Tensor Network Methods in 2D at Finite Temperature

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Entanglement in Strongly Correlated Systems
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Menú del día

Primer plato

- Frustrated Spin Systems at Finite Temperature in 2D

Segundo plato

- Purification and Ancilla

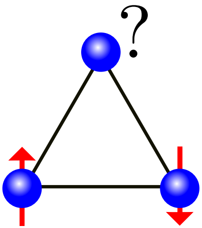
Postre

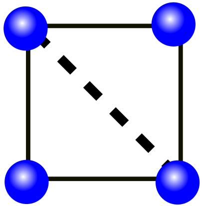
- METTS and XTRG

Contents

Frustrated magnetism

- magnetic insulators
- competing magnetic interactions
- no classical configuration fulfilling all local constraints

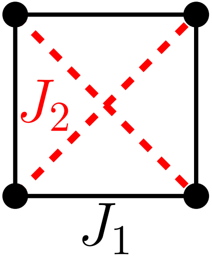




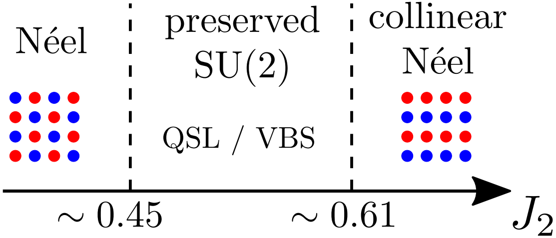
- exotic physics: quantum spin liquids, residual entropy, order by disorder…
- highly relevant experimentally
- numerically challenging (sign problem)

$J_1 - J_2$ Heisenberg model

- spin-1/2 on the square lattice
- $J_1 = 1$ first neighbor interaction
- $J_2 > 0$ second neighbor: magnetic frustration
- possible spin liquid realization
- describes iron-base superconductors magnetism



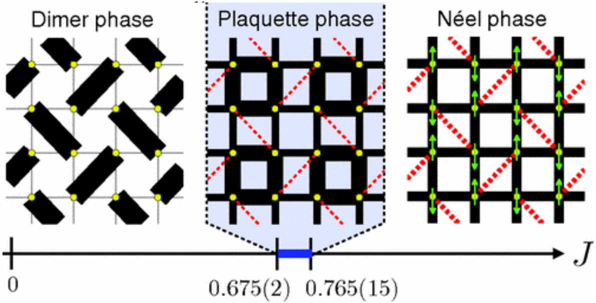
$$\mathcal{H} = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

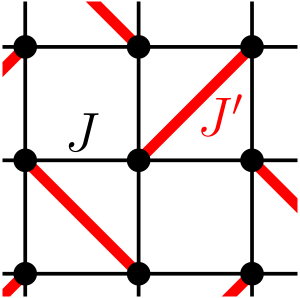


[Chandra & Douçot, 1988]
[Ferrari & Becca, 2020]
[Liu et al., 2022]
[Nomura & Imada, 2021]

- $J_D = 1$ dimer interaction
- J' square lattice interaction
- exact dimer product ground state for small J'
- experimental realization in $SrCu_2(BO_3)_2$

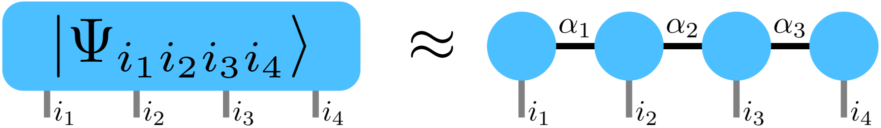
$$\mathcal{H} = J_D \sum \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum \mathbf{S}_i \cdot \mathbf{S}_j$$





[Shastry & Sutherland, 1981]
[Kageyama et al., 1999]
[Corboz & Mila, 2013]

Tensor description of a wavefunction

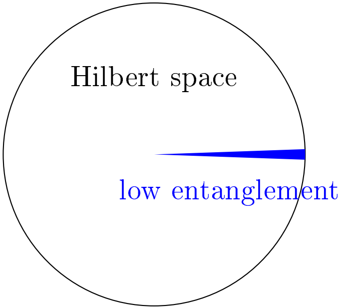


- virtual variables of dimension D
- coefficients obtained by summing over virtual variables:

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

- $D = 1$: product state (mean-field)
- virtual variables carry entanglement

Entanglement entropy and area law



Most of the Hilbert space is junk!

- reduced density matrix of subregion A:

$$\rho_A = \mathrm{Tr}_{\bar{A}} \left|\Psi\right\rangle \left\langle\Psi\right|$$

$$S_{\mathrm{ent}}(A) = -\,\mathrm{Tr}\,\rho_A \ln \rho_A$$

- random state obey volume law $S_{\mathrm{ent}}(A) \propto |A|$
- low energy states of local Hamiltonians obey **area law**:

$$S_{\mathrm{ent}}(A) \propto |\partial A|$$

- tensor networks: $S_{\mathrm{ent}}(A) \leq \ln D$

Tensor networks provide efficient representation of low-entanglement states!

The problem

Tensor networks provide very good ansatze for low-energy *states*.
How to construct finite temperature *density matrix*?

$$\rho(\beta) = \frac{1}{Z(\beta)} \exp(-\beta \mathcal{H})$$

3 main solutions:

- purification
- typical state sampling
- direct contraction of MPO/PEPO

sweet: can implement any continuous symmetry for 2D systems!

Contents

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

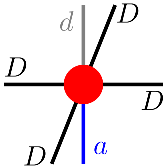
$$\rho(\beta) = \mathrm{Tr}_{\mathrm{auxiliary}} |\Psi(\beta)\rangle \langle\Psi(\beta)|$$

- use imaginary time evolution to reach thermal states

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

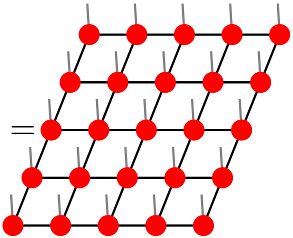
Thermal tensor networks with ancilla

- 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



- Matrix Product States (MPS) on the cylinder
- 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, García-Ripoll, & Cirac, 2004]
[Verstraete & Cirac, 2004]

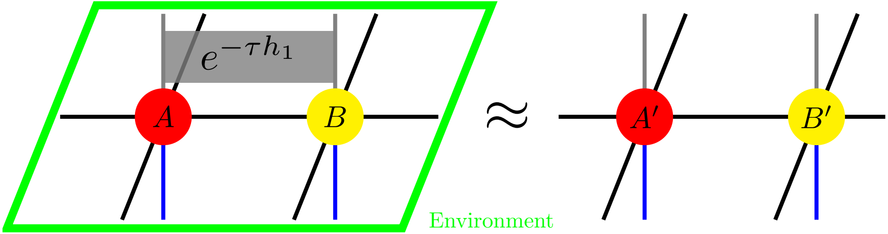
Purification: cooking recipe

1. choose tensor network geometry (MPS, PEPS)
2. finite or repeated unit cell
3. start from exact product state at $\beta = 0$
4. imaginary time evolve up to $\beta = 1/T$
   (TEBD, TDVP, SU, NTU, FU, eeFU, ...)
5. trace over auxiliary variables
6. contract the tensor network and compute observables
   (CTMRG, TRG, VUMPS, ...)
7. enjoy with lettuce and olive oil

Imaginary time evolution

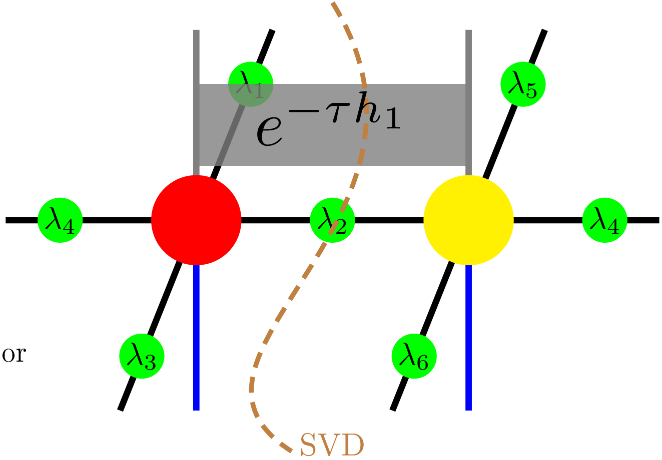
- Trotter-Suzuki decomposition: $\exp(-\beta\mathcal{H}) \approx \prod e^{-\tau h_i}$ with small τ
- start from $|\Psi(D)\rangle$
- apply gate on physical legs: obtain $\left|\Psi'(d^2 D)\right\rangle$
- renormalize tensors: find $|\Psi''(D)\rangle$ that maximizes fidelity with $|\Psi'\rangle$

- 2D: no optimal gauge! [Czarnik & Dziarmaga, 2018]
- need (approximated) metric tensor [Czarnik, Dziarmaga, & Corboz, 2019]



Simple update

- contract only involved tensors
- apply gate $e^{-\tau h}$
- diagonal weights λ_b as environment
- get new set of weights λ_b

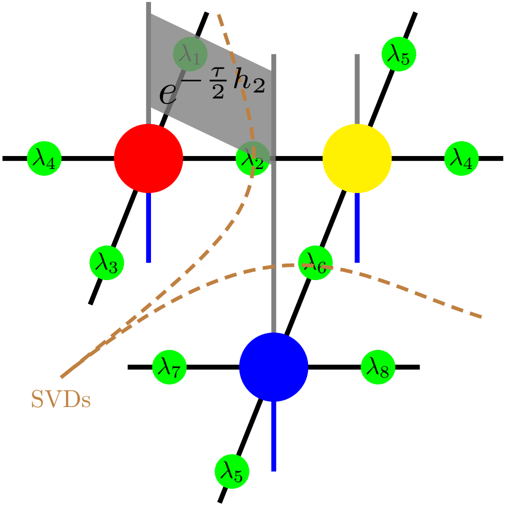


- cheap
- stable
- automatically selects symmetry sector
- not well controlled (short range)

[Jiang, Weng, & Xiang, 2008]

Simple update: next nearest neighbor

- similar for J_2 with intermediate site
- apply twice $e^{-\frac{\tau}{2}h_2}$ with different proxy
- C_{4v} asymmetric
- need to renormalize non-involved intermediate tensor

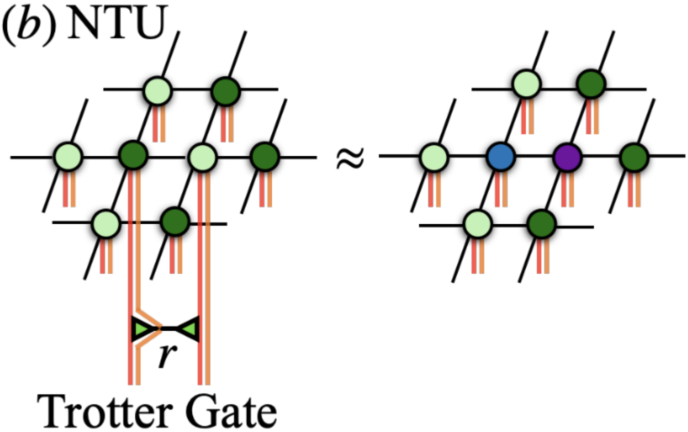


[Corboz, Jordan, & Vidal, 2010]

Neighborhood Tensor Update

- use single layer of tensor environment as metric tensor

- stable
- moderately expensive
- cost of second neighbor update?
- better than SU (still short range)

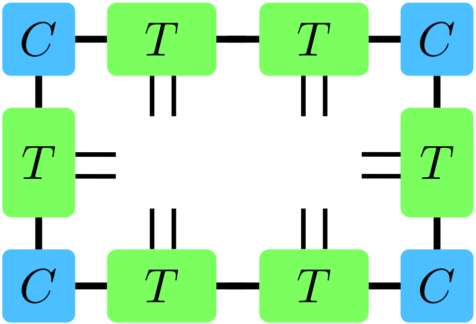


[Dziarmaga, 2021]
[Sinha et al., 2022]

Full Update

- use converged environment (CTMRG...)

- rigorous and controlled
- second neighbor with intermediate sites
- extremely expensive
- instable

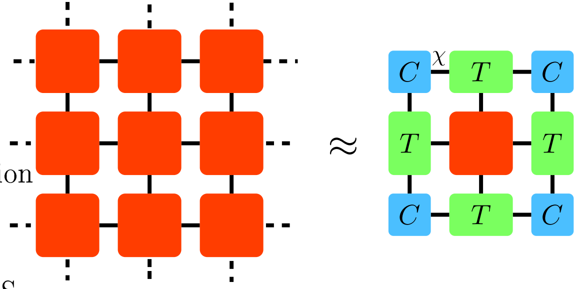


[Corboz et al., 2010]
[Phien et al., 2015]

Corner Transfer Matrix Renormalization Group

- 2D: contraction is hard
- define bilayer tensor
- construct environment tensors
- corner dimension χ *controls* approximation
- most expensive part: $O(D^{12})$

- other algorithms: TRG, iTEBD, VUMPS

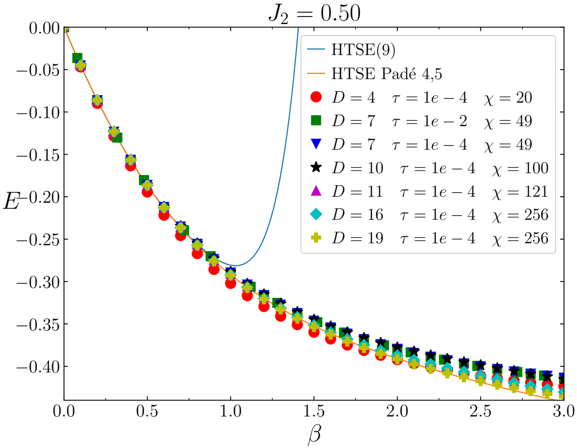


Work directly in the thermodynamic limit!

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

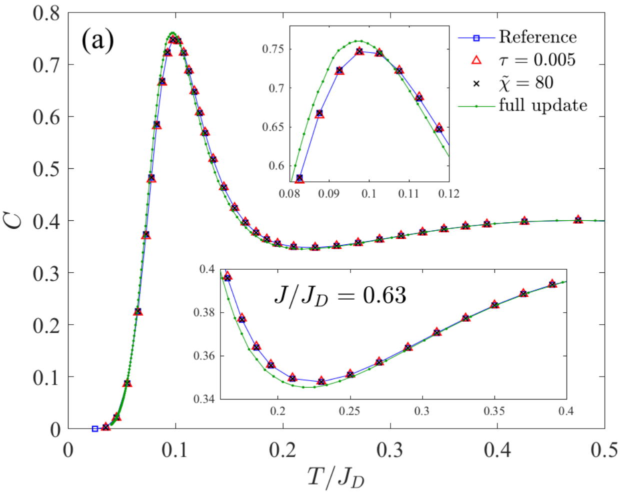
Benchmark: High Temperature Series Expansion

- $J_1 - J_2$ model with $J_2 = 0.50$
- Padé approximant for lower temperature
- perfect agreement at high temperature



[Rosner et al., 2003]

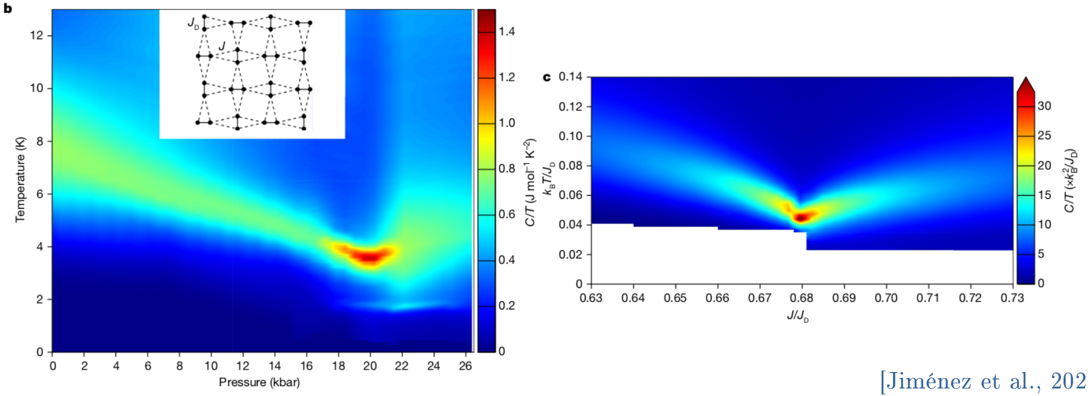
- Shastry Sutherland model
- dimer phase
- surprisingly good performances with SU



[Wietek et al., 2019]

Critical point in the Shastry-Sutherland

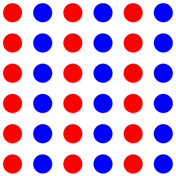
- First order transition between dimer an plaquette phases
- Finite temperature: first order line and critical point
- Experimentally observed in $SrCu_2(BO_3)_2$!

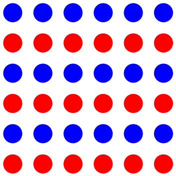


[Jiménez et al., 2021]

Finite temperature phase transition in the $J_1 - J_2$

- Mermin–Wagner: SU(2) symmetry cannot be broken at $T > 0$
- finite temperature Ising transition





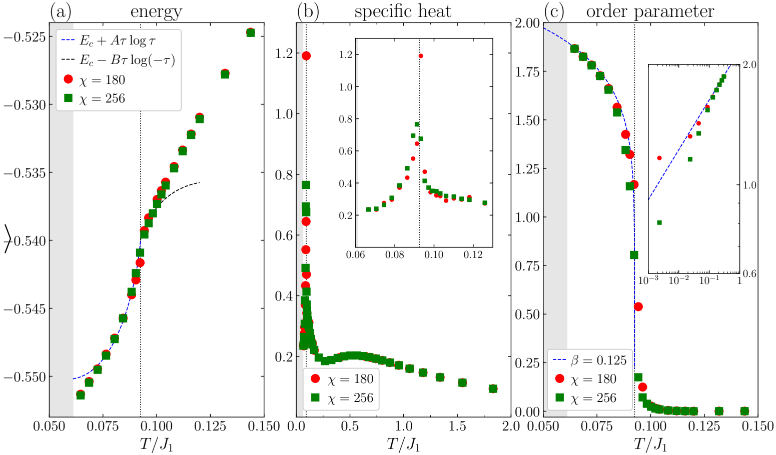
- stripe direction selected *before* Néel order appears
- spontaneous $\mathbb{Z}_2$ symmetry breaking
- Ising transition in Heisenberg magnet

[Chandra, Coleman, & Larkin, 1990]

Energy, specific heat and order parameter

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

$J_2 = 0.85 \quad D = 16$

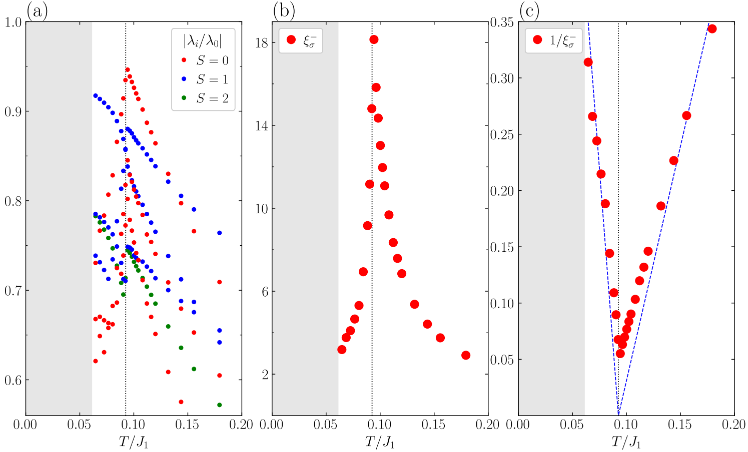


[Gauthé & Mila, 2022]

Correlation lengths

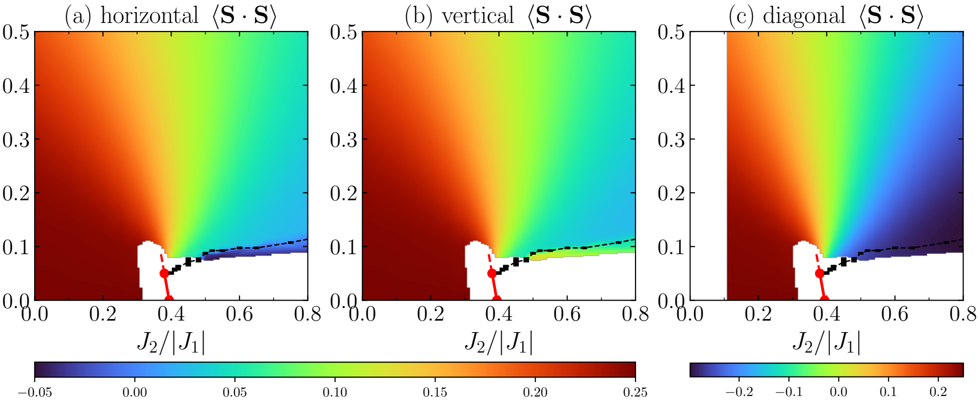
- compute transfer matrix spectrum
- define $\xi_i = -1/\ln(|\lambda_i/\lambda_0|)$
- multiplet decomposition
- leading singlet: $\nu = 1$

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



teaser: ferro$J_1 - J_2$

- $J_1 - J_2$ with ferromagnetic $J_1 < 0$
- difficulties to directly probe first order transition



See my poster!

Any drawback?

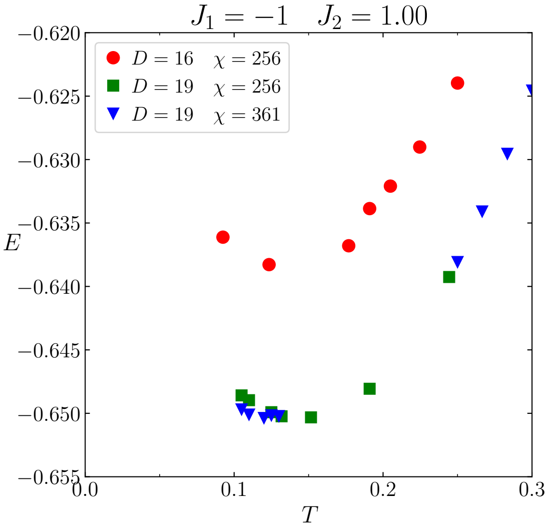
- iPEPS is very expensive
- converging the environment sometimes fails
- D extrapolation is complicate

Any drawback?

- iPEPS is very expensive
- converging the environment sometimes fails
- D extrapolation is complicate
- **results can be totally wrong**

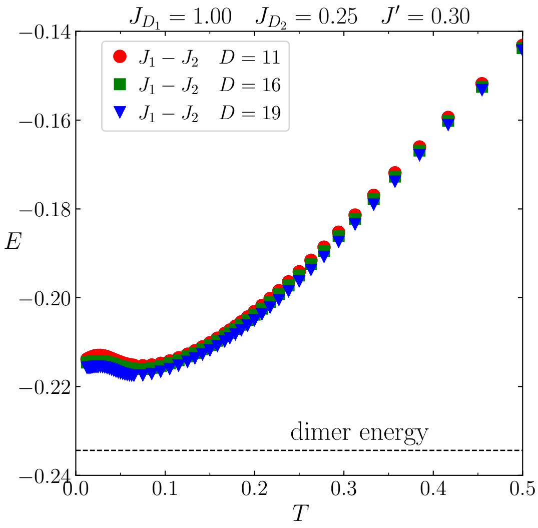
Problem: reaching low temperature

- energy rises at low T
- end of validity
- link with problem for Lorentzian PEPS?
- prevents any D scaling

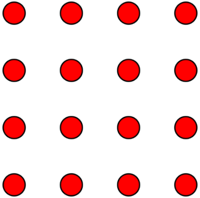
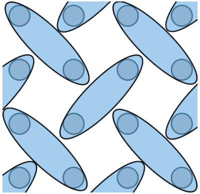
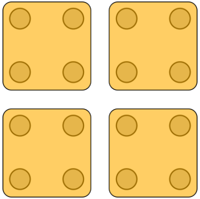


Problem: results validity

- asymmetric Shastry-Sutherland
- $J_{D_1} \neq J_{D_2}$
- D looks converged
- cannot find dimer ground state



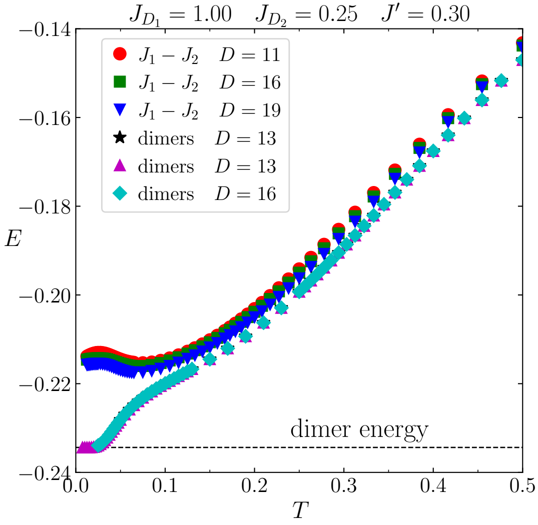
Different PEPS setups

$J_1 - J_2$ **setup**	**dimer setup**	**plaquette setup**
1 tensor = 1 site	1 tensor = 2 sites	1 tensor = 4 sites
$d = 2$	$d = 4$	$d = 16$
favors Néel	favors dimers	favors plaquettes
		

- $T = 0$: energy can be compared
- finite temperature: uncontrolled bias

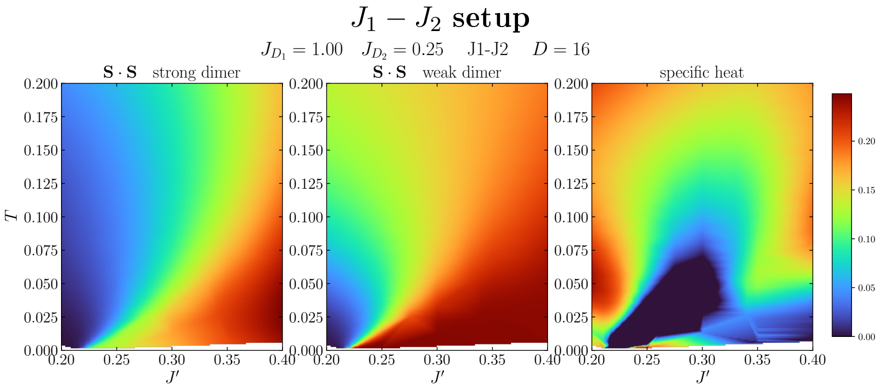
Setup effects

- $J_1 - J_2$ setup imposes Néel like correlations
- the *phase* was wrong
- dimer setup is correct
- $\xi < 2$ here!



Setup effects: $J_1 - J_2$ for Shastry-Sutherland

- asymmetric Shastry-Sutherland
- $J_{D_1} \neq J_{D_2}$
- specific heat is negative

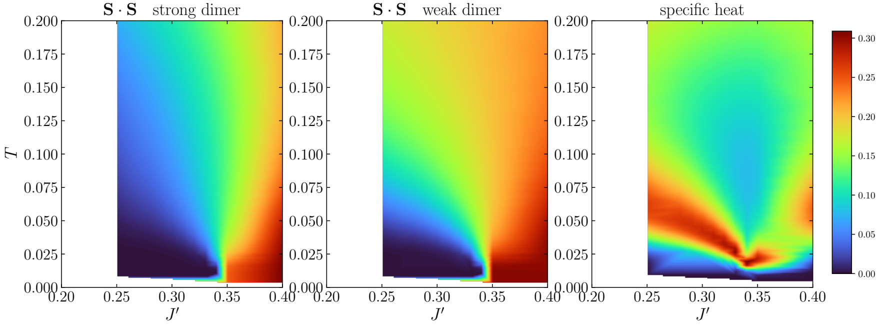


Setup effects: dimers for Shastry-Sutherland

- asymmetric Shastry-Sutherland
- $J_{D_1} \neq J_{D_2}$
- clean critical point

dimer setup

$J_{D_1} = 1.00 \quad J_{D_2} = 0.25 \quad$ orthodimers $\quad D = 16$



Conclusion on purification

- nearly exact at high temperature
- probes critical points and second order transition
- first order transition harder but possible

- hard to reach very low temperatures
- highly setup dependent: effect stronger than finite D
- requires knowledge of zero temperature phase
- problem when phase boundary matches setup validity

Contents

Typicality

- many-body Hilbert space is huge
- a random state is typical with probability 1 for large systems

$$Z(\beta) = \sum_i \langle i | e^{-\beta H} | i \rangle$$

- sample states instead of full computation (TPQ)
- how to deal with entanglement?

Minimally Entangled Typical Thermal States

- idea: use classical product state as sampling basis
- describe pure state as a MPS
- no purification needed: gain factor d for each tensor!
- able to reach very low temperature
- currently cylinder MPS method (see Aritra Sinha's talk for 2D)
- finite size systems

[Stoudenmire & White, 2010]
[Wietek et al., 2021]

METTS: cooking recipe

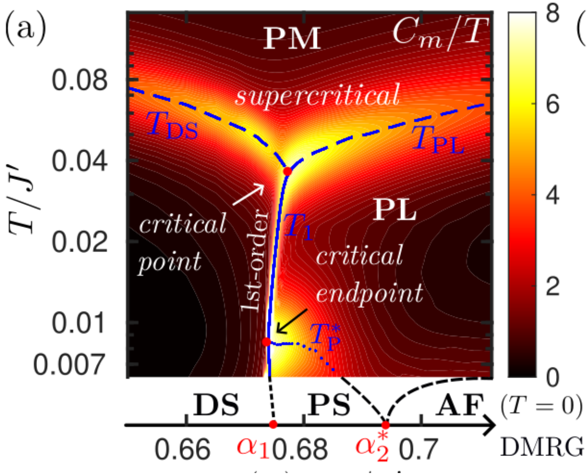
- start from random product state
- imaginary time evolve MPS up to β
  - compute observables
- project back to classical product state
  - collapse each site at a time with probability given by overlap
  - choose maximally mixed basis every other step
- iterate Markov process

XTRG

- construct an MPO for $e^{-\tau H}$ with series expansion
- square the MPO: double τ
- renormalize MPO bond dimension
- reach exponentially fast any β
- cylinder MPS
- 2D generalization not straightforward

[Chen et al., 2018]

- plaquettes appear at finite temperature
- lattice symmetry breaking
- extremely low temperature: $\beta > 100$
- $W = 6 \quad L = 4W$



[Wang et al., 2023]

Conclusion

- tensor networks are a powerful tool to simulate finite temperatures
- methodological developments still needed
- purification is best at high temperature
- only naturally 2D method
- setup may lead to incorrect phase
- METTS and XTRG in 2D?

Acknowledgements

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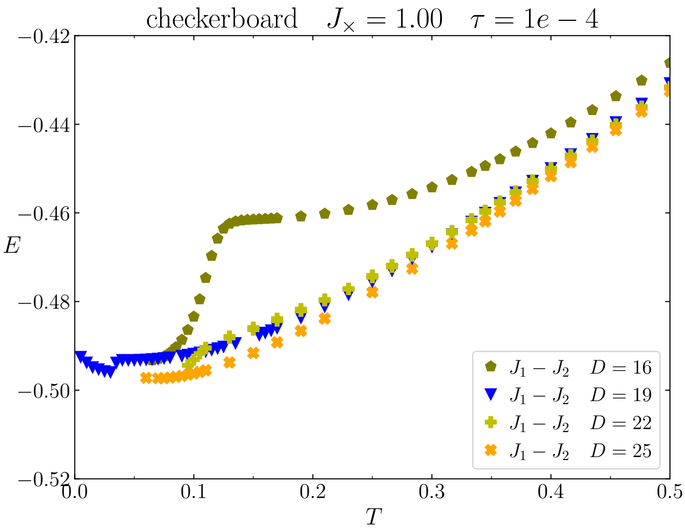
Alexander Wietek

Thank you for your attention!

Problem: results validity

- $J_1 - J_2$ model on the checkerboard lattice
- $D = 16$ is off
- $D \geq 19$ effects still strong



Setup effects

- $J_1 - J_2$ setup imposes Néel like correlations
- the *phase* was wrong
- $\xi < 2$ here!
- plaquette setup looks correct