Thermal Ising transition in the spin-1/2 $J_1 - J_2$ Heisenberg model

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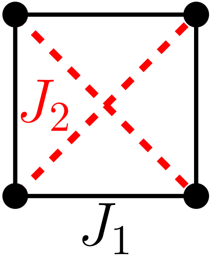
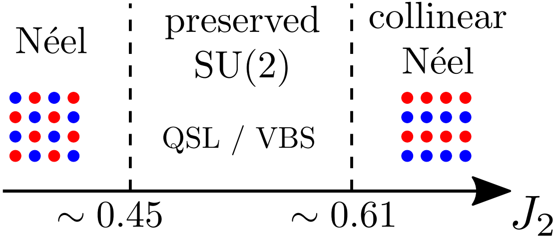
$J_1 - J_2$ Heisenberg model

- spin-1/2 on the square lattice
- $J_1 = 1$ first neighbor interaction
- $J_2 > 0$ second neighbor: magnetic frustration
- [Chandra & Doucot, 1988]: spin liquid realization



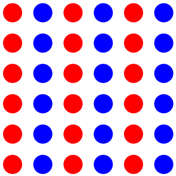
$$\mathcal{H} = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

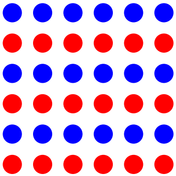


[Ferrari & Becca, 2020]
[Liu et al., 2020]
[Nomura & Imada, 2021]

Finite temperature phase transition

- Mermin–Wagner: SU(2) symmetry cannot be broken at $T > 0$
- [Chandra et al., 1990]: finite temperature Ising transition





- spontaneous C_{4v} symmetry breaking
- stripe direction selected *before* Néel order appears
- [Weber et al., 2003]: classical phase diagram
- [Capriotti et al., 2004]: semi-classical theory based on classical results
- 30 years after, no direct numerical evidence

Thermal ensemble and purification

- density matrix ρ obtained from *purified* wavefunction $|\Psi\rangle$
- $|\Psi\rangle$ lives in enlarged Hilbert space $\tilde{H} = H \otimes H'$

$$|\Psi\rangle = \sum \sqrt{p_i}\,|i\rangle \otimes |i'\rangle$$

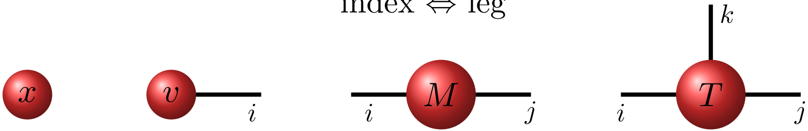
- trace over auxiliary degrees of freedom to recover thermal ensemble

$$\rho(\beta) = \mathrm{Tr}_{\mathrm{auxiliary}} |\Psi(\beta)\rangle \langle\Psi(\beta)|$$

- use imaginary time evolution to reach thermal states

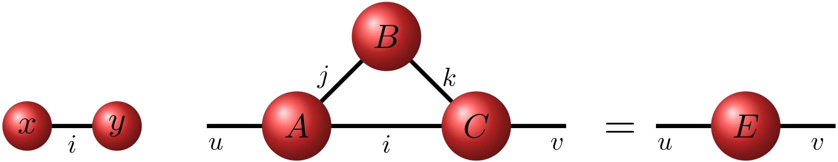
$$|\Psi(\beta)\rangle = e^{-\frac{1}{2}\beta\mathcal{H}}\,|\Psi(0)\rangle$$

index ⇔ leg



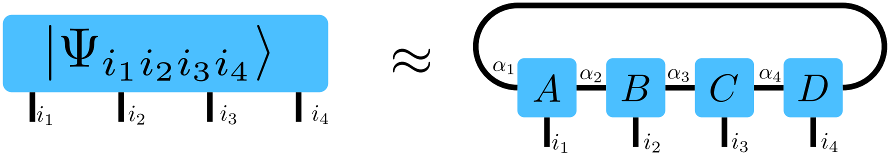
scalar x vector v_i matrix M_{ij} T_{ijk}

merge legs ⇔ sum over index



$$\sum_i x_i y_i \qquad \sum_{ijk} A_{uij} B_{ijk} C_{ikv} = E_{uv}$$

Tensor description of a wavefunction



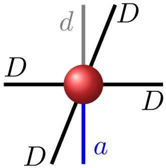
- virtual variables of dimension D
- coefficients obtained by summing over virtual variables:

$$c_{i_1 i_2 i_2 i_4} = \mathrm{Tr}\left[A^{i_1} B^{i_2} C^{i_3} D^{i_4}\right].$$

- $D = 1$: product state (mean-field)
- virtual variable carry entanglement
- efficient representation of low-entanglement states

Thermal tensor networks

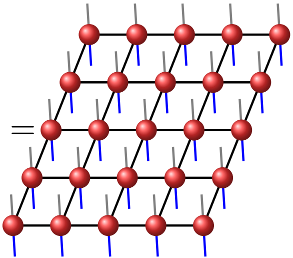
- thermal equilibrium: area law for entanglement
- weakly entangled $|\Psi\rangle$: tensor networks ✓
- each site described by local tensor w. ancilla
- virtual dimension D *controls* approximation



- 2D: Projected Entangled Pair States (PEPS)

$$\Psi_{123\ldots} = \sum_{\text{virtual}} A^{[1]}_{abcd} A^{[2]}_{defg} A^{[3]}_{behi} \cdots$$

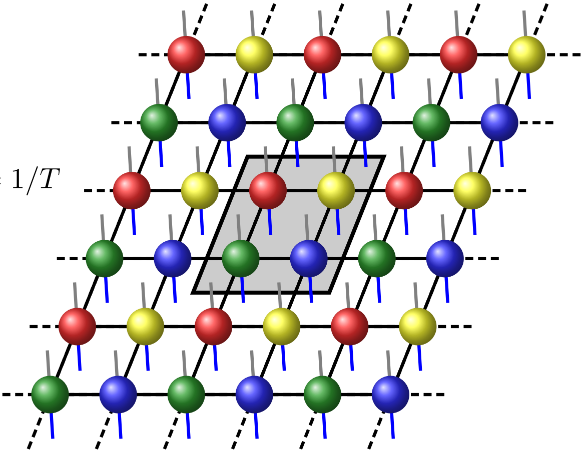
$|\Psi\rangle =$



[Verstraete et al., 2004]
[Verstraete & Cirac, 2004]

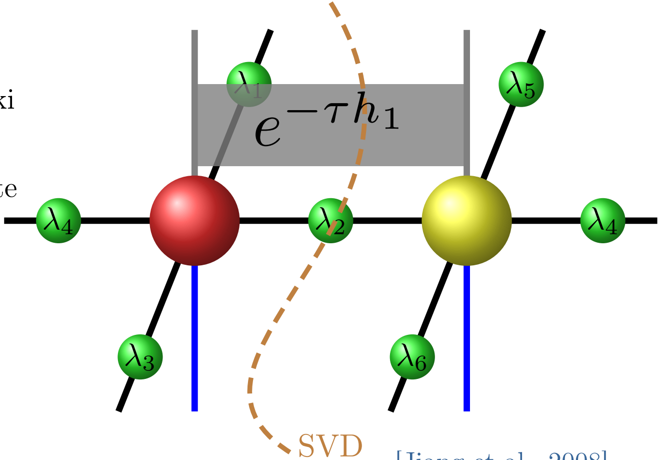
iPEPS algorithm

- define 2×2 plaquette
- start from exact product state at $\beta = 0$
- imaginary time evolve tensors up to $\beta = 1/T$
- contract tensor network
- compute observables



Simple update

- decompose $e^{-\beta\mathcal{H}}$ with Trotter-Suzuki
- apply gate $e^{-\tau h}$
- search for best tensor to approximate updated wavefunction $|\Psi'\rangle$
- diagonal weights λ_b as environment
- get new set of weights λ_b

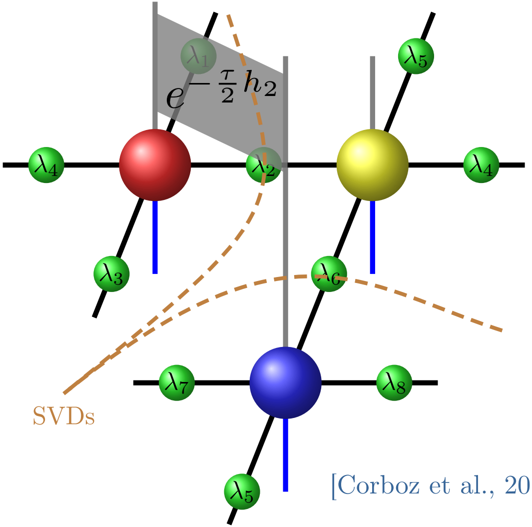


[Jiang et al., 2008]

Simple update: next nearest neighbor

- similar for J_2 with proxy site
- apply twice $e^{-\frac{\tau}{2}h_2}$ with different proxy

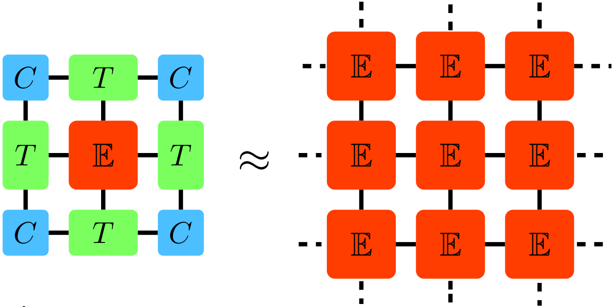
- cheap
- C_{4v} asymmetric
- not well controlled



[Corboz et al., 2010]

Corner Transfer Matrix Renormalization Group

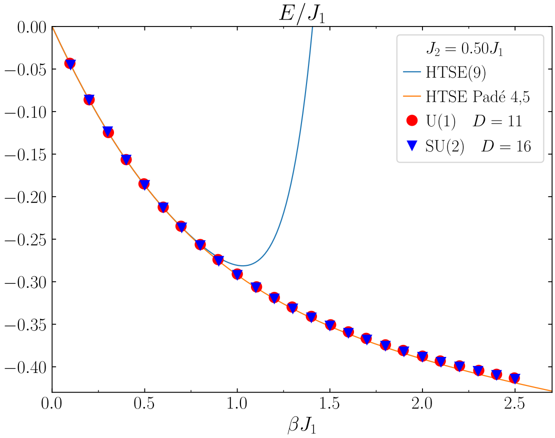
- define bilayer tensor
- construct environment tensors
- fully asymmetric CTMRG
- corner dimension χ controls approximation
- most expensive part $O(D^{12})$



[Nishino & Okunishi, 1996]
[Orús & Vidal, 2009]
[Corboz et al., 2011]

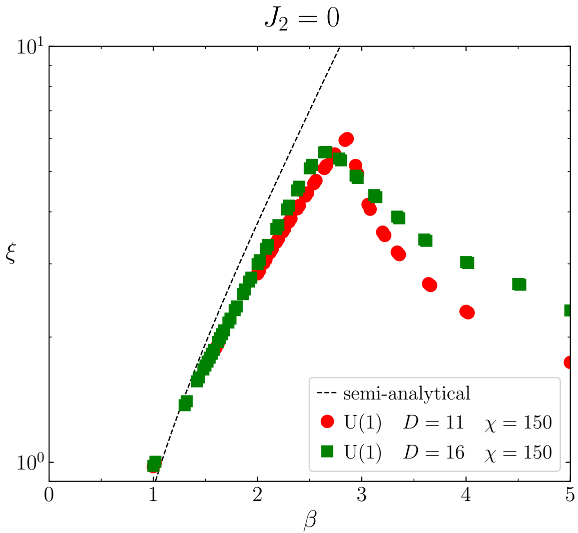
HTSE benchmark

- high temperature series expansion
- Padé approximant for lower temperature
- perfect agreement at high temperature



[Rosner et al., 2003]

Signs of trouble



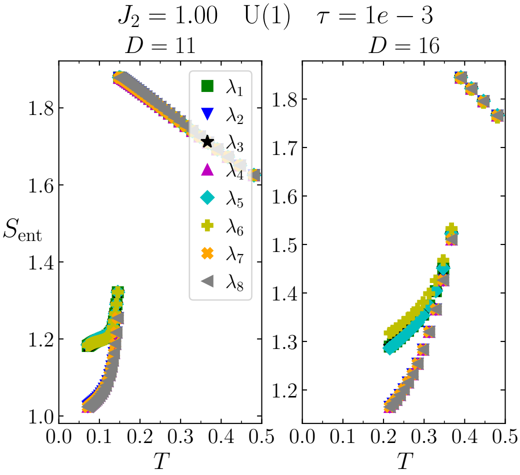
- correlation length for $J_2 = 0$
- should diverge at $T = 0$

Symmetry breaking artifact

- qualitative measure of entanglement

$$S^b_{\text{ent}} = -\sum_i \lambda^b_i \ln \lambda^b_i$$

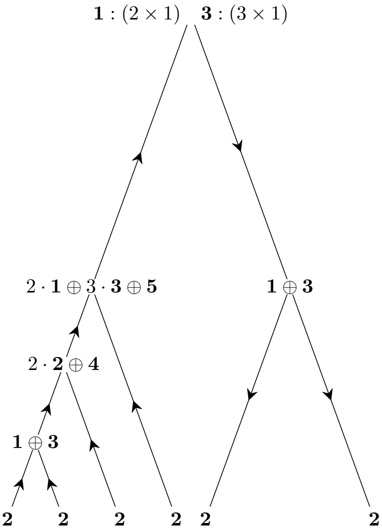
- also check multiplet structure
- finite temperature SU(2) breaking
- hides Ising transition



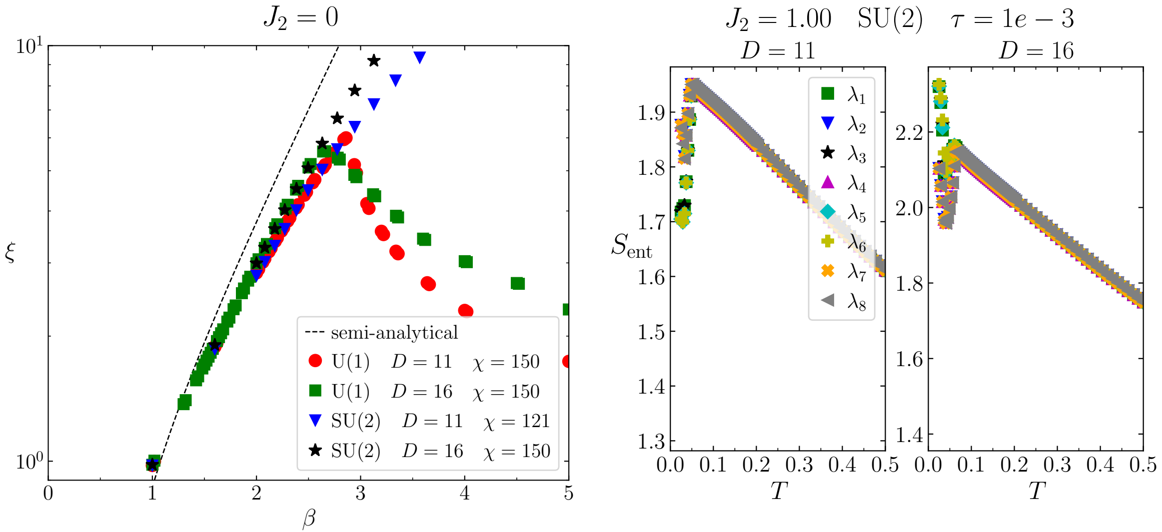
Symmetries

- SU(2) symmetry for simple update
  - prevents any SU(2) breaking
  - expensive unitary transformations
  - imposes $D \in \{11, 16, 19, 22\}$

- U(1) for CTMRG
  - reduced contraction and SVD complexity
  - reduced memory use
  - allows to reach large D

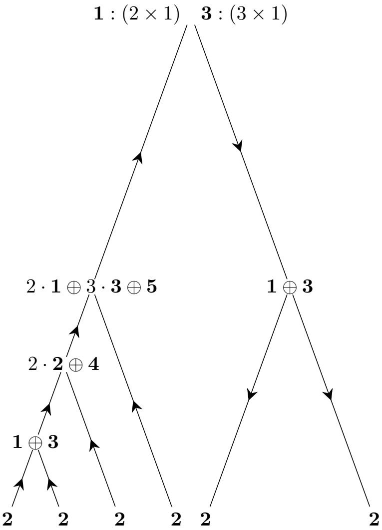


Problem solved?

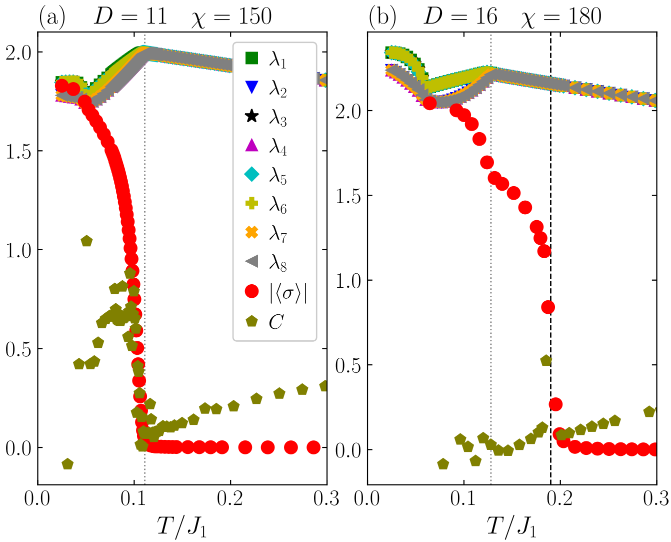


Symmetries

- SU(2) symmetry for simple update
  - prevents any SU(2) breaking
  - expensive unitary transformations
  - imposes $D \in \{11, 16, 19, 22\}$
- U(1) for CTMRG
  - reduced contraction and SVD complexity
  - reduced memory use
  - allows to reach large D
- C_{4v} lattice symmetry not enforced
  - still *explictly* broken in simple update
  - low enough temperature to get results



The real transition

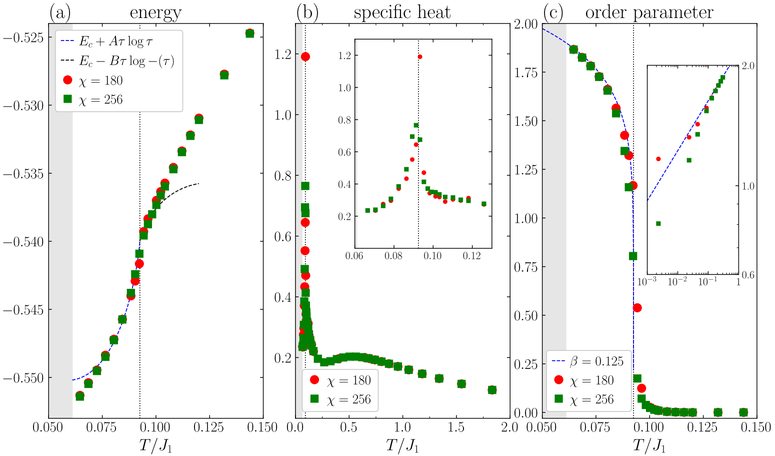


- requires $D \geq 16$
- $|\Psi\rangle$ stays C_{4v} symmetric
- symmetry breaking in the *observables* only

Energy, specific heat and order parameter

- $C = \partial E / \partial T$
  $\alpha = 0$
- $\sigma = \sum_{\langle i,j \rangle |} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_{\langle i,j \rangle -} \mathbf{S}_i \cdot \mathbf{S}_j$
  $\beta = 1/8$

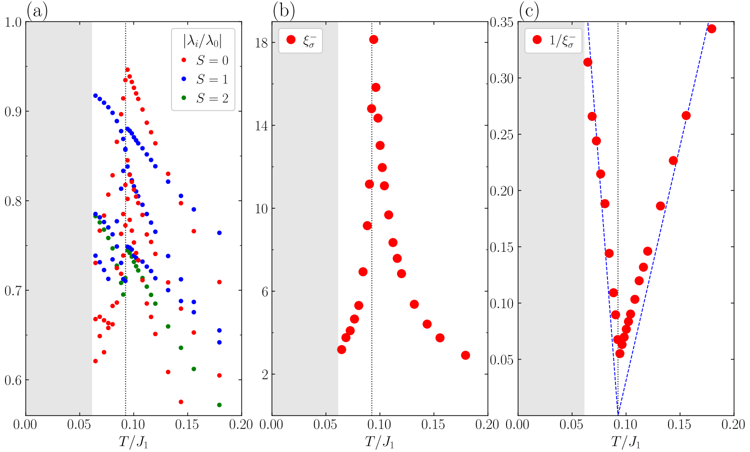
$J_2 = 0.85 \quad D = 16 \quad \chi = 256$



Correlation lengths

$J_2 = 0.85 \quad D = 16 \quad \chi = 256$

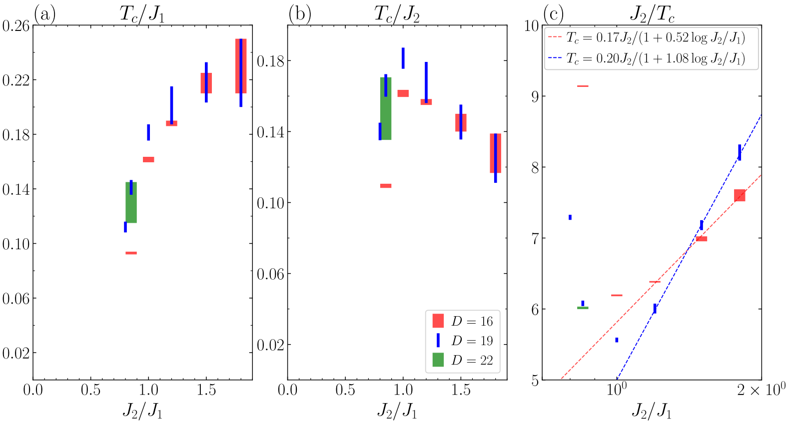
- compute transfer matrix spectrum
- define $\xi_i = -1/\ln(|\lambda_i/\lambda_0|)$
- multiplet decomposition
- leading singlet: $\nu = 1$



Phase diagram

- compatible with $T_c = 0$ for $J_{2c} \sim 0.61$
- finite slope: differs from classical
- T_c/J_2 decreases at large J_2

$J_2 = 0.85 \quad D = 16 \quad \chi = 256$



Conclusion

- finite temperature study of $J_1 - J_2$ model
- numerical evidence for finite temperature phase transition
- compatible with Ising 2D universality class
- confirm [Chandra et al., 1990] predictions
- limited by explicit symmetry breaking
- very large D are required
- SU(2) implementation is crucial

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