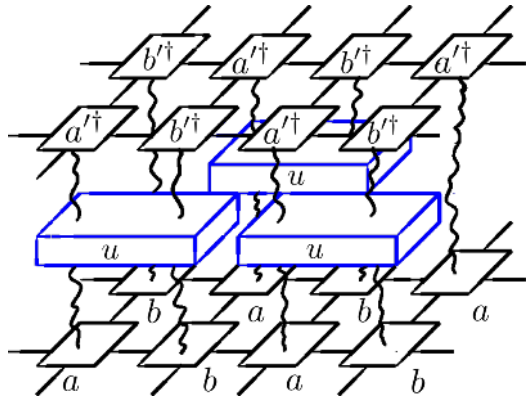
(I) Find the **fixed point** of **imag. time evolution** ...

$$U(\tau) = exp(-\tau H)$$





... use **Trotter decomposition**



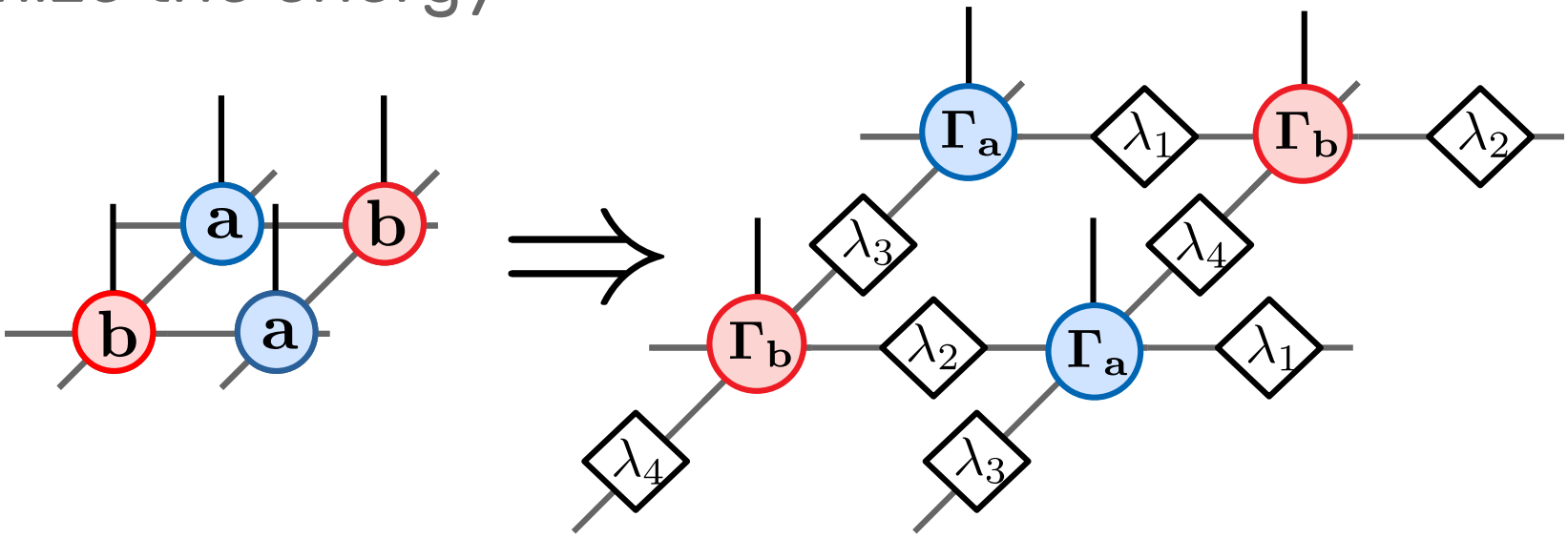
Simple and **Full Update** contract layer by layer

Jordan et al., Phys. Rev. Lett. 101, 250602, (2008); Phien et al., Phys. Rev. B 92, 035142 (2015)

iPEPS Optimization: Simple update

2-site Simple update (SU)

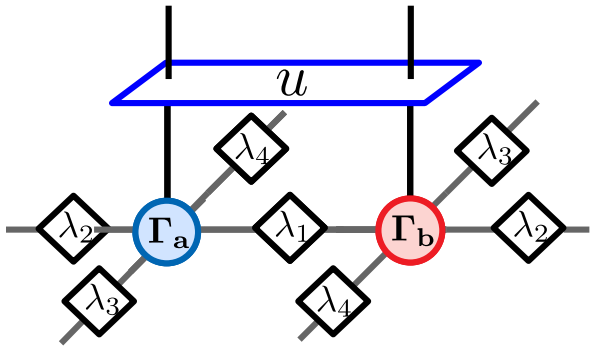
- Direct generalization of iTEBD from 1D to 2D
- Due to the absence of canonical form for PEPS, **does not** minimize the energy



- Ansatz for NN Hamiltonian: breaks spatial symmetries and requires CTM for generic unit cells to contract
- **Useful to find viable symmetry sectors !**

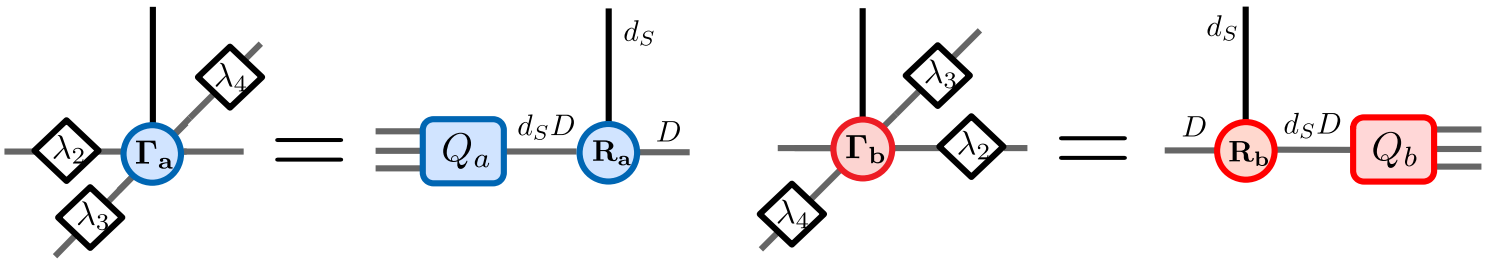
iPEPS Optimization: Simple update

2-site Simple update (SU)

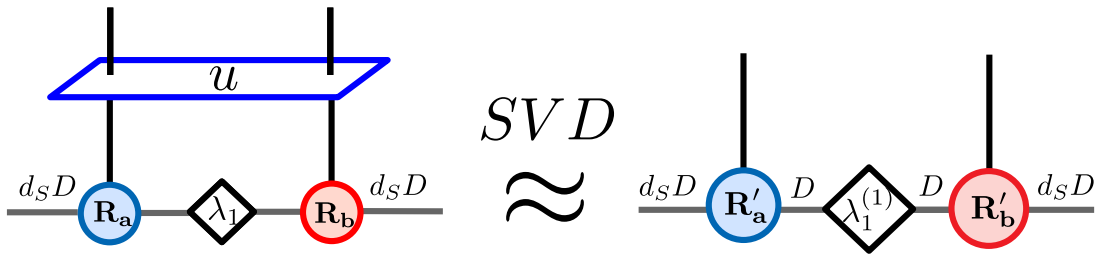


- Single gate application. Repeat for λ_2, λ_3, and λ_4

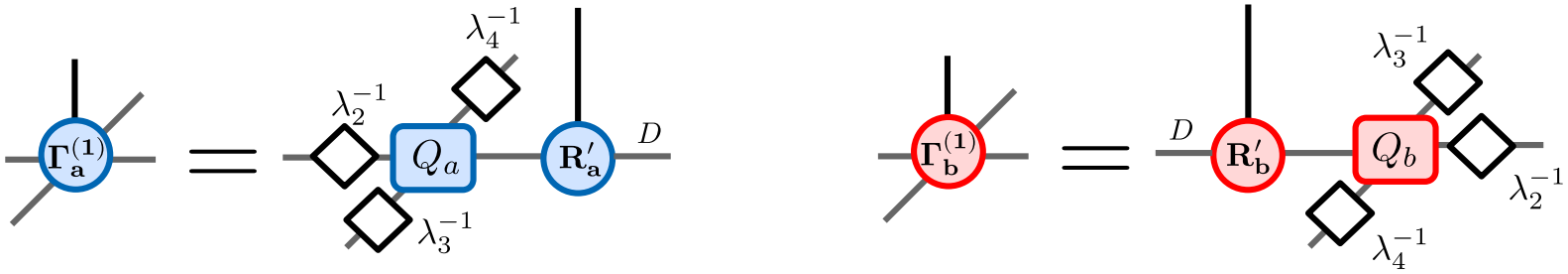
I.



II.



III.



iPEPS Optimization: gradient descent

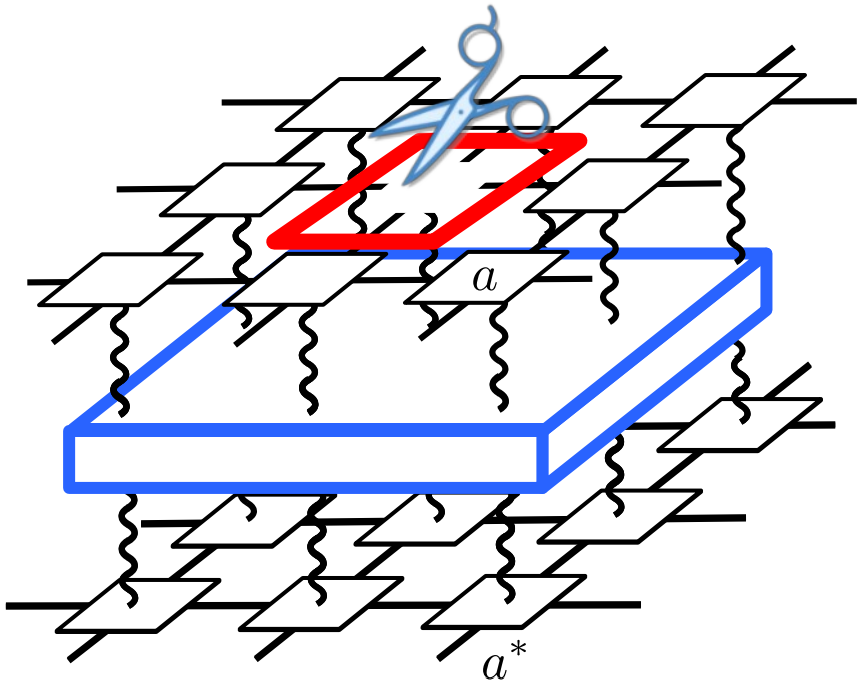
Direct energy minimization

$$min\langle\psi|H|\psi\rangle$$

1. get **gradient**

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

2. steepest descent, CG, L-BFGS, ...



How to evaluate the gradient for **iPEPS** ?

- Finite-Difference: simple, but only for few parameters
  D. Poilblanc and M. Mambrini, Phys. Rev. B 96, 014414 (2017)
- Summation schemes: harder with increasing range of *H*-terms
  P. Corboz, Phys. Rev. B 94, 035133 (2016); Vanderstraeten et al., Phys. Rev. B 94, 155123 (2016)
- **Algorithmic/Automatic differentiation** (AD)
  Liao et al., Phys. Rev. X 9, 031041 (2019)

Algorithmic differentiation: Core

Central question:

How to evaluate the gradient of a complicated scalar function of many variables ?

Simple model of a variational energy:

$$E : \mathbb{R}^N \xrightarrow{F^1} \mathbb{R}^{M_2} \xrightarrow{F^2} \mathbb{R}^{M_3} \xrightarrow{F^3} \mathbb{R}^{M_4} \xrightarrow{F^4} \mathbb{R}$$

$$F^4(F^3(F^2(F^1(\mathbf{x})))) = F^4(F^3(F^2(\mathbf{v}^2))) = F^4(F^3(\mathbf{v}^3)) = F^4(\mathbf{v}^4) =: E$$

Option 1: **Finite difference**

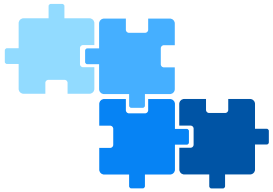
pick a direction $\mathbf{e}_i$ in the space of parameters and a small *h*

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

- finite precision error, **complexity O(N) x O(E)**

Primer: Algorithmic differentiation

Core premise of Algorithmic differentiation:



Functions are ultimately composed of (many) simple operations as +, -, /, *, exp, log, sin, ...

Assume that **Jacobians** are known: $J^n(\mathbf{v}_0^n) = \left(\frac{\partial F^n}{\partial \mathbf{v}^n}\right)\Big|_{\mathbf{v}^n=\mathbf{v}_0^n}$.

The **forward mode** AD

$$
\begin{aligned}
&\mathbf{x}_0 \equiv \mathbf{v}_0^1 \quad \rightarrow \mathbf{v}_0^2 = F^1(\mathbf{v}_0^1) \quad \rightarrow \mathbf{v}_0^3 = F^2(\mathbf{v}_0^2) \quad \rightarrow \mathbf{v}_0^4 = F^3(\mathbf{v}_0^3) \\
&\qquad\qquad \rightarrow E = F^4(\mathbf{v}_0^4), \\
&\mathbf{e}_i \equiv \mathbf{g}_{0,i}^1 \quad \rightarrow \mathbf{g}_{0,i}^2 = J^1(\mathbf{v}_0^1)\cdot \mathbf{g}_{0,i}^1 \quad \rightarrow \mathbf{g}_{0,i}^3 = J^2(\mathbf{v}_0^2)\cdot \mathbf{g}_{0,i}^2 \quad \rightarrow \mathbf{g}_{0,i}^4 = J^3(\mathbf{v}_0^3)\cdot \mathbf{g}_{0,i}^3 \\
&\qquad\qquad \rightarrow (\mathbf{g}_0)_i = J^4(\mathbf{v}_0^4)\cdot \mathbf{g}_{0,i}^4.
\end{aligned}
$$

In short: $(\mathbf{g}_0)_i = J^4(\mathbf{v}_0^4)\cdot(J^3(\mathbf{v}_0^3)\cdot(J^2(\mathbf{v}_0^2)\cdot(J^1(\mathbf{x}_0)\cdot\mathbf{e}_i)))$ Cost: **O(N) x O(E)**

Primer: Algorithmic differentiation

The **reverse mode** AD

I. Evaluate E($\mathbf{x}_0$) and **store all the intermediate variables**

$$\mathbf{x}_0 \equiv \mathbf{v}_0^1 \rightarrow \ \mathbf{v}_0^2 = F^1(\mathbf{v}_0^1) \rightarrow \ \mathbf{v}_0^3 = F^2(\mathbf{v}_0^2) \rightarrow \ \mathbf{v}_0^4 = F^3(\mathbf{v}_0^3) \rightarrow \ E = F^4(\mathbf{v}_0^4)$$

II. Accumulate the gradient in the reverse order

$$1 \cdot J^4(\mathbf{v}_0^4) = \bar{\mathbf{v}}_0^4 \rightarrow \bar{\mathbf{v}}_0^4 \cdot J^3(\mathbf{v}_0^3) = \bar{\mathbf{v}}_0^3 \rightarrow \bar{\mathbf{v}}_0^3 \cdot J^2(\mathbf{v}_0^2) = \bar{\mathbf{v}}_0^2 \rightarrow \bar{\mathbf{v}}_0^2 \cdot J^1(\mathbf{x}_0) = \bar{\mathbf{x}}_0$$

Observe: $\bar{\mathbf{x}}_0$ holds all components of the gradient

$$\bar{\mathbf{x}}_0 \cdot \mathbf{e}_i = (((J^4(\mathbf{v}_0^4) \cdot J^3(\mathbf{v}_0^3)) \cdot J^2(\mathbf{v}_0^2)) \cdot J^1(\mathbf{x}_0)) \cdot \mathbf{e}_i = (\mathbf{g}_0)_i$$

Define vector-matrix products - **Adjoint functions**

$$\bar{F}^n : \mathbb{R}^{M_n} \times \mathbb{R}^{M_{n+1}} \xrightarrow{\bar{F}^n} \mathbb{R}^{M_n}$$
$$\bar{F}^n(\mathbf{v}^n, \bar{\mathbf{v}}^{n+1}) := \bar{\mathbf{v}}^{n+1} \cdot J^n(\mathbf{v}^n) = \bar{\mathbf{v}}^n$$

$$\Rightarrow \quad F^4(F^3(F^2(F^1(\mathbf{x}_0)))) \qquad \bar{F}^1(\mathbf{x}_0, \bar{F}^2(\mathbf{v}_0^2, \bar{F}^3(\mathbf{v}_0^3, \bar{F}^4(\mathbf{v}_0^4, 1)))) = \bar{\mathbf{x}}_0$$

Primer: Algorithmic differentiation

A (central) example of the **adjoint function**

$$C = f(A,B) \longrightarrow \mathrm{d}C = \frac{\partial f}{\partial A}\mathrm{d}A + \frac{\partial f}{\partial B}\mathrm{d}B \qquad E = E(C) \longrightarrow \mathrm{d}E =: Tr\left(\overline{C}^T \mathrm{d}C\right)$$

$$dE = Tr\left(\overline{C}^T \frac{\partial f}{\partial A}\mathrm{d}A\right) + Tr\left(\overline{C}^T \frac{\partial f}{\partial B}\mathrm{d}B\right) \longrightarrow \begin{cases} \overline{A} = \left(\frac{\partial f}{\partial A}\right)^T \overline{C} \\ \overline{B} = \left(\frac{\partial f}{\partial B}\right)^T \overline{C} \end{cases}$$

Take **matrix multiplication** (= tensor contraction)

$$C = AB \longrightarrow \mathrm{d}C = \mathrm{d}AB + A\mathrm{d}B \longrightarrow \begin{cases} \overline{A} = \overline{C}B^T \\ \overline{B} = A^T\overline{C} \end{cases}$$

Many other matrix functions (ED, SVD, Inverse, …)

M. Giles, https://people.maths.ox.ac.uk/gilesm/files/NA-08-01.pdf

Recent developments: Complex SVD, Lanczos, …

Z.Q. Wan, S.X. Zhang arXiv:1909.02659; H. Xie, J.G. Liu, L. Wang, Phys. Rev. B 101, 245139 (2020)

Algorithmic Differentiation

- Both **Forward mode** and **Reverse mode** evaluate derivatives with **machine precision**

- **Forward mode** has complexity O(N) * O(E)

- **Reverse mode has complexity O(1) * O(E)**

- Caveat: Memory requirements **are not bounded** !
- Implemented in major machine-learning frameworks: **TensorFlow**, **PyTorch**, **JAX, ...**

  ... or in one of the libraries for your favorite language Fortran, C++, Julia, etc. (see http://www.autodiff.org)

IPEPS – Thermodynamic limit

Addressing thermodynamic limit

Q: Adressing thermodynamic limit ?

- iPEPS lack **physical size ...**

How to use **finite bond** and **environment** dimension (D,χ) data to provide thermodynamic estimates ?

A: Finite correlation length scaling (FCLS)

- use **ξ** as the length scale

Rader and Lauchli, Phys. Rev. X, (2018)
Corboz, Czarnik, Kapteijns, and Tagliacozzo, Phys. Rev. X (2018)

$$e(L) = e(\infty) + \frac{b}{L^3} + O\left(\frac{1}{L^4}\right) \Leftrightarrow e(\xi) = e(\infty) + \frac{\beta}{\xi^3} + O\left(\frac{1}{\xi^4}\right)$$

$$m^2(L) = m^2(\infty) + \frac{a}{L} + O\left(\frac{1}{L^2}\right) \Leftrightarrow m^2(\xi) = m^2(\infty) + \frac{\alpha}{\xi} + O\left(\frac{1}{\xi^2}\right)$$

Q: Adressing thermodynamic limit ?

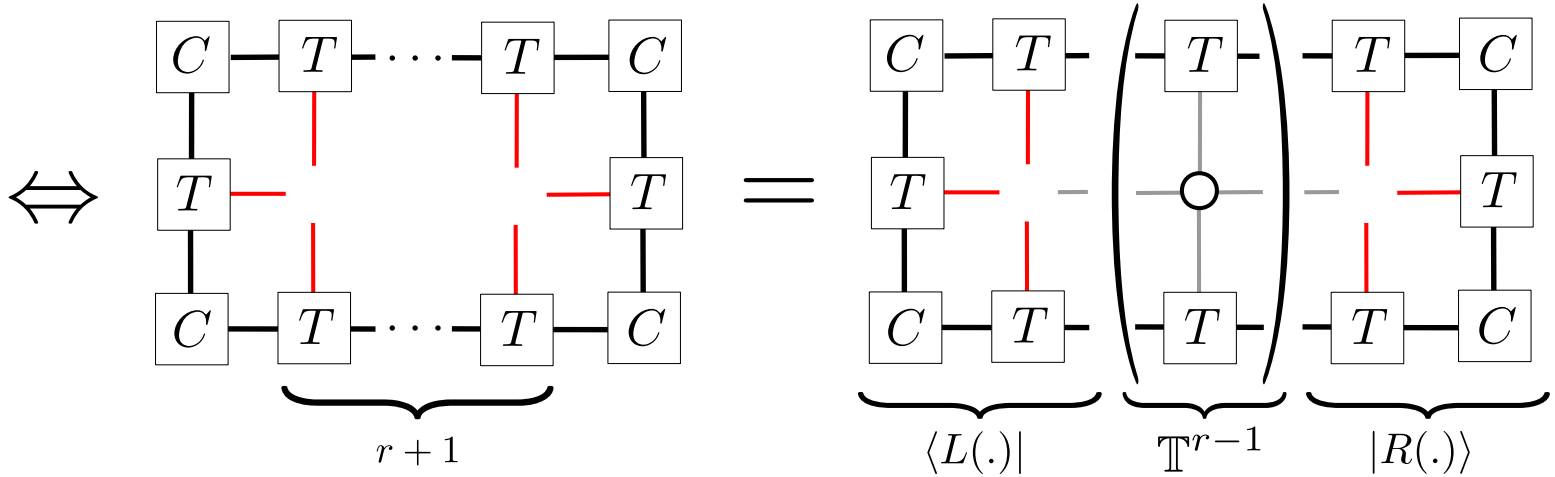
- iPEPS lack **physical size ...**

How to use **finite bond** and **environment** dimension (D,χ) data to provide thermodynamic estimates ?

A: Finite correlation length scaling (FCLS)

- use **ξ** as the length scale

$$\langle O_1(0)O_2(r)\rangle - \langle O_1(0)\rangle\langle O_2(r)\rangle = \sum_{i>0} \lambda_i^{r-1}\langle L|O_1|l_i\rangle\langle r_i|O_2|R\rangle \Leftrightarrow$$



Nishino, Phys. Lett. A, (1996); M. M. Rams, P. Czarnik, and L. Cincio Phys. Rev. X 8, (2018)

iPEPS in action

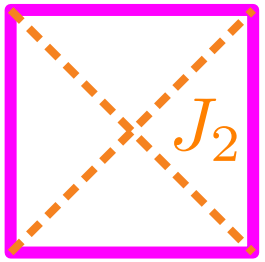
Application to J1-J2 model
on square lattice

JH, D. Poilblanc, F. Becca, SciPost Phys. (2021)

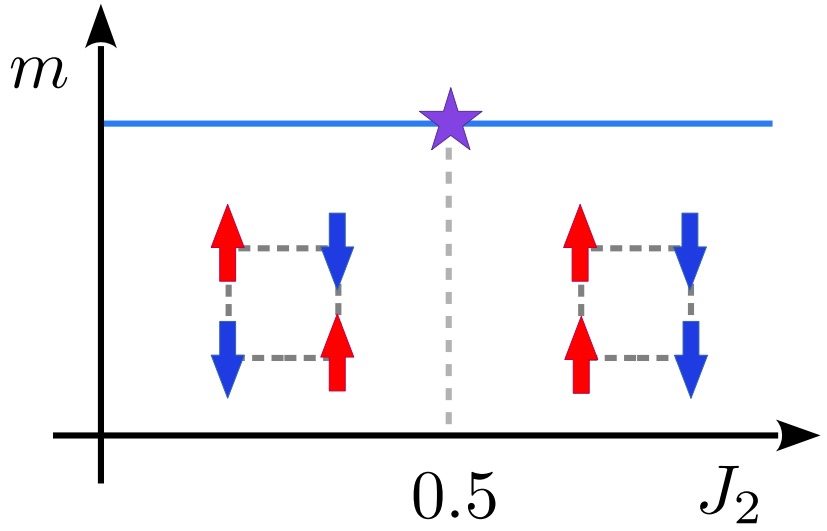
Intro: Square Lattice J1-J2 Model

Paradigmatic example of a frustrated magnet (J_1, J_2>0)

$$H = J_1 \sum_{\langle i,j \rangle} S_i.S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i.S_j$$



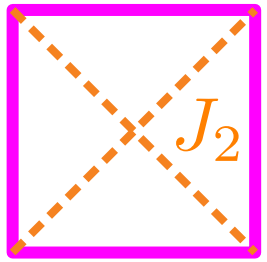
- Classically: transition at **$J_2/J_1 = 0.5$**, where macroscopic degeneracy appears



Intro: Square Lattice J1-J2 Model

Paradigmatic example of a frustrated magnet (J_1, J_2>0)

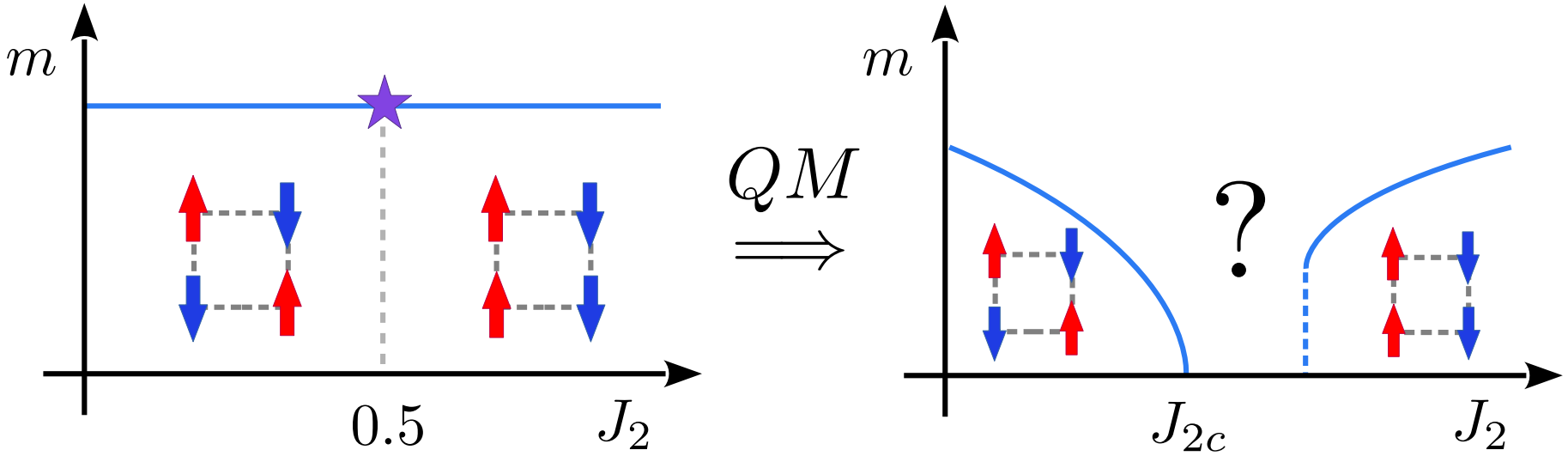
$$H = J_1 \sum_{\langle i,j \rangle} S_i.S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i.S_j$$



Spin waves:

P. Chandra and B. Doucot, Phys. Rev. B 38, 9335 (1988)

- **Transition** from **Néel** to **paramagnetic** phase near maximally frustrated point **$J_2/J_1 \approx 0.5$**
- For **$J_2/J_1 \gtrsim$ 0.6** system orders again in stripes



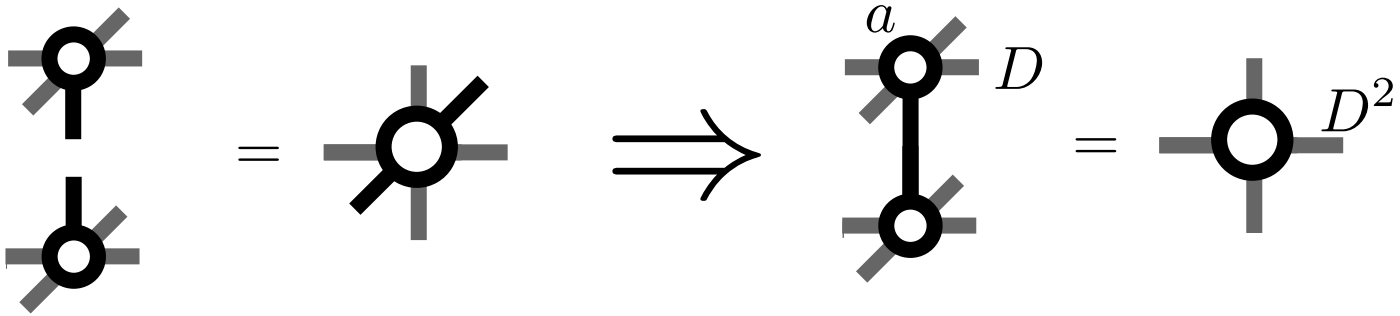
Protocol

Single-site iPEPS with **real C_{4v} symmetric** on-site tensor a + AF structure by sub-lattice rotation

1. Optimize iPEPS tensors with increasing D
   i. Given a, compute environments E and reduced density matrices ϱ
   ii. Evaluate energy <=> few unique Hamiltonian terms
   iii. Compute gradient (AD) and update a
2. With optimal iPEPS for set of D
   i. Extrapolate observables to $\chi \to \infty$ (infinite system size): energies, order params (m^2), and correlation lengths ξ
   ii. Apply finite correlation-length scaling to get thermodynamic estimates for $\xi \to \infty$

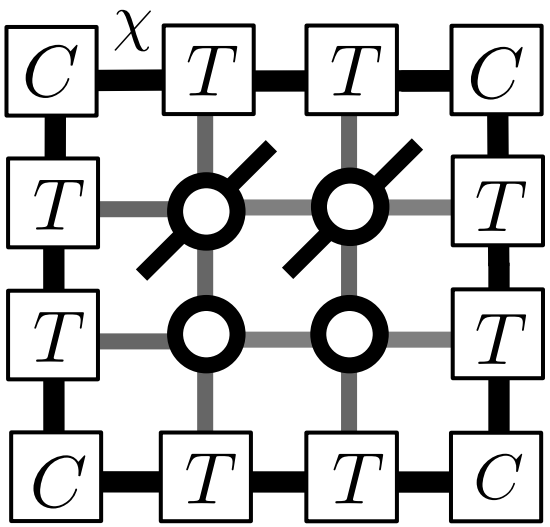
Evaluating energy of J1-J2 model

How to evaluate the energy ?

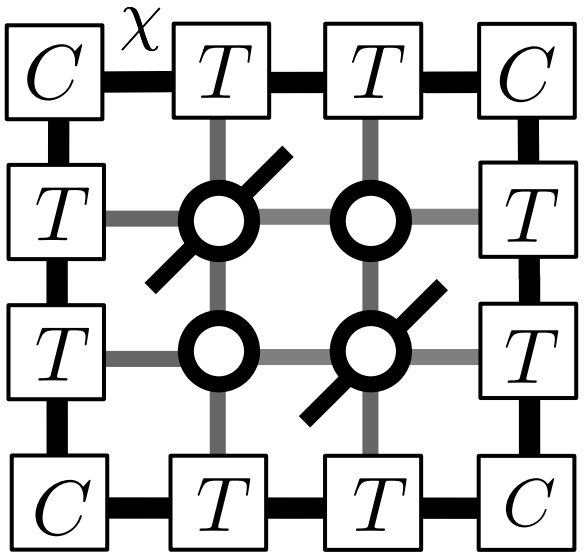


Perform **CTMRG** to build following RDMs:

$\rho_{\chi}^{(NN)} =$



$\rho_{\chi}^{(NNN)} =$

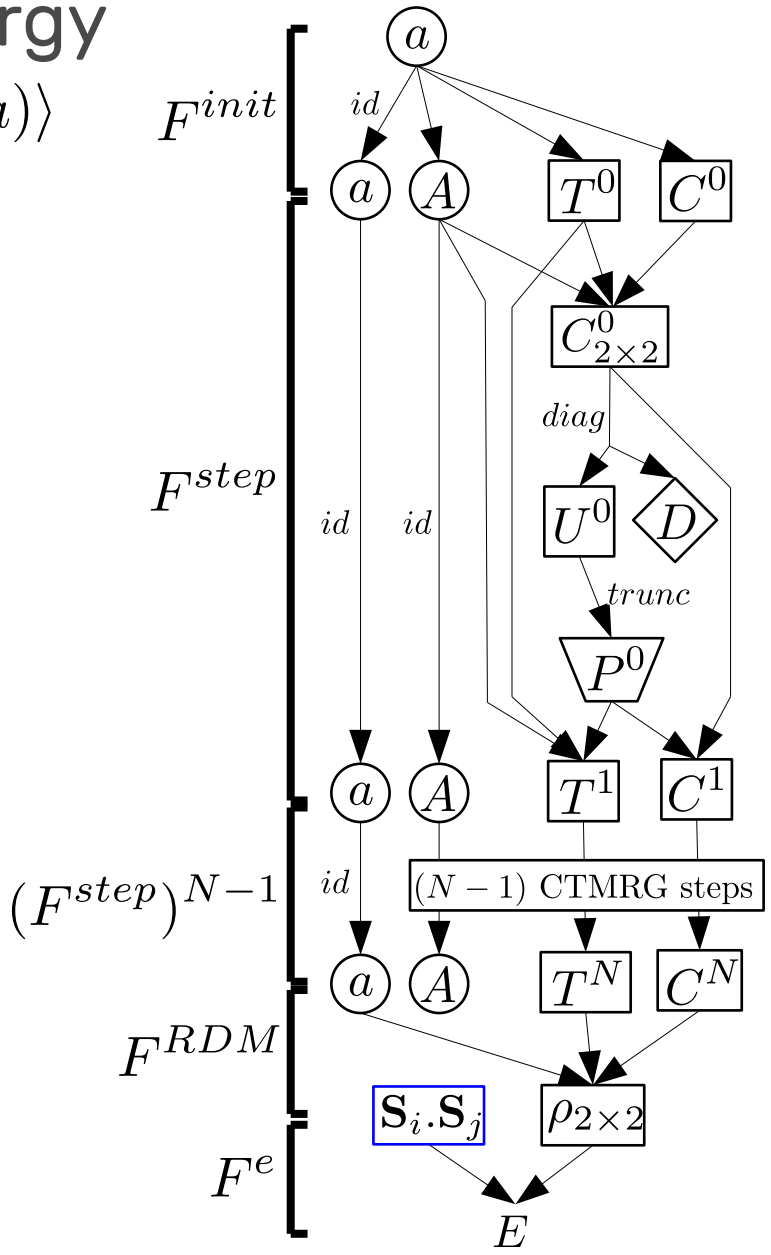


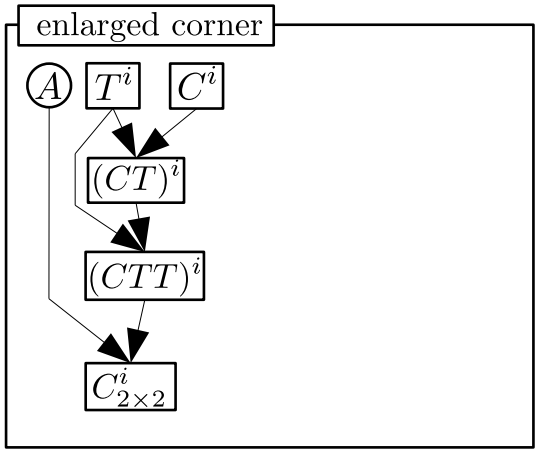
Evaluate the spin-spin interactions and invoke AD

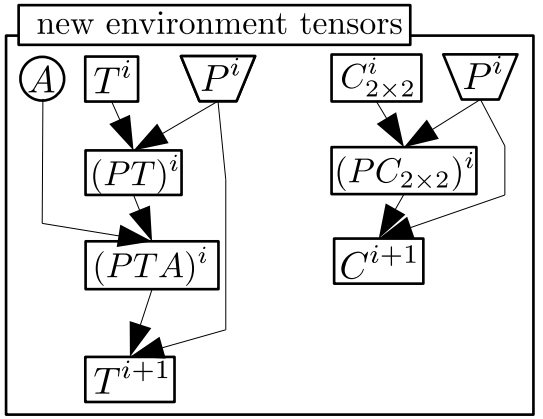
Single-site iPEPS: Energy as DAG

Variational energy

$$E(a) = \langle \psi(a) | H | \psi(a) \rangle$$



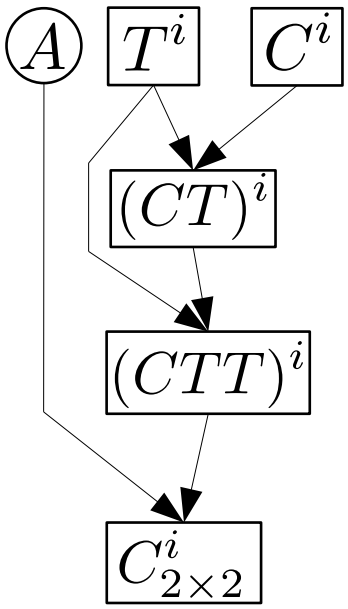




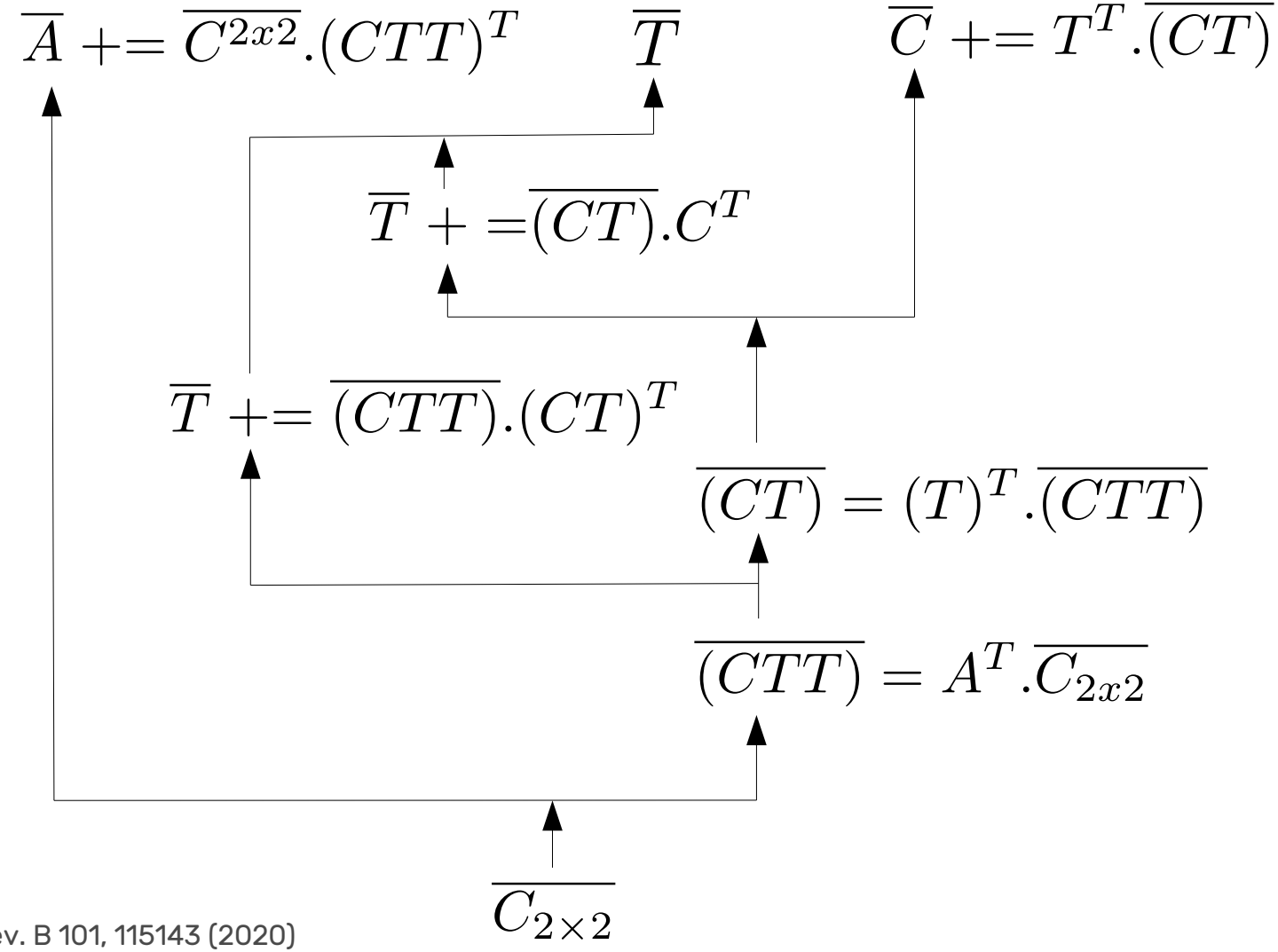
Single-site iPEPS: Energy as DAG

Enlarged corner

Forward



Backward



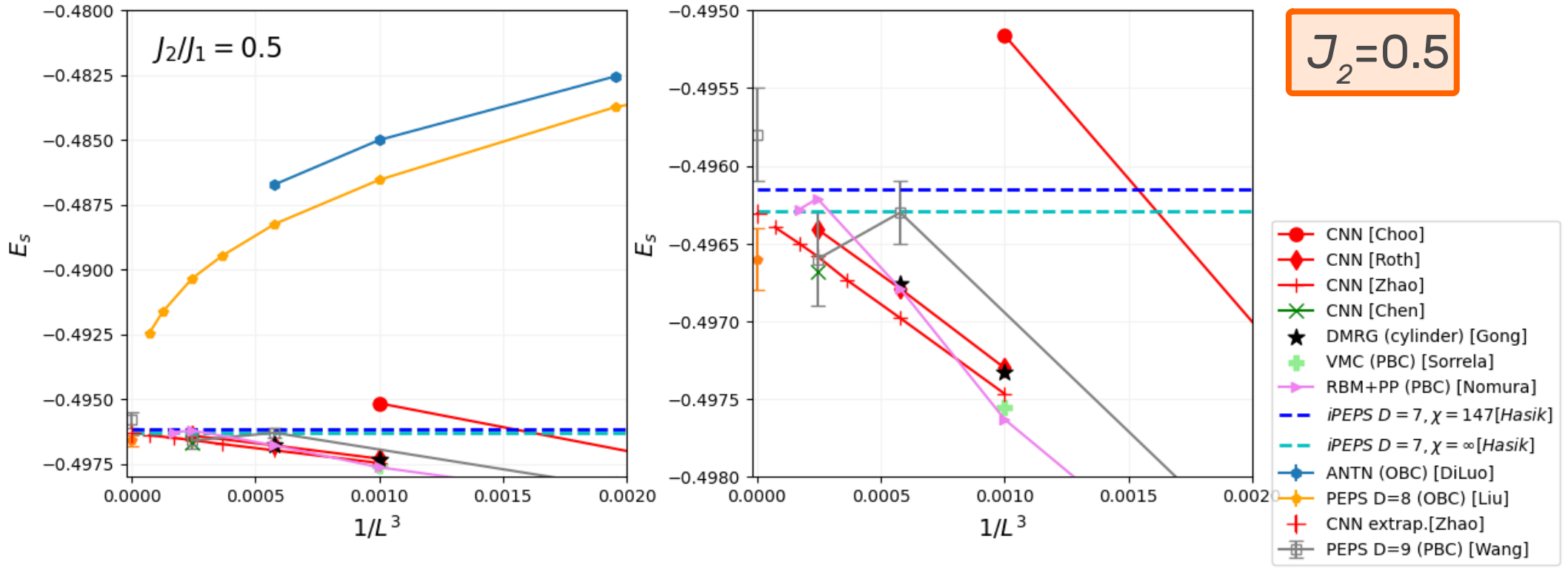
Analogy ?

S.P.G. Crone and P. Corboz, Phys. Rev. B 101, 115143 (2020)

J2=0.5 Point - Energetics

Strict upper bound for **thermodynamic limit**

- Point-group + U(1) sym D=7 iPEPS: **167** parameters



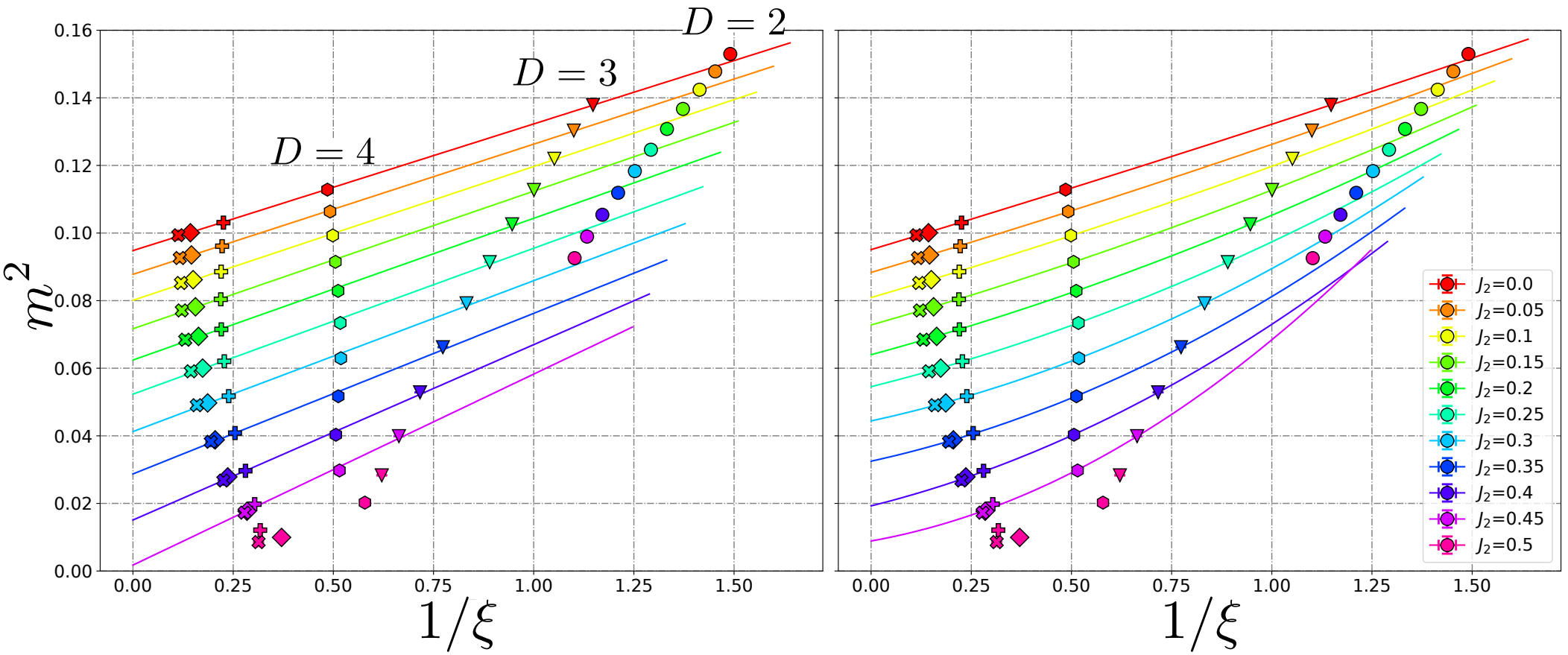
Néel phase of J1-J2 Model

Extrapolate (staggered) magnetization* m^2 to thermodynamic limit as:

$$m^2(\xi) = m^2(\infty) + \frac{B}{\xi} + O\left(\frac{1}{\xi^2}\right)$$

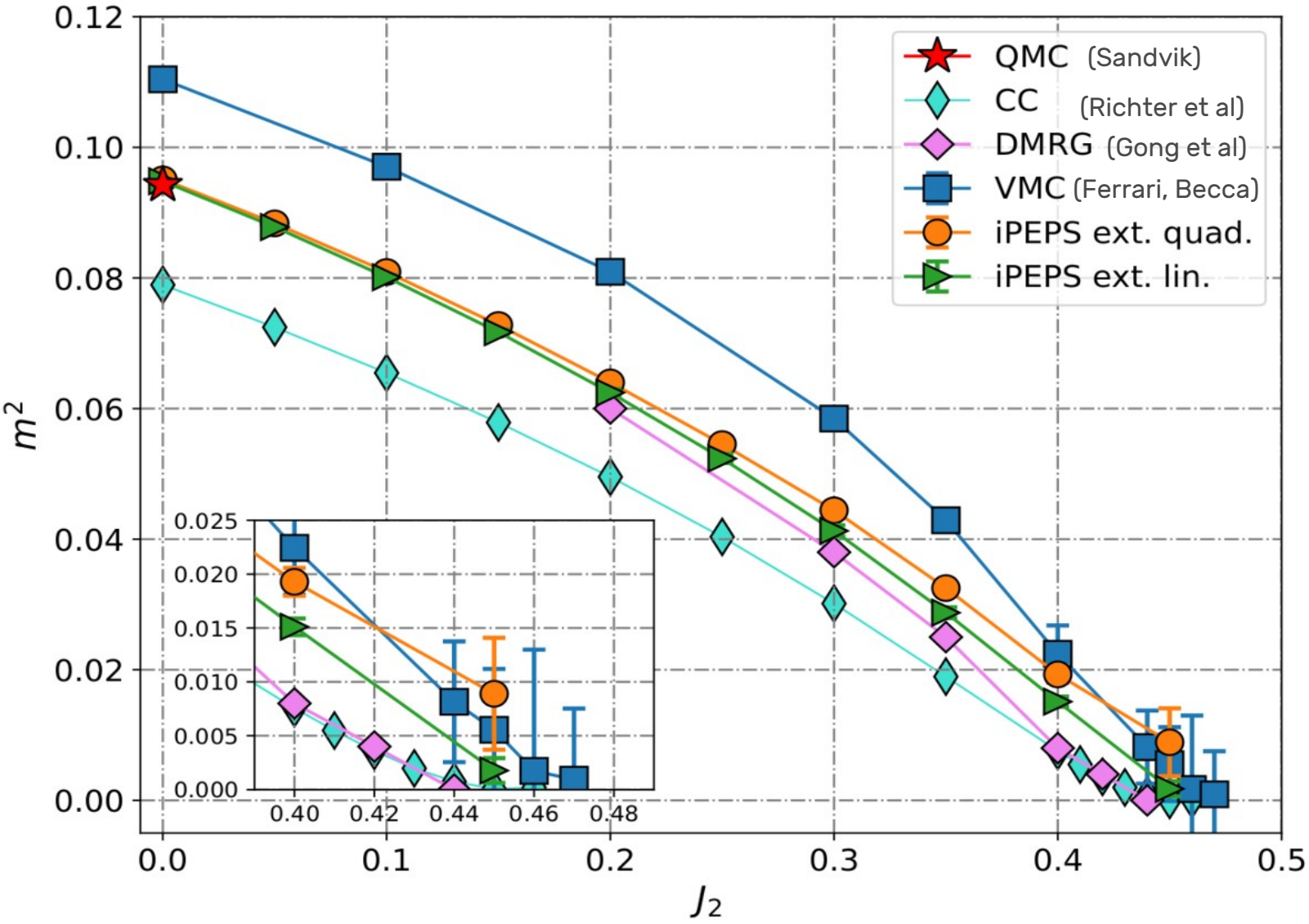
*** Resolve U(1) !**

(Rader and Lauchli, Corboz et al. 2018)



Néel phase of J1-J2 Model

Magnetization curve vanishing around $J_{2c} = 0.46(1)$

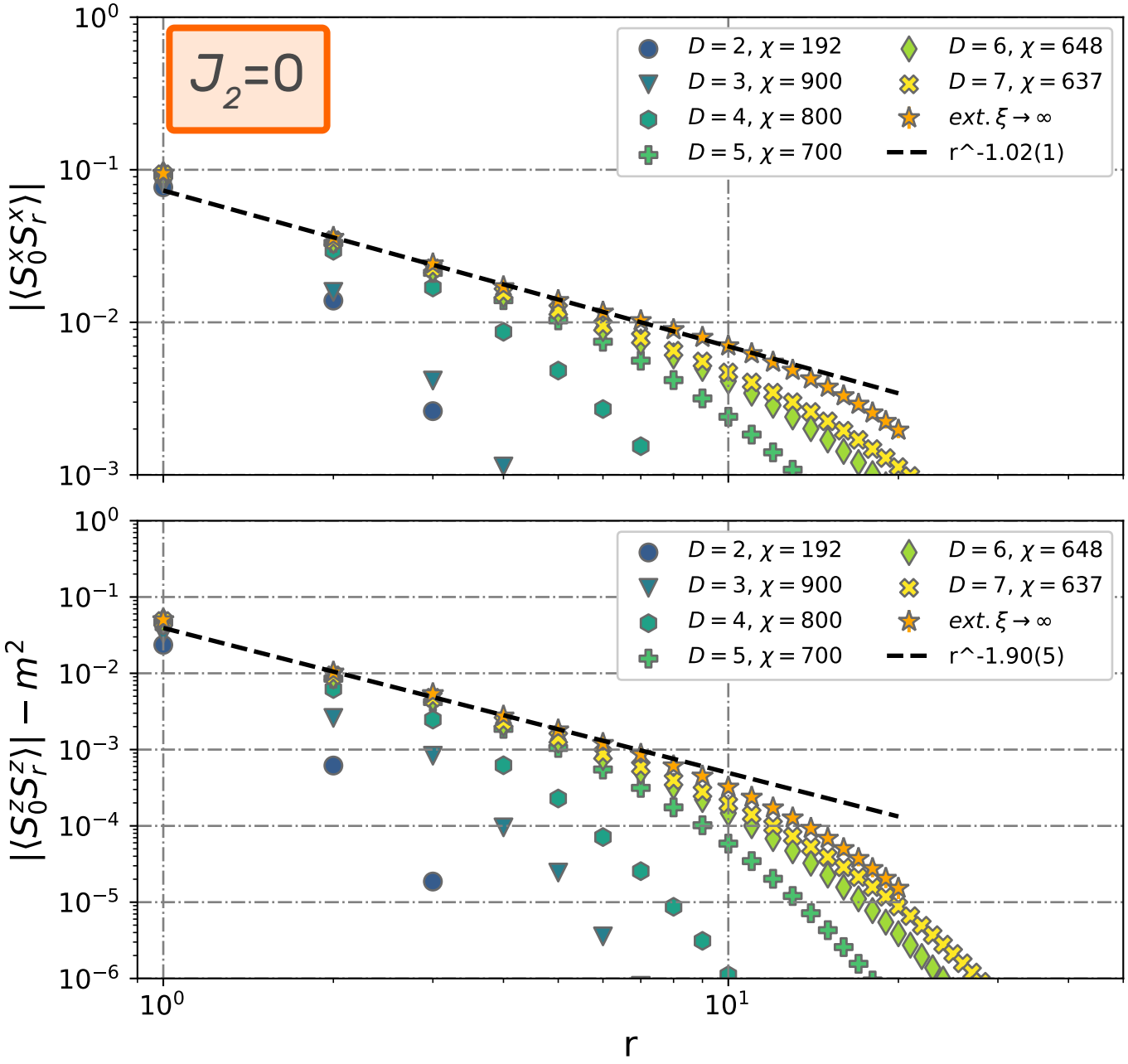


Néel phase of J1-J2 Model

Spin-resolved 2-point corr. F

Short-range
Power law decay

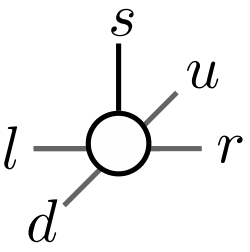
T $\propto r^{-1.02(1)}$
L $\propto r^{-1.90(5)}$



Inferring the *U(1)* structure

Proposition: Resolve minima by imposing *U(1)* symmetry on the on-site tensor

$$a(\vec{\lambda}) = \sum_i \lambda_i t_i \quad \Longleftrightarrow \quad a^s_{uldr} =$$



- $\{t_0, t_1, \ldots\}$ are elementary representatives of A_1 irrep and chosen *U(1)* class
- *U(1)* class $\Leftrightarrow$ charges $\vec{u} = (u^{\uparrow}, u^{\downarrow})$ and $\vec{v} = (v_0, \ldots, v_{D-1})$ assigned to indices *s* and *u,l,d,r*

Conservation law: $u^s + v_u + v_l + v_d + v_r = N$

Q: How to choose charge sector, that is, $\vec{u}, \vec{v}$?

Inferring the $U(1)$ structure

Observation: unrestricted optimization for small J_2 leads to an almost U(1)-symmetric states (S.S(r), Transfer matrix spectrum)

- Solve the system of constraints given by **the largest elements** of tensor *a* from unrestricted optimization (pre-process by HOSVD)
- Example for D=3: $(\vec{u}, \vec{v}) = (1, -1, 0, 2, 0)$ with *N*=1

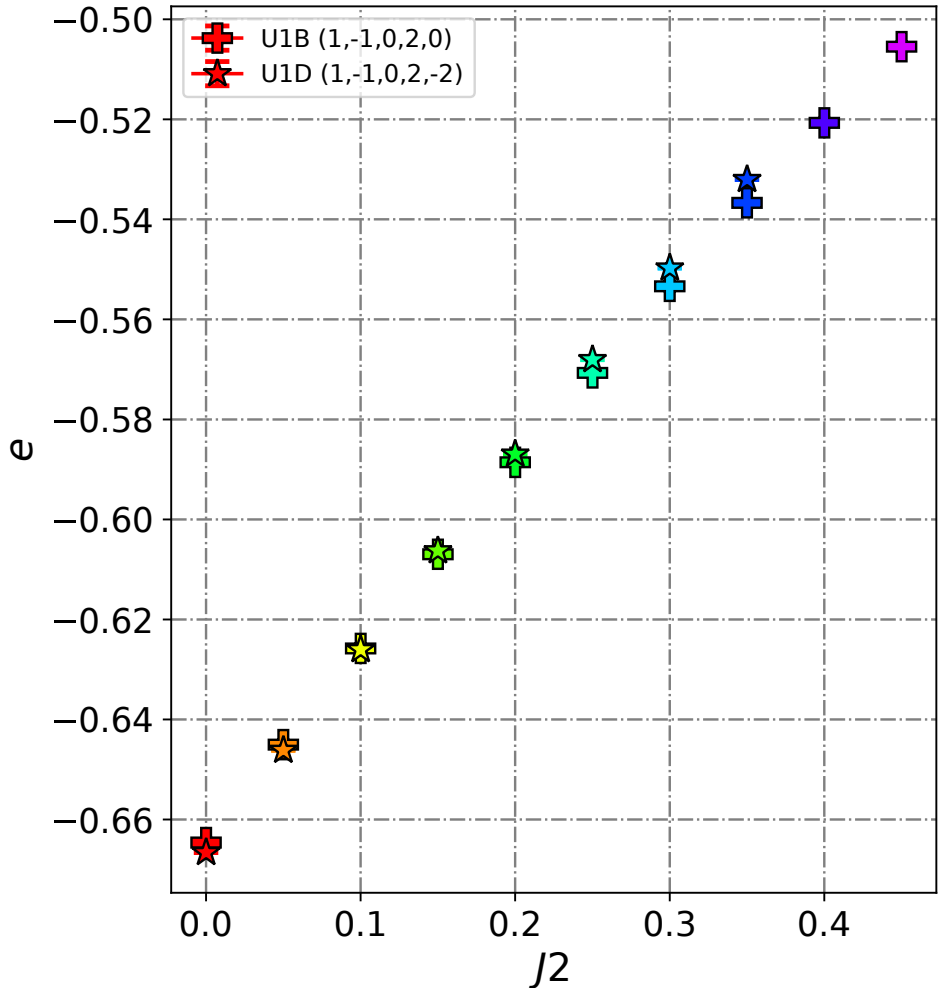
$$\begin{array}{ll} \vec{n}(a^{\uparrow}_{0000}) & \to \\ \vec{n}(a^{\downarrow}_{0001}) & \to \\ \vec{n}(a^{\uparrow}_{0002}) & \to \\ \vec{n}(a^{\uparrow}_{2222}) & \to \\ \vec{n}(a^{\uparrow}_{0222}) & \to \end{array} \begin{bmatrix} 1 & 0 & 4 & 0 & 0 \\ 0 & 1 & 3 & 1 & 0 \\ 1 & 0 & 3 & 0 & 1 \\ 1 & 0 & 0 & 0 & 4 \\ 1 & 0 & 1 & 0 & 3 \end{bmatrix} \cdot \begin{bmatrix} u^{\uparrow} \\ u^{\downarrow} \\ v_0 \\ v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} N \\ N \\ N \\ N \\ N \end{bmatrix} .$$

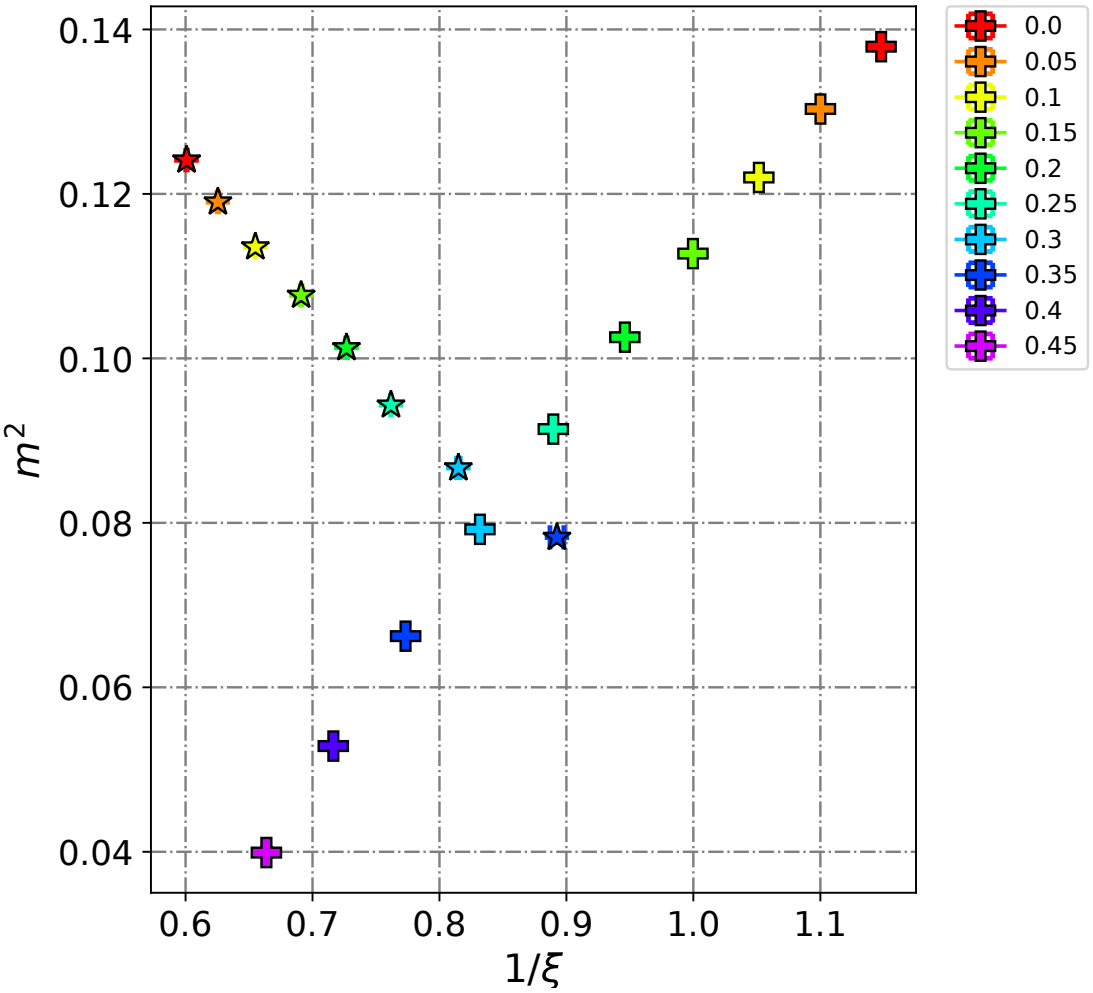
Solve within integer domain by **Smith normal form**

Inferring the *U(1)* structure

Competition between different U(1) classes appears

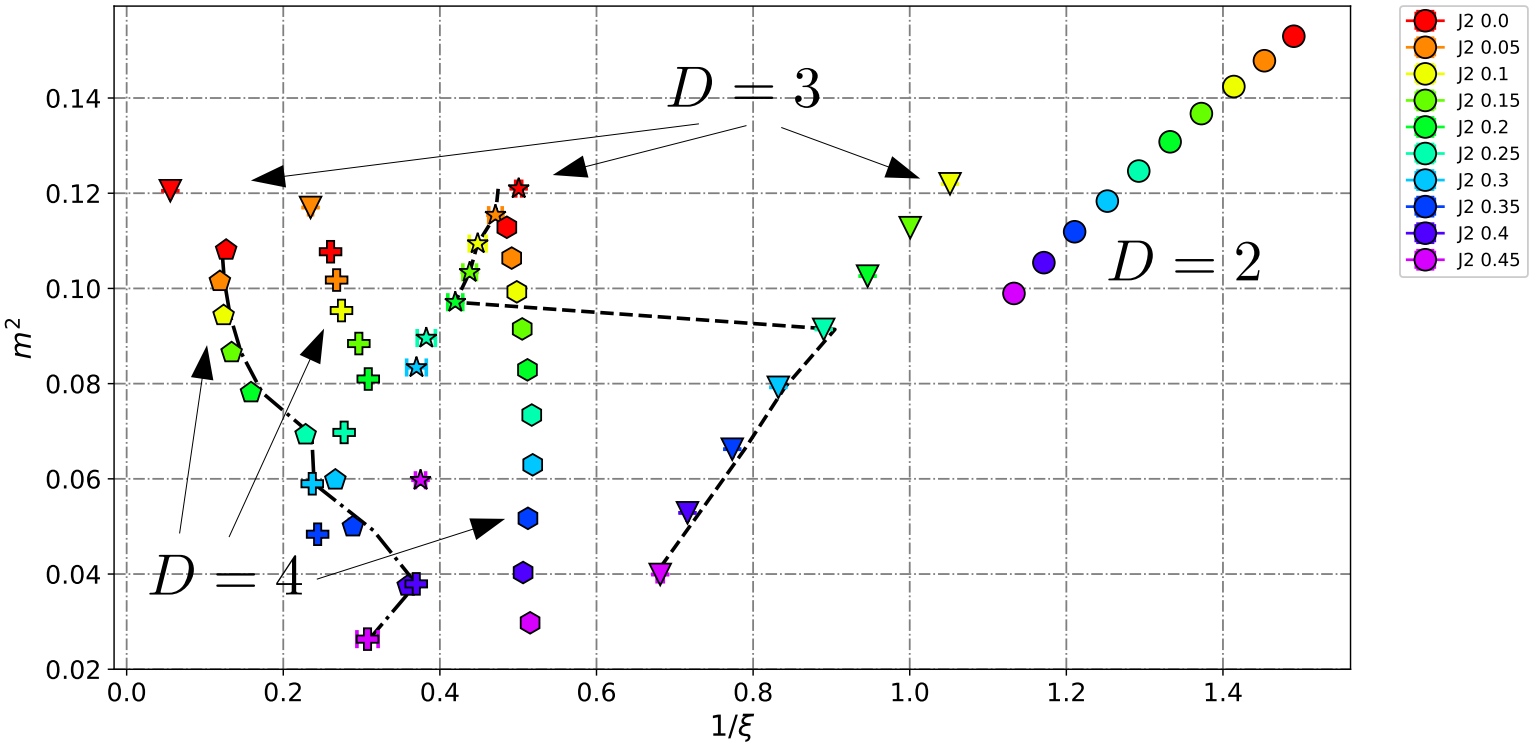
- Example for D=3 (also D=4)





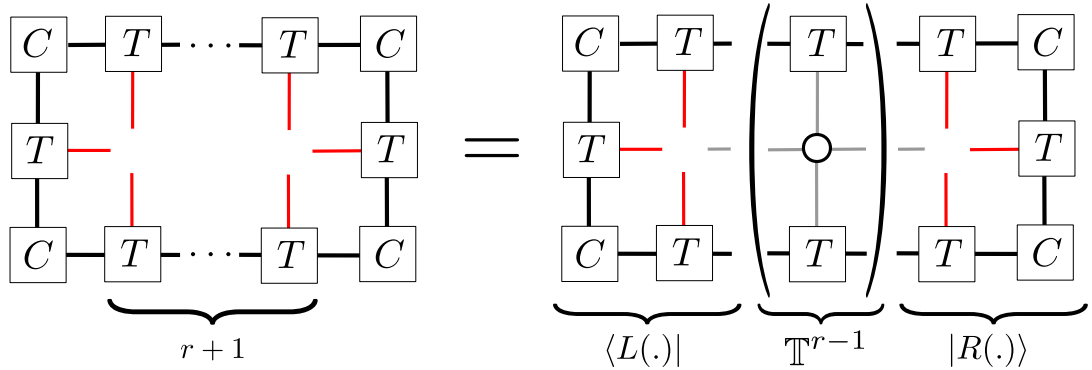
Application to J1-J2 Model

Complication: Presence of distinct local minima



Corr. Length:

$$f^C(r)_{O_1O_2} = \sum_{i>0} \lambda_i^{r-1} \langle L|l_i\rangle\langle r_i|R\rangle \Leftrightarrow$$



Nishino, Phys. Lett. A, (1996); M. M. Rams, P. Czarnik, and L. Cincio Phys. Rev. X 8, (2018)