Tensor-network study of frustrated Heisenberg model

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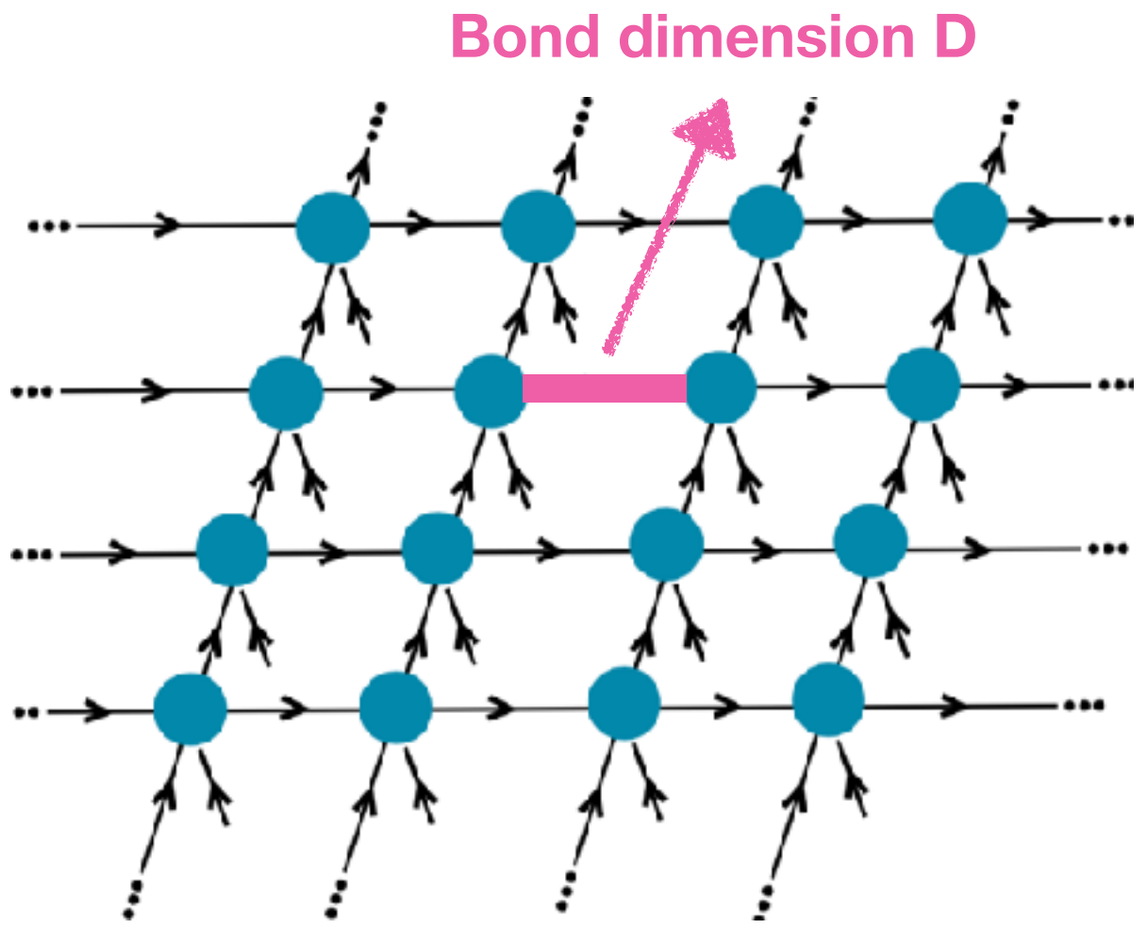
infinite projected entangled-pair states (iPEPS) ansatz

It works directly in the thermodynamic limit

No boundary effect and finite-size scaling

Only essential parameter is the amount of entanglement: bond dimension D

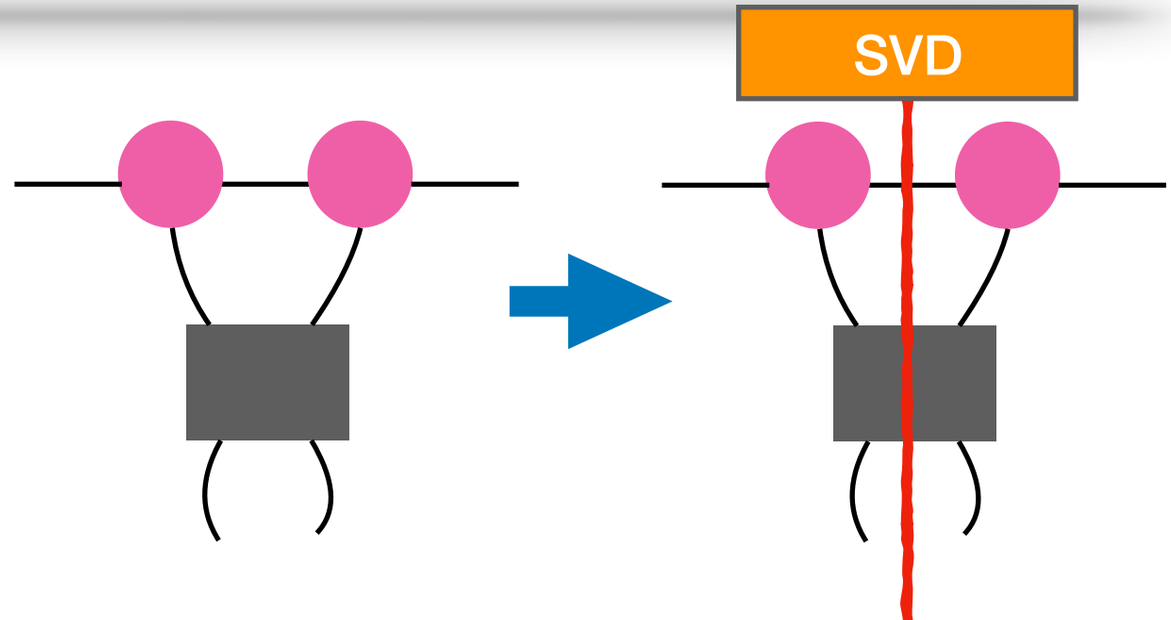


A U(1)-symmetric iPEPS ansatz reproduces entanglement area-law in 2D

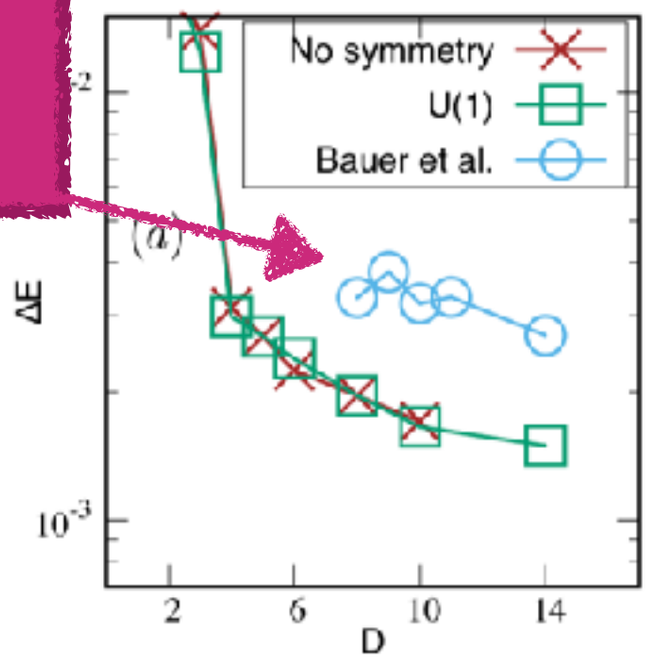
How to implement symmetry into iPEPS?

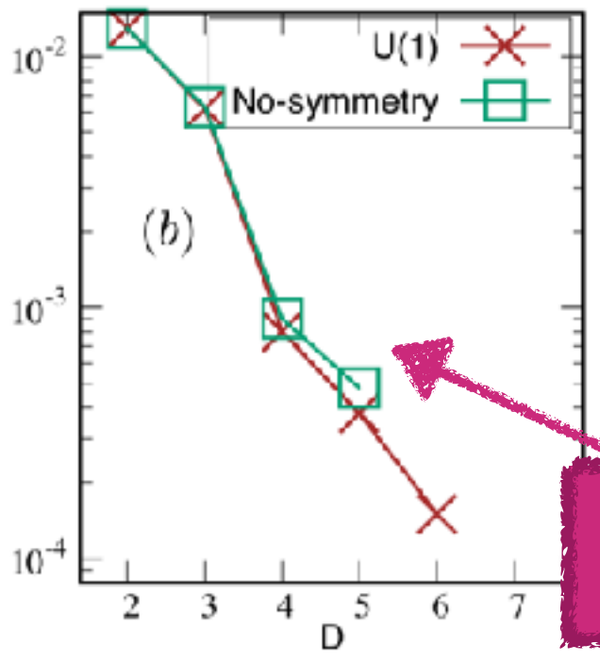
Use ***SVD*** in simple-update simulation to select the symmetry sectors for each virtual bond

Use a non-homogeneous structure: each virtual bond takes different symmetric sectors from another one



The homogeneous structures are not accurate



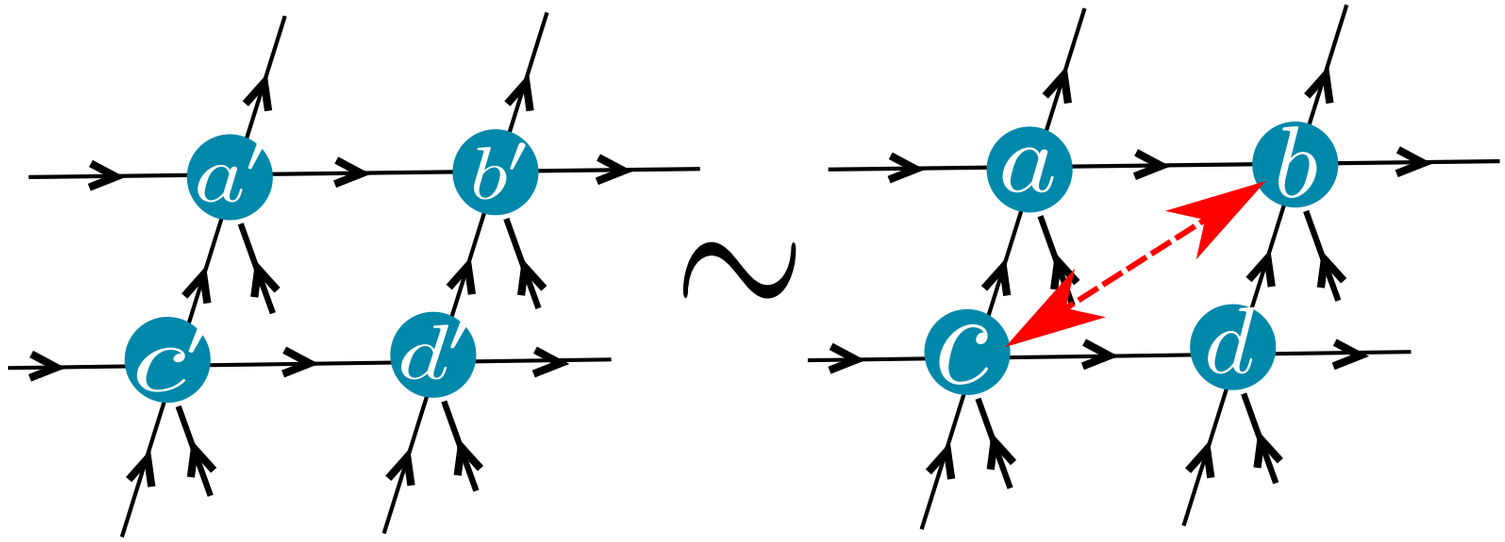


Full-update simulation: no loss of accuracy

How to improve optimization in the presence of second-neighbor interactions?

How to efficiently obtain tensors $\{a', b', c', d'\}$?

$$|\psi'(a', b', c', d')\rangle \quad \sim \quad U|\psi(a, b, c, d)\rangle$$

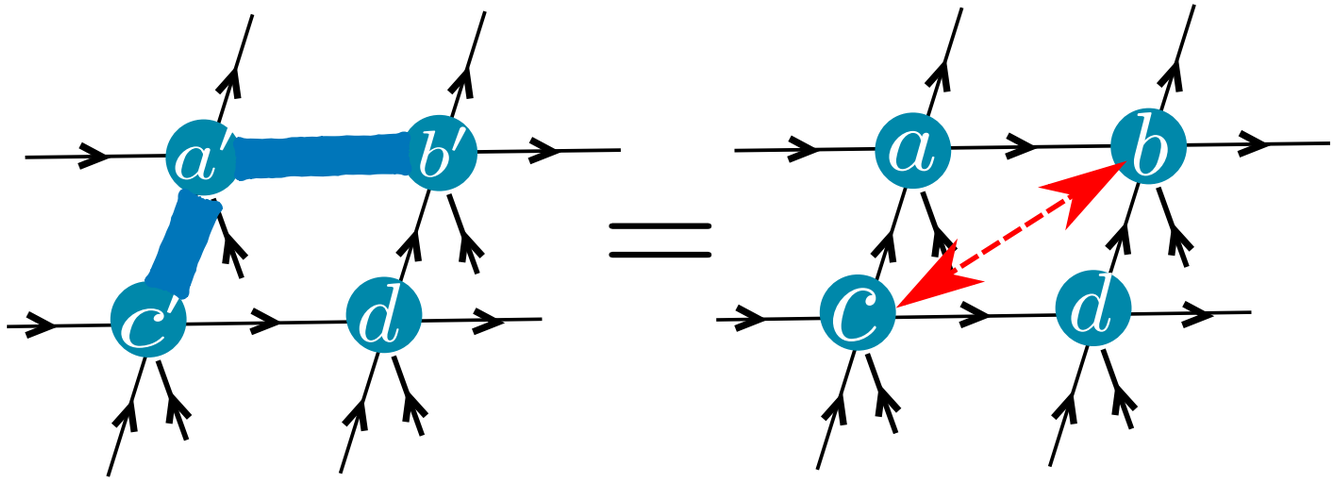


We use **positive approximant** and **reduced tensors** in an

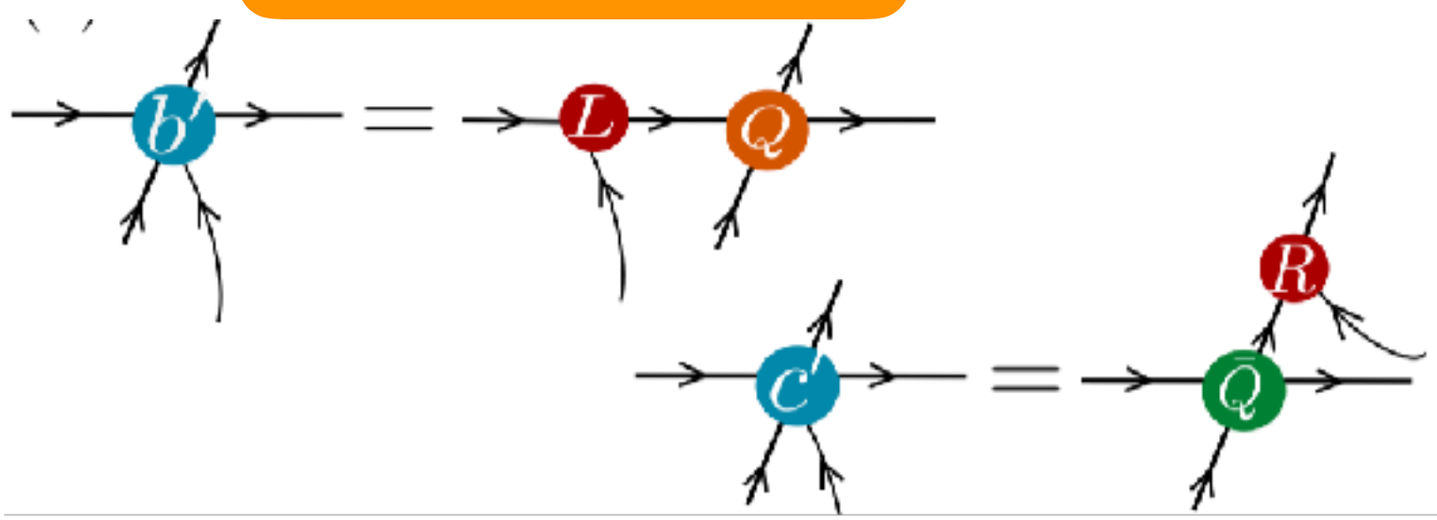
iterative way to improve accuracy and convergence rate of optimization algorithm

Basic Idea: reduced tensors

Reduced tensors: Interaction only effects the blue bonds!!!



LQ and QR decomposition



We only need to optimze reduced tensors {L, R} and tensor {a'}, which hugely reduces computational time.

Basic idea: positive approximant

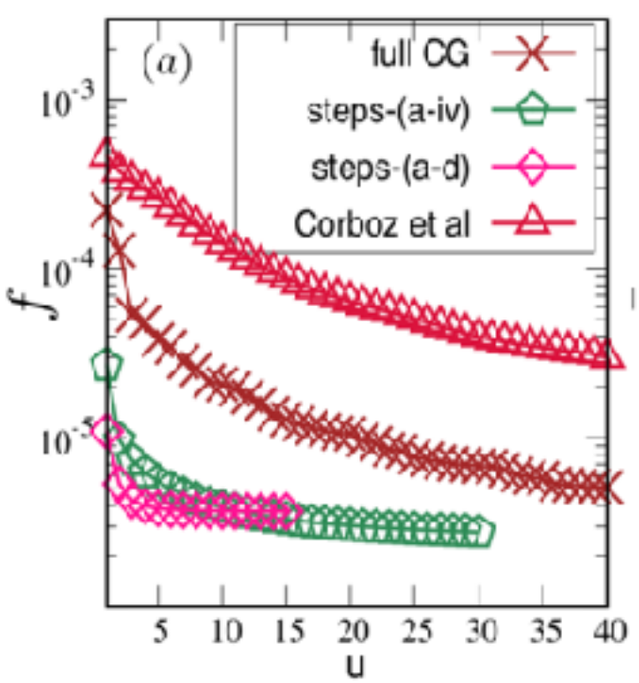
The square distance

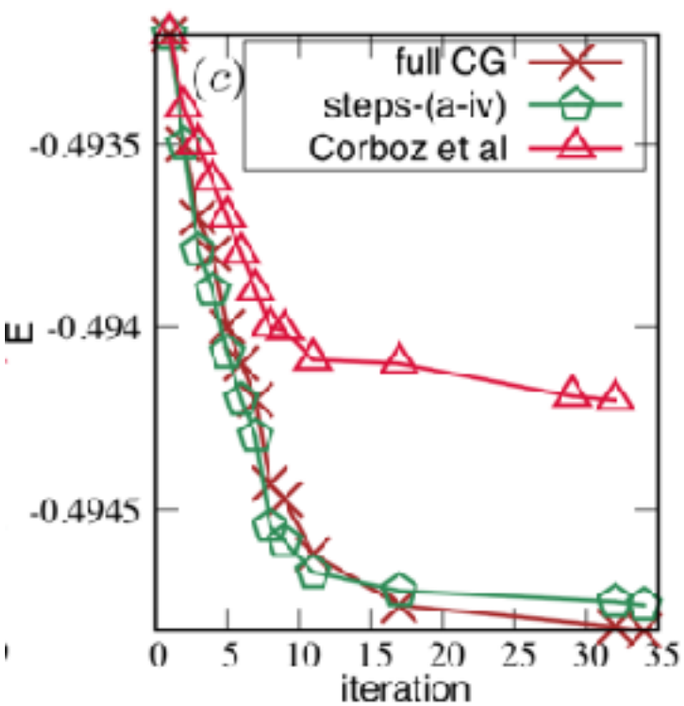
$$f = \langle\psi|U^\dagger U|\psi\rangle + \langle\psi'|\psi'\rangle - \langle\psi'|U|\psi\rangle - \langle\psi|U^\dagger|\psi'\rangle.$$

$$\min_{\{a',r,l\}} f = const + r^\dagger a'^\dagger l^\dagger \mathcal{N} l a' r - r^\dagger a'^\dagger l^\dagger \bar{\mathcal{N}} - \bar{\mathcal{N}}^\dagger r a' l,$$

We explicitly eliminate negative part of Norm tensor, enforcing it to be positive square distance: $\mathcal{N} \rightarrow \mathcal{N}_+$

better convergence rate



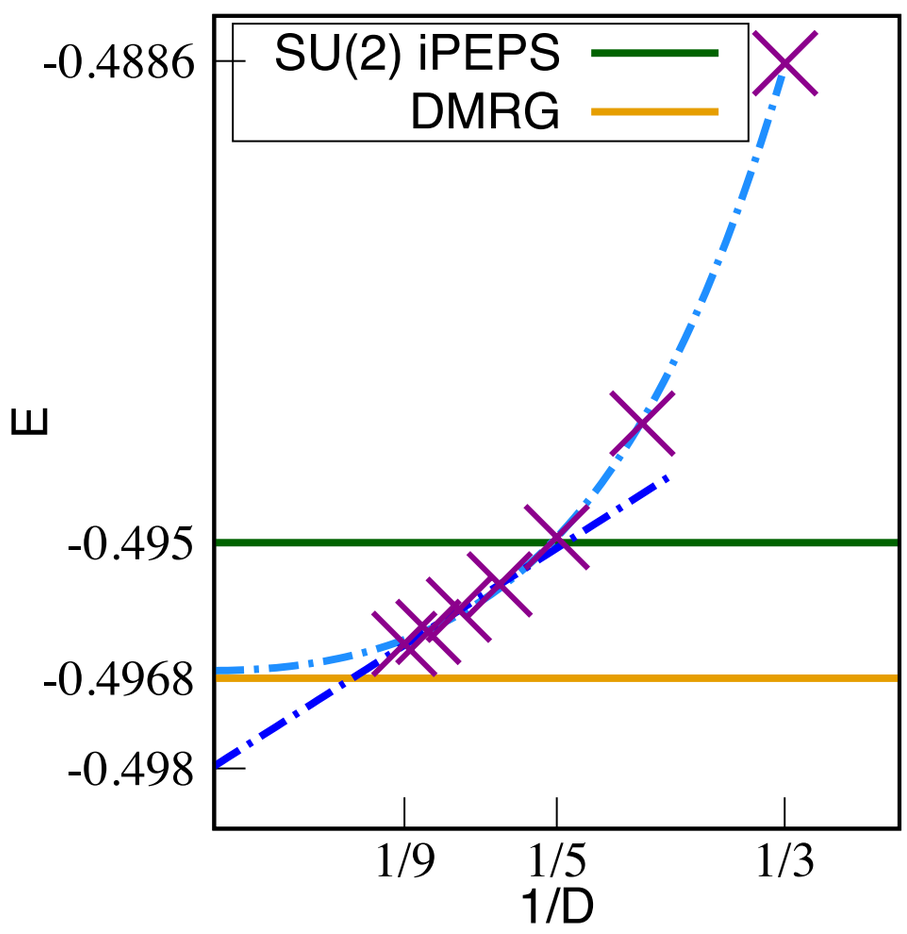


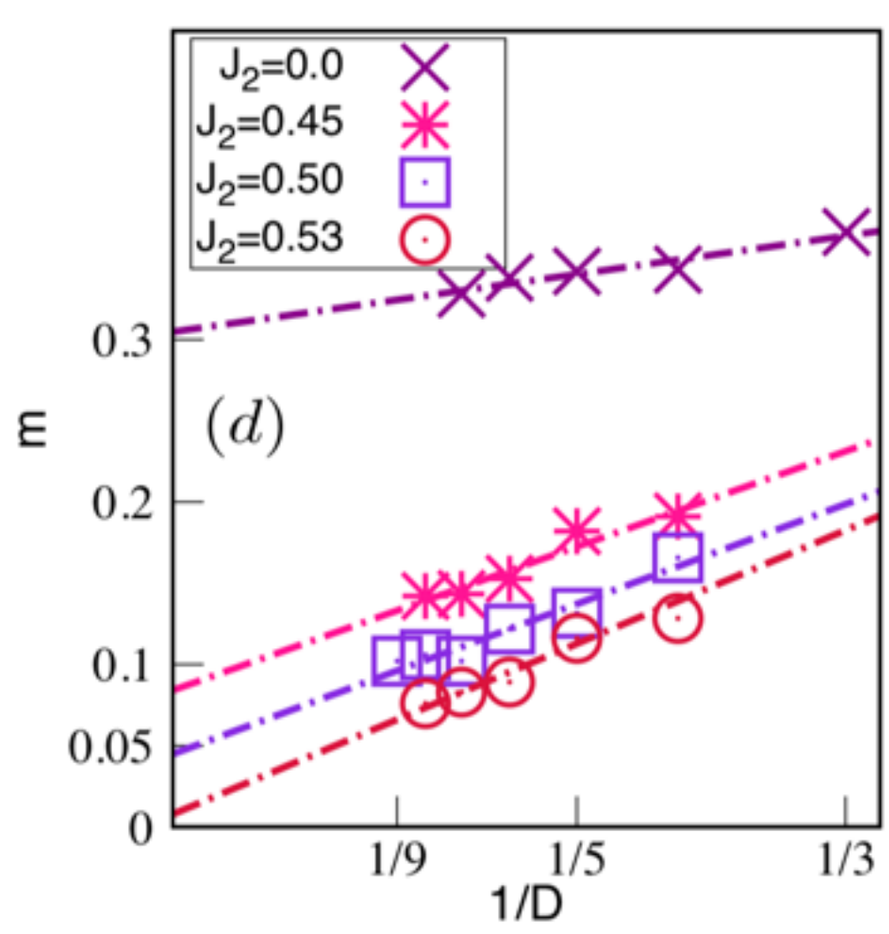
better accuracy

The spin-1/2 square J_1-J_2 Heisenberg model

The U(1)-symmetric iPEPS variational energy is compatible with DMRG at the highly frustrated point J_2=0.50

The Neel order parameter **m** as a function of **1/D**. A linear fit in large-D limit reveals **m** vanishes at point J_2=0.53



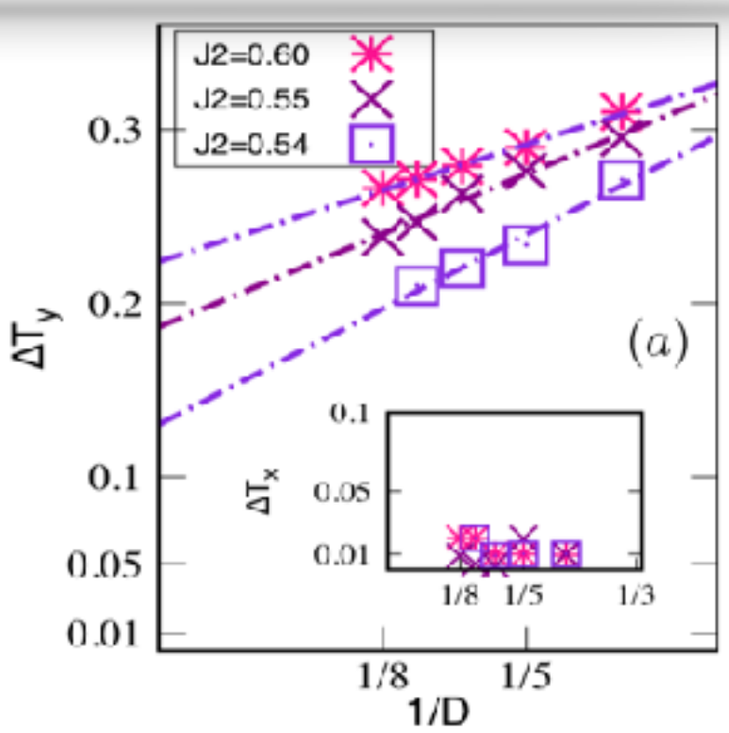


The columnar valence bond solid as intermediate phase

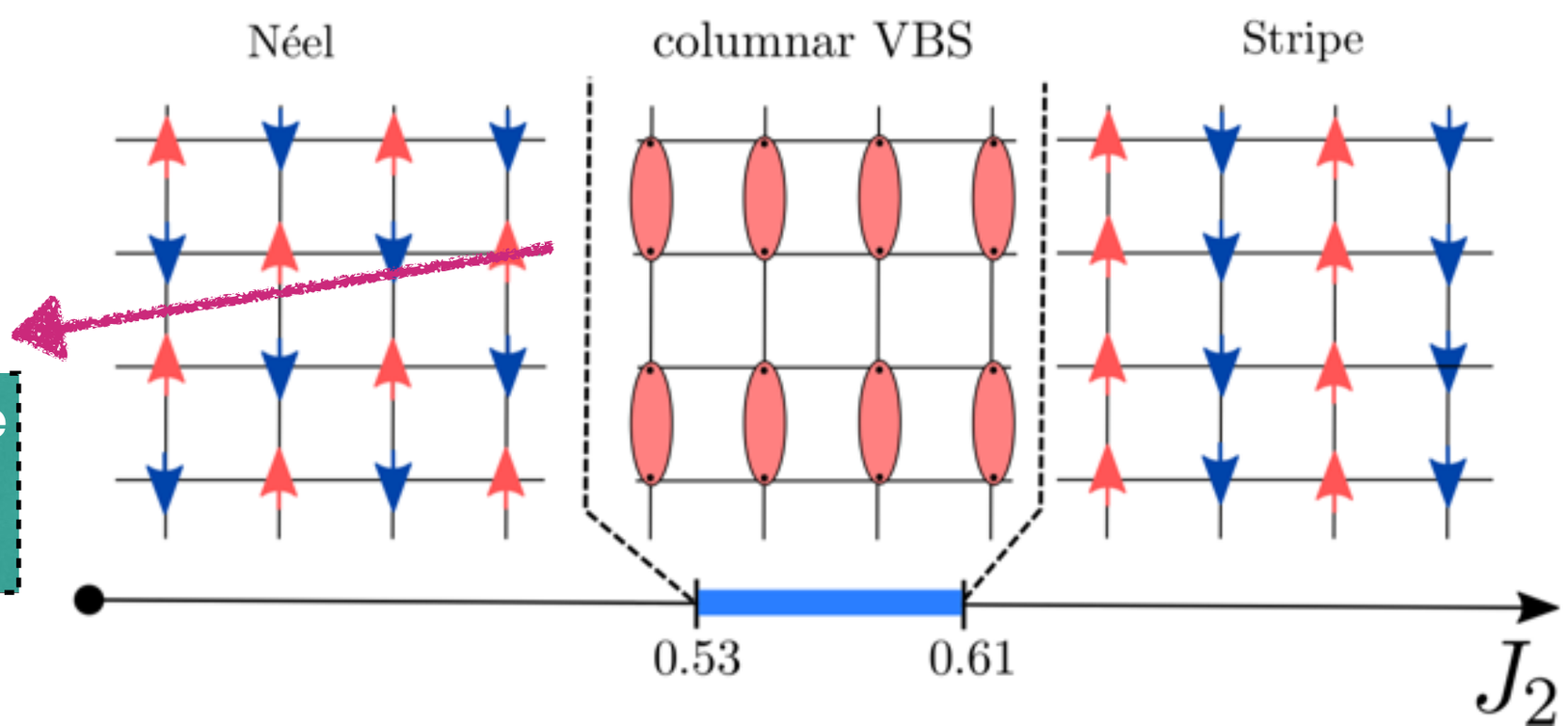
The iPEPS predicts a columnar VBS order as intermediate phase

$$\Delta T_y = \max(E_y) - \min(E_y)$$

$$\Delta T_x = \max(E_x) - \min(E_x)$$



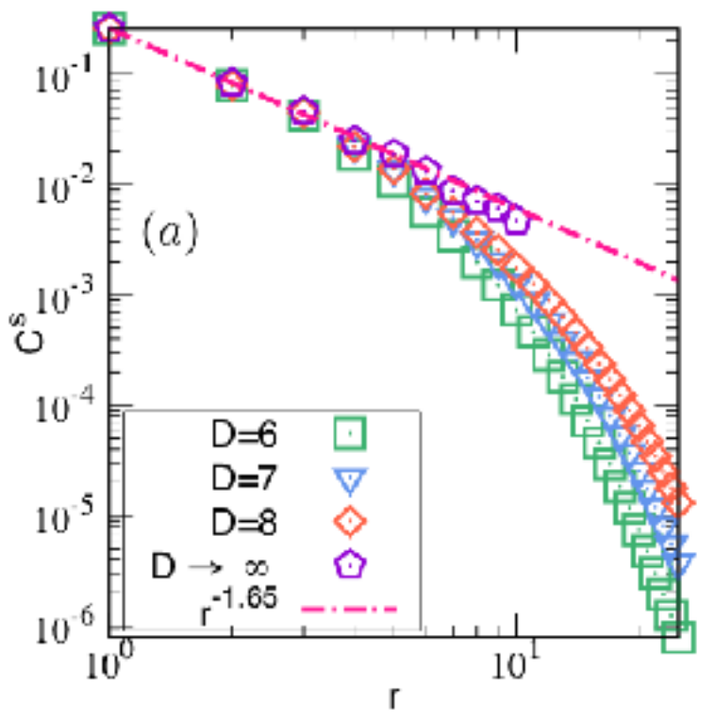
What is the nature of the quantum phase transition?

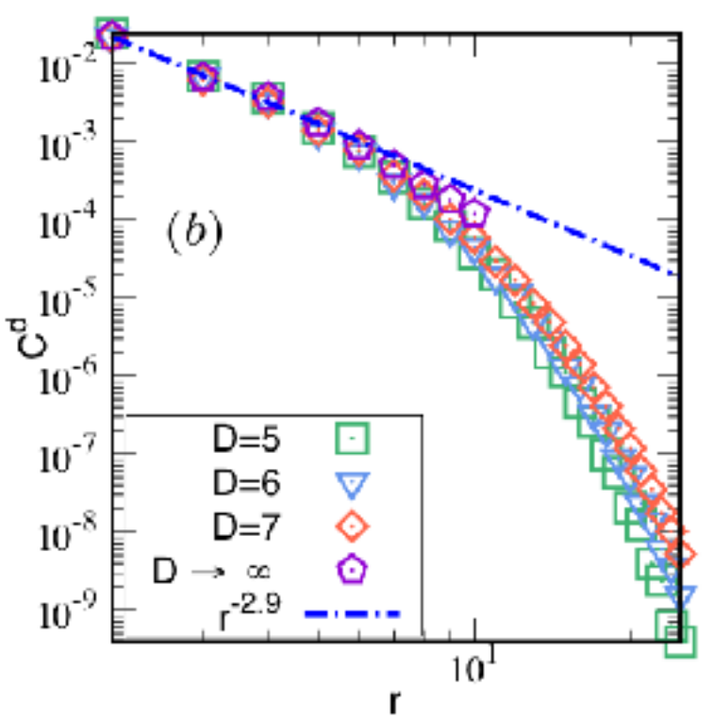


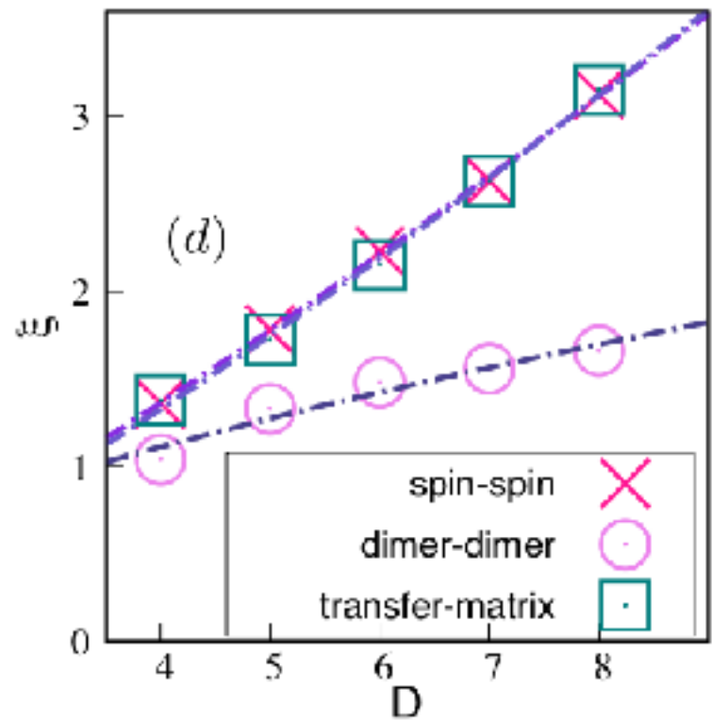
The Spin-spin and dimer-dimer Correlation functions

The critical exponents for spin-spin and dimer-dimer are, respectively, {0.65, 1.9}; showing strong deviation from J-Q models

The spin correlation length diverges like $\xi \sim D^{1.2}$ which is more rapidly than dimer correlation length





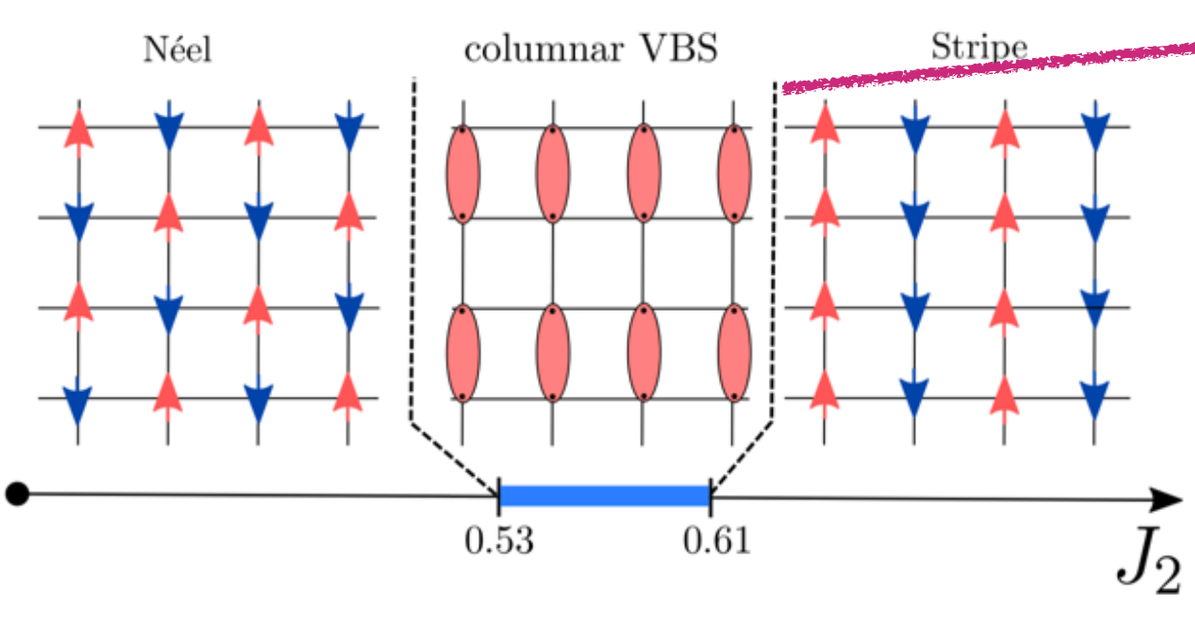


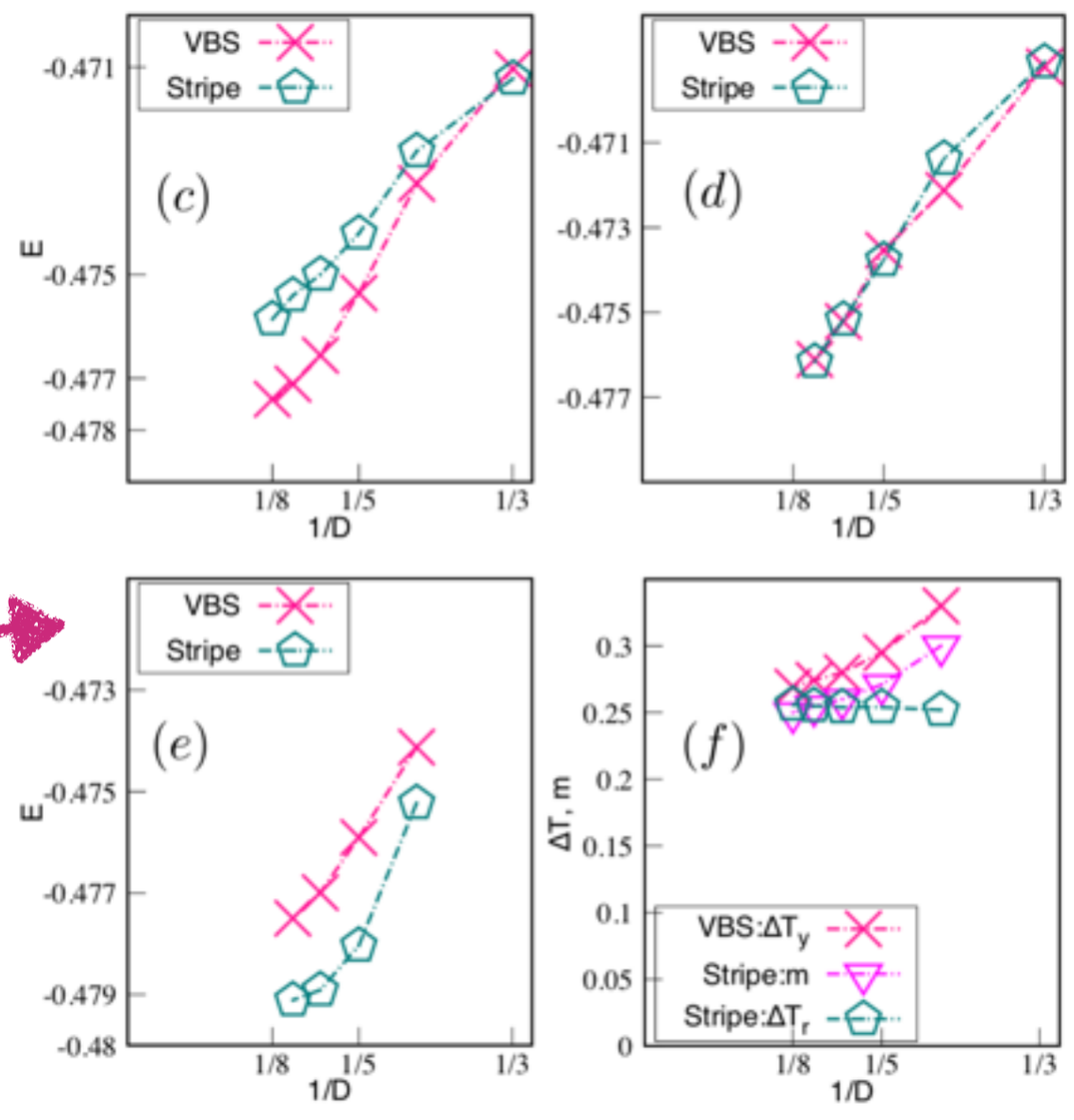
The first-order phase transition: hysteresis analysis

✓ we initialize the iPEPS ansatz by competitive ordered states in the vicinity of the critical point energy

✓ The columnar VBS energy crosses the Stripe one around ~ 0.61

✓ The order parameter always remains non-zero

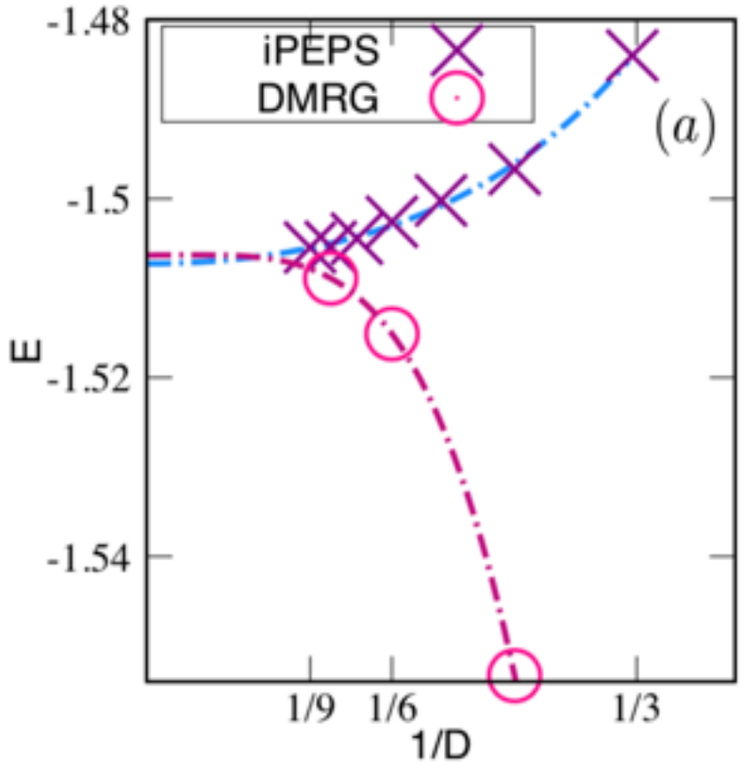


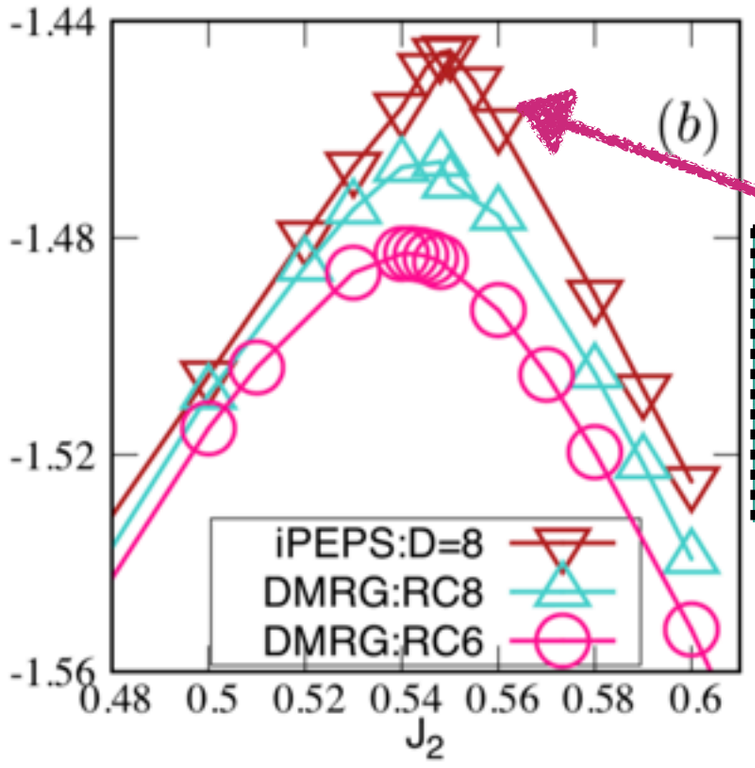


The spin-1 square J_1-J_2 Heisenberg model

Is there any non-magnetic intermediate phase?

What is the nature of the phase transition?





A sharp peak might suggest a firs-order transition

hysteresis analysis

Is there any non-magnetic intermediate phase?

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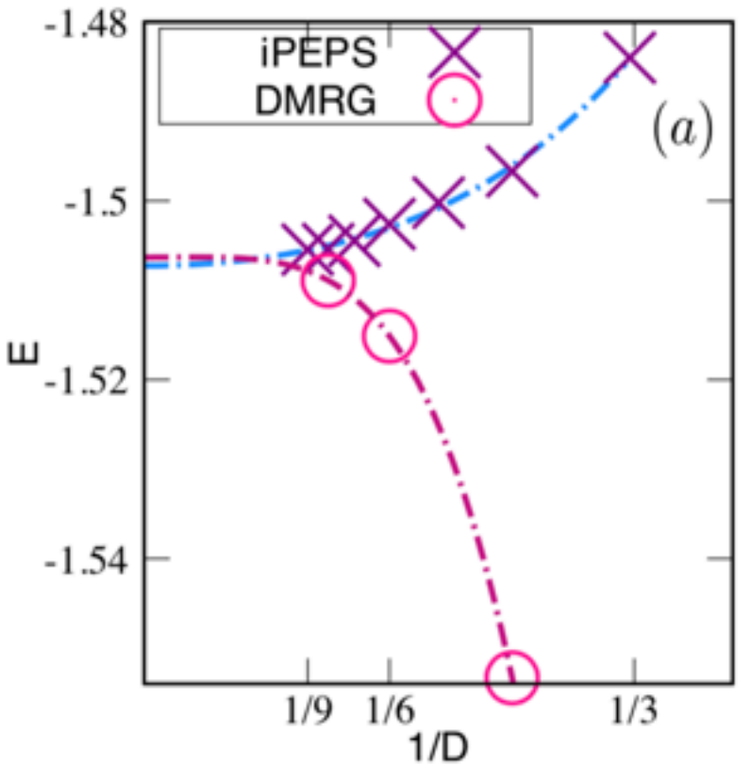
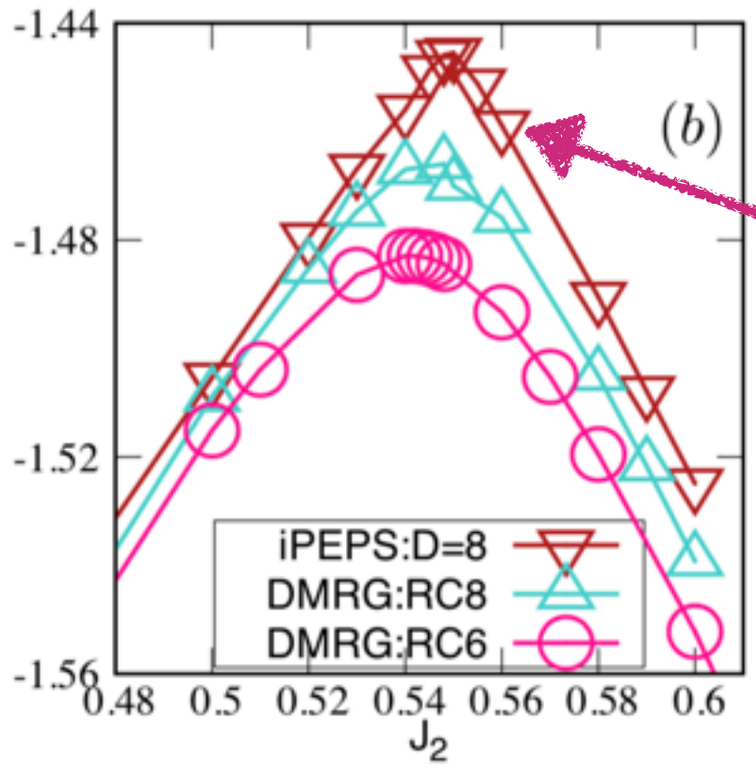
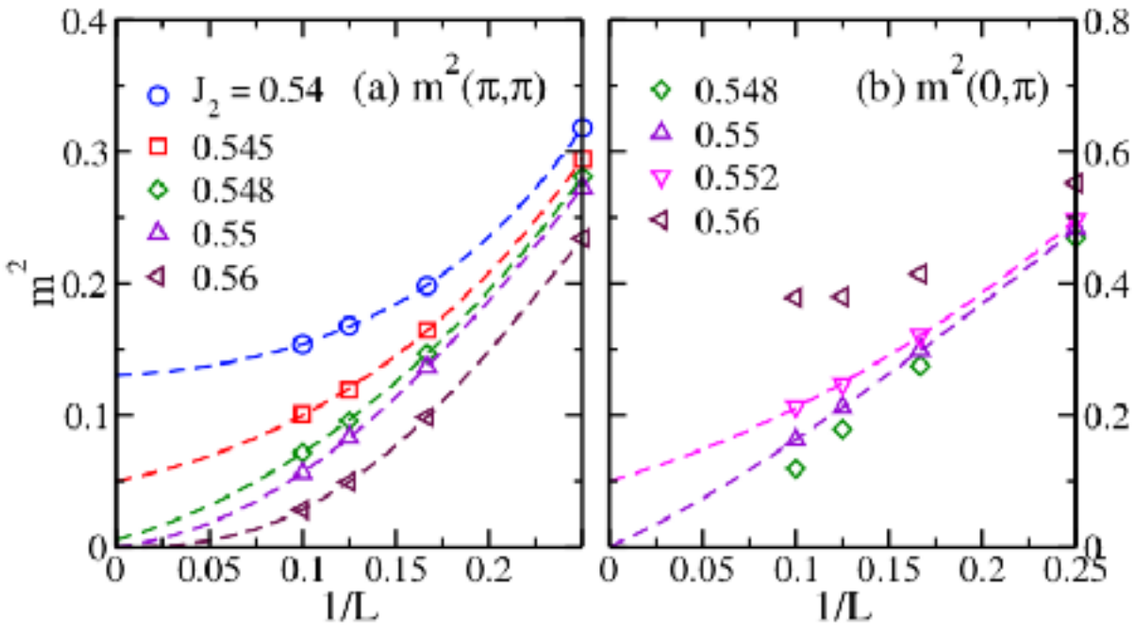




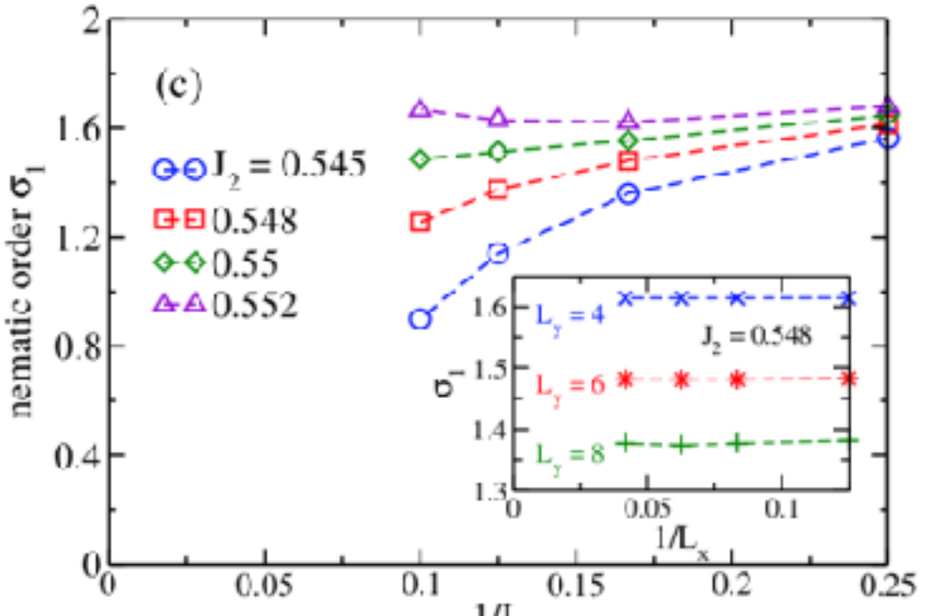
A sharp peak might suggest a firs-order transition

DMRG: order parameters

✔The DMRG calculation shows the Need and the Stripe phases persist up to a very tiny region



✔The nematic order parameter is also consistent with the Need and the Stripe phase



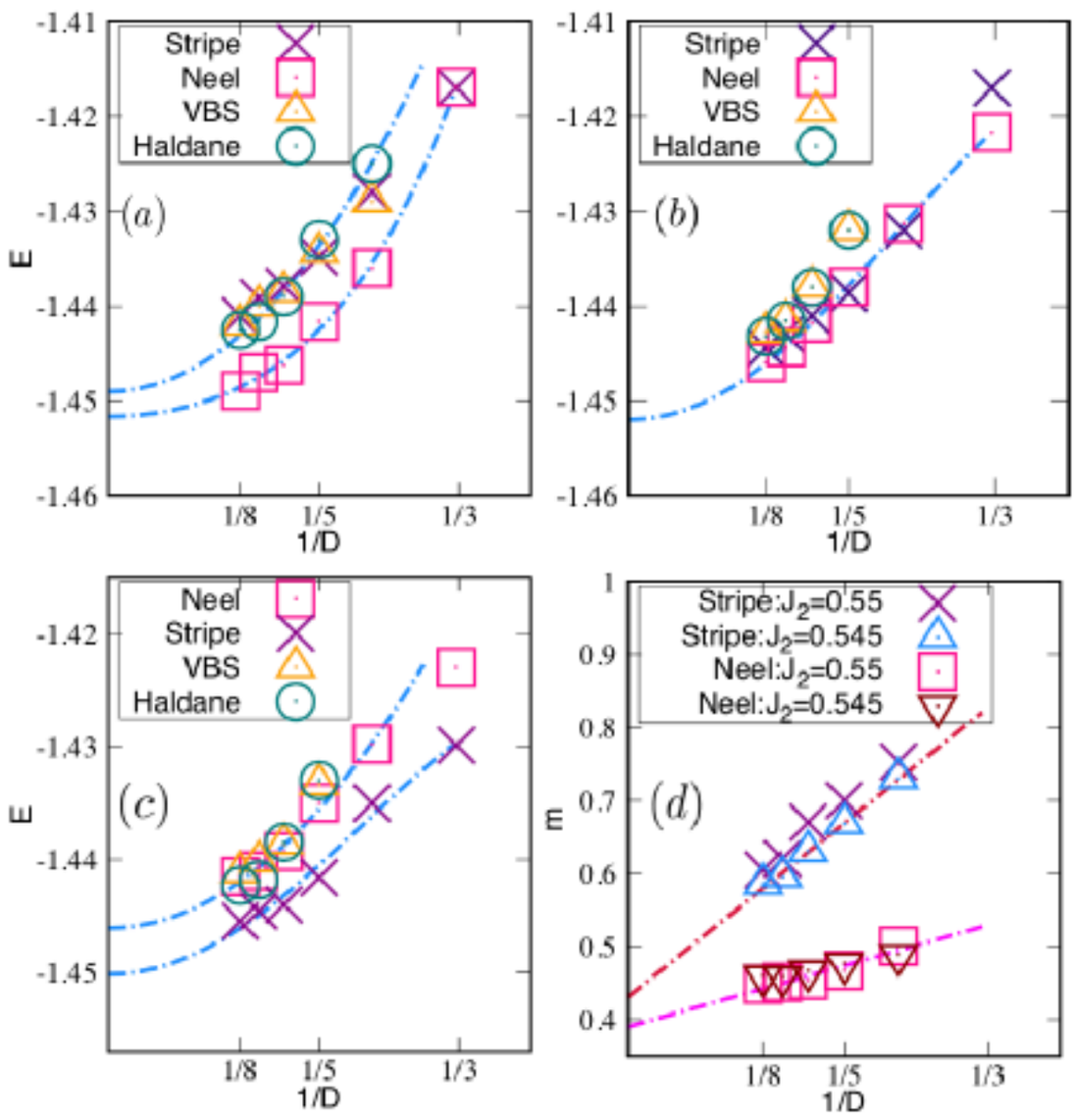
The iPEPS results

✔ The iPEPS energy with different competitive ordered states, as Need, Stripe, VBS and Haldane

✔ In this region, the columnar VBS and the Haldane states never provide the lower energy than magnetically ordered states

✔ The energies of the Neel and Stripe cross each other around 0.549

✔ The magnetically order parameters always remain non-zero



The iPEPS results: correlation length

✓ The correlation length does not illustrate a quantitive changes through the quantum phase transition, Supporting a first order phase transition