Cluster Expansion of Thermal States using Tensor Networks

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Introduction

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- Overview condensed matter physics

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- Strongly correlated materials [1]
  - Superconductors
  - Quantum spin liquids
  - Strange metals
  - Quantum Criticality
  - Correlated topological matter

Introduction

- Overview condensed matter physics
- Strongly correlated materials
- How to proceed
  - Material synthesis and discovery
  - Numerical methods
  - Analytical methods

Simulating Quantum Many-body Systems

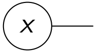
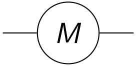
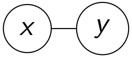
- Equations are known
- Curse of dimensionality
- Tensor networks

Tensor Networks: Introduction

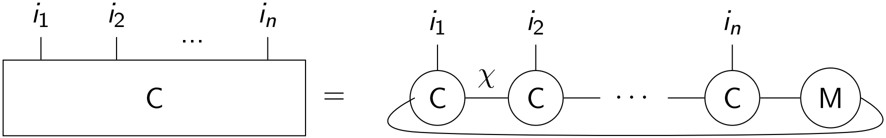
$$|\Psi\rangle = \sum_{i_1 i_2 \cdots i_n} C^{i_1 i_2 \cdots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle . \tag{1}$$

$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M). \tag{2}$$

Tensor Networks: Graphical Notation

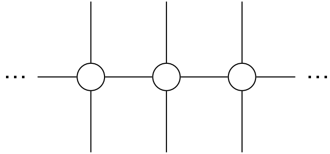
conventional	Einstein	tensor notation
$\vec{x}$	x_α	
M	$M_{\alpha\beta}$	
$\vec{x} \cdot \vec{y}$	$x_\alpha y_\alpha$	

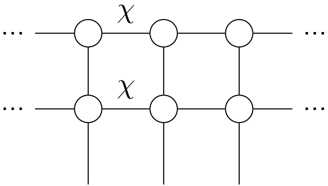
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M) \tag{3}$$

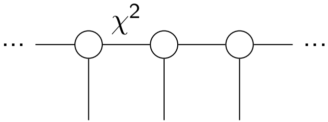


(4)

Tensor Networks: Operators

$\hat{O} =$  (5)

$\hat{O}\,|\Psi\rangle =$ 

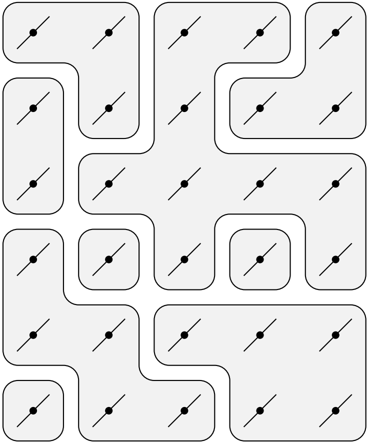
$=$ 

(6)

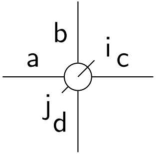
Operator exponential

- (Real) Time eveolution: $\hat{O} = e^{-i\hat{H}t}$
- Statistical ensembles: $\hat{O} = e^{-\beta\hat{H}}$

Cluster Expansion

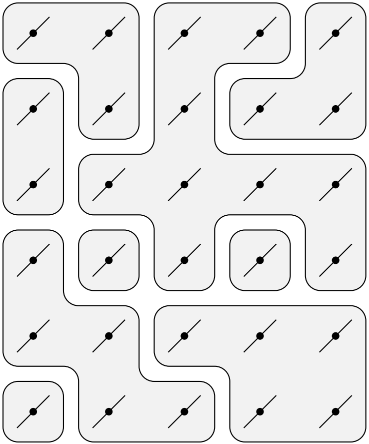


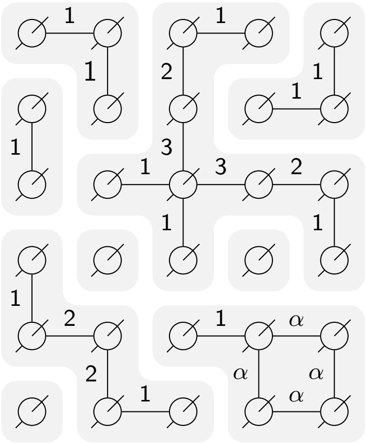
- $\sum_{\{B_i\}} \bigotimes_i B_i = e^{-\beta \hat{H}}$
- Increase size patches
- Thermodynamic limit
- Patches encoded by 1 tensor:



(7)

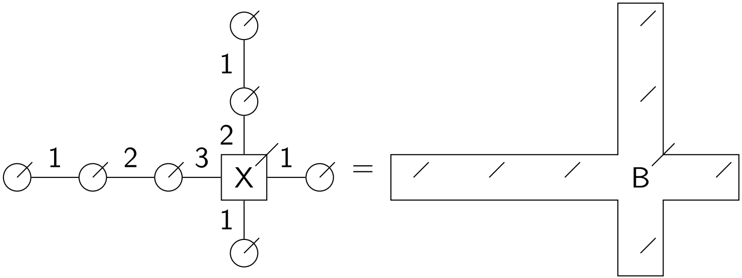
Cluser Exapansion





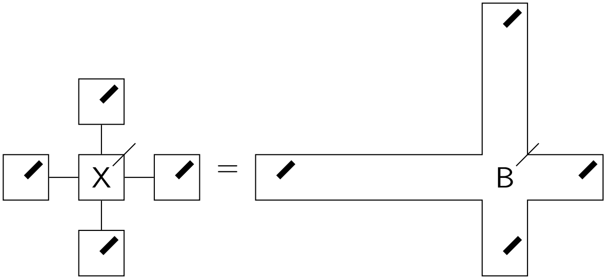
Solvers

Linear Solver: Standard Form



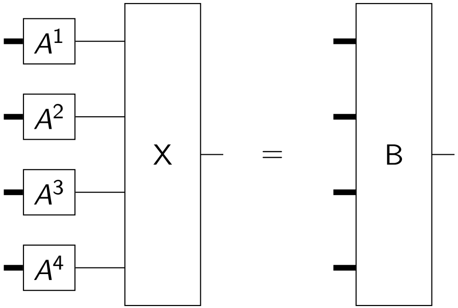
(7)

Linear Solver: Standard Form



(7)

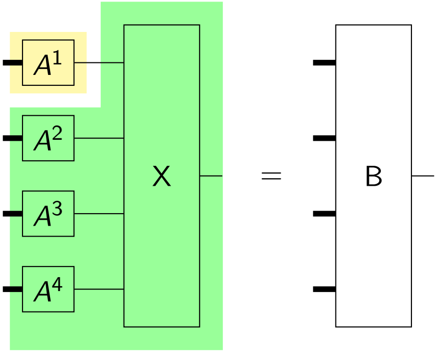
Linear Solver: Standard Form



(7)

Linear Solver: Inversion Scheme

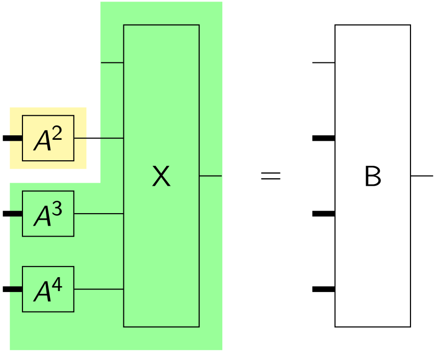
- Invert A^i separately
  - Fast
  - Numerically unstable



(8)

Linear Solver: Inversion Scheme

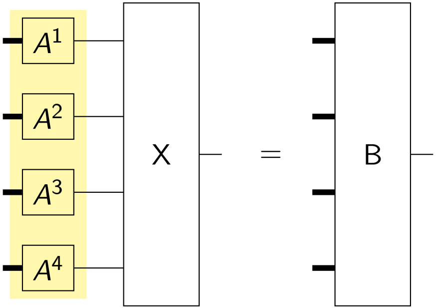
- Invert A^i separately
  - Fast
  - Numerically unstable



(8)

Linear Solver: Inversion Scheme

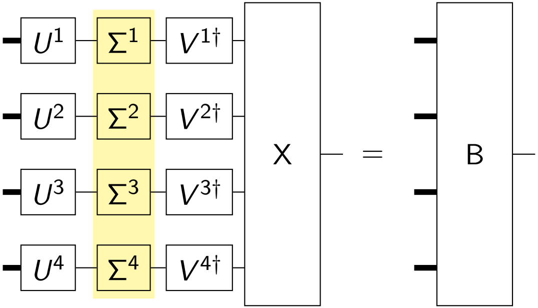
- Invert A^i separately
- Full inversion
  - Slow
  - Stable for pseudoinverse



(8)

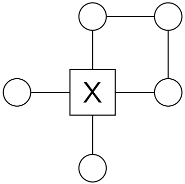
Linear Solver: Inversion Scheme

- Invert A^i separately
- Full inversion
- Sparse full inversion
  - $A^i = U^i \Sigma^i V^{i\dagger}$

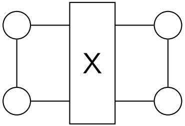


(8)

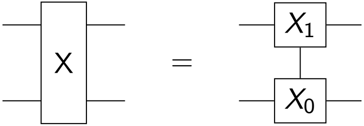
Linear Solver: Applicability



(9)



(10a)



(10b)

Nonlinear Solver

- Nonlinear least squares
- Jacobian
- Permutations

Sequential Linear Solver

- Based on linear solver
- Sweep over unknown tensors
- Permutations

Results

1D: Transverse Field Ising

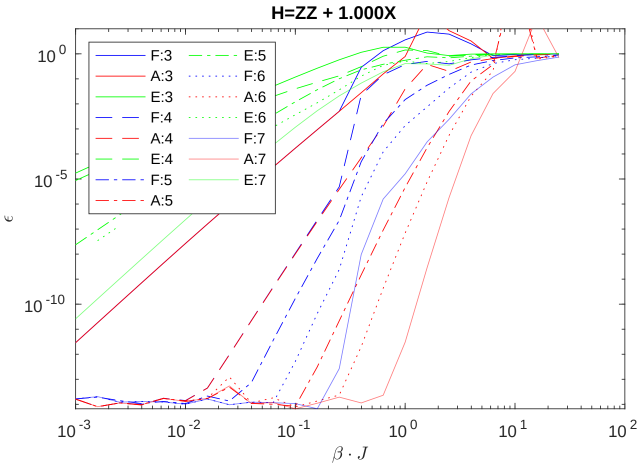
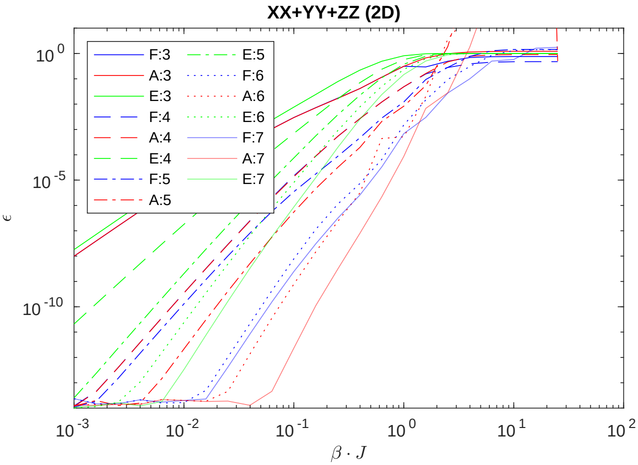


Table: χ

	A	E/F
3	5	10
5	21	42
7	85	170

1D: Heisenberg XXX



2D: TFI

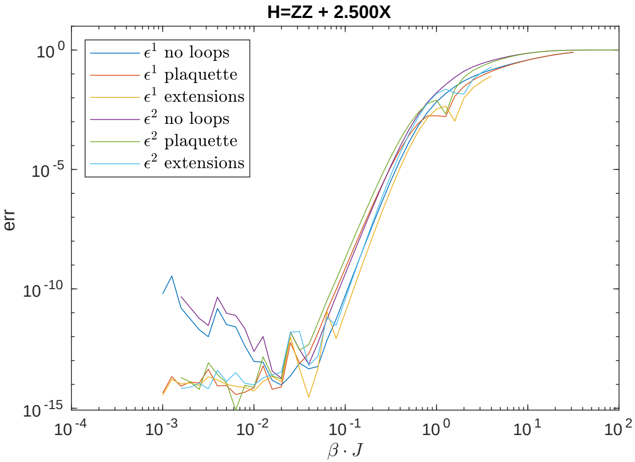


Table: χ

no loops	21
loops	27
extensions	43

2D: TFI

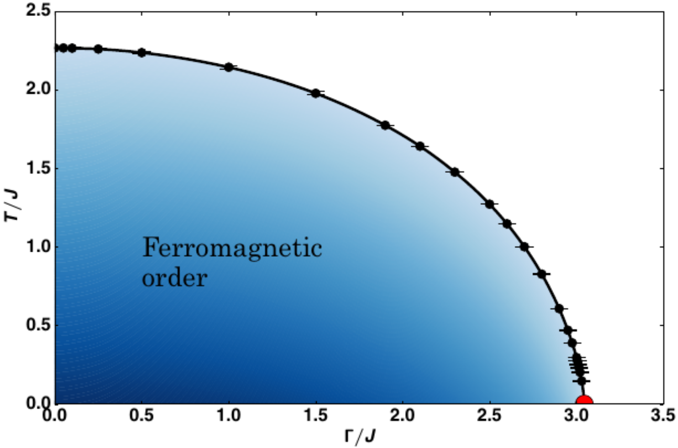
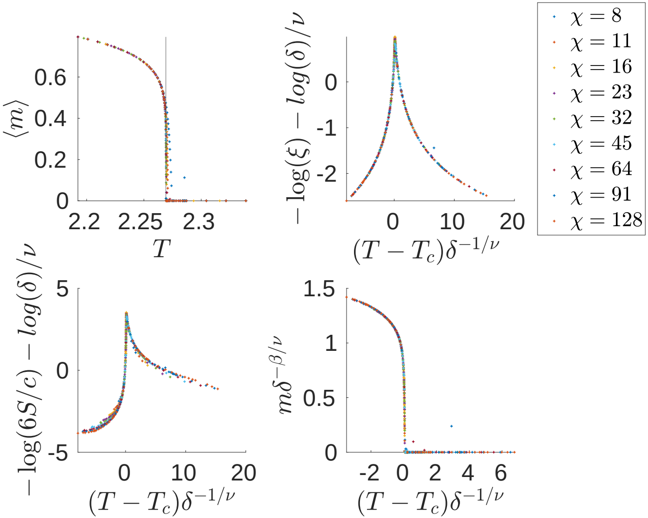


Figure: Figure taken from [2]

2D: Classical Ising



	T_c
Fit	2.691(9)
Exact	2.691853

2D: TFI $g = 2.5$

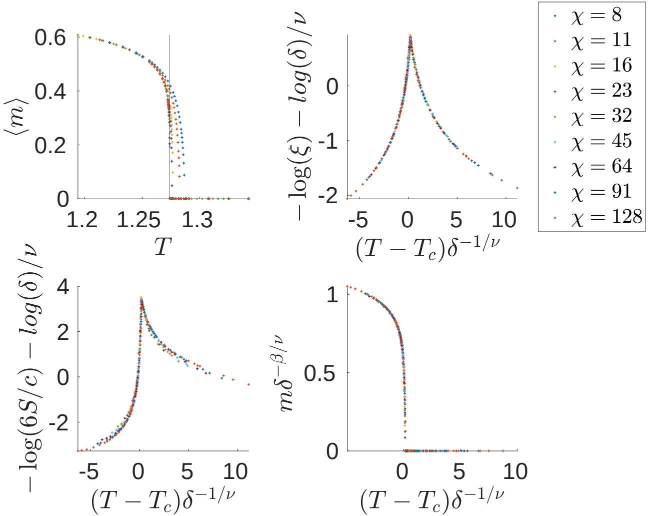


Table: Data from [3]

	T_c
Fit	1.2736(6)
QMC	1.2737(6)
TN	1.2737(2)

Conclusion

References I

A. Alexandradinata, N. P. Armitage, A. Baydin, W. Bi, Y. Cao, H. J. Changlani, E. Chertkov, E. H. d. S. Neto, L. Delacretaz, I. E. Baggari, G. M. Ferguson, W. J. Gannon, S. A. A. Ghorashi, B. H. Goodge, O. Goulko, G. Grissonnanche, A. Hallas, I. M. Hayes, Y. He, E. W. Huang, A. Kogar, D. Kumah, J. Y. Lee, A. Legros, F. Mahmood, Y. Maximenko, N. Pellatz, H. Polshyn, T. Sarkar, A. Scheie, K. L. Seyler, Z. Shi, B. Skinner, L. Steinke, K. Thirunavukkuarasu, T. V. Trevisan, M. Vogl, P. A. Volkov, Y. Wang, Y. Wang, D. Wei, K. Wei, S. Yang, X. Zhang, Y.-H. Zhang, L. Zhao, A. Zong, The Future of the Correlated Electron Problem (oct 2020).
arXiv:2010.00584.
URL http://arxiv.org/abs/2010.00584

References II

S. Hesselmann, S. Wessel, Thermal Ising transitions in the vicinity of two-dimensional quantum critical points, PHYSICAL REVIEW B 93 (2016) 155157.
doi:10.1103/PhysRevB.93.155157.

P. Czarnik, P. Corboz, Finite correlation length scaling with infinite projected entangled pair states at finite temperature, Physical Review B 99 (2019) 245107.
doi:10.1103/PhysRevB.99.245107.