Cluster Expansion of Thermal States using Tensor Networks

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Introduction

Introduction

- Overview condensed matter physics

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- Overview condensed matter physics
- 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

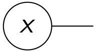
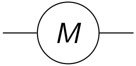
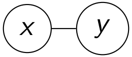
- Equations are known
- Curse of dimensionality
- Tensor networks

Tensor Networks: Introduction

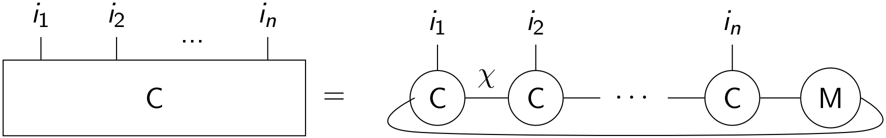
$$|\Psi\rangle = \sum_{i_1 i_2 \cdots i_n} C^{i_1 i_2 \cdots i_n} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \, . \tag{1}$$

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

Tensor Networks: Graphical Notation

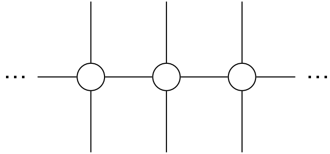
conventional	Einstein	tensor notation
$\vec{x}$	x_α	
M	$M_{\alpha\beta}$	
$\vec{x} \cdot \vec{y}$	$x_\alpha y_\alpha$	

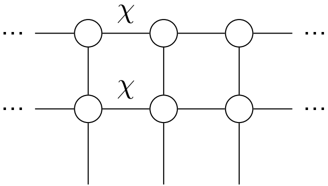
$$C^{i_1 i_2 \cdots i_n} = Tr(C^{i_1} C^{i_2} \cdots C^{i_n} M) \tag{3}$$

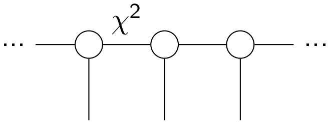


(4)

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

General idea

$$\bigcirc = \exp\left(-\beta H(\bigcirc)\right) \tag{7}$$

$$\begin{aligned} \bigcirc\!\overset{1}{\frac{}{}}\!\bigcirc &= \exp -\beta H(\bigcirc\!\frac{}{}\!\bigcirc) \\ &\quad - \bigcirc\!\overset{0}{\frac{}{}}\!\bigcirc \end{aligned} \tag{8}$$

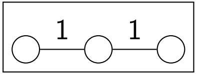
General idea

$$
\begin{aligned}
\bigcirc\overset{1}{\text{——}}\bigcirc\overset{1}{\text{——}}\bigcirc = \exp -\beta H(&\bigcirc\text{——}\bigcirc\text{——}\bigcirc) \\
-&\bigcirc\overset{0}{\text{——}}\bigcirc\overset{0}{\text{——}}\bigcirc \\
-&\bigcirc\overset{1}{\text{——}}\bigcirc\overset{0}{\text{——}}\bigcirc \\
-&\bigcirc\overset{0}{\text{——}}\bigcirc\overset{1}{\text{——}}\bigcirc
\end{aligned}
\tag{9}
$$

General idea

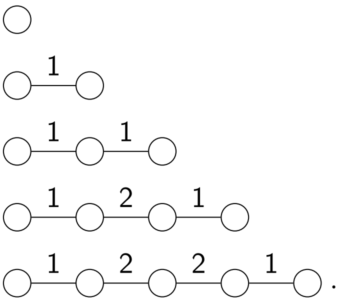
$$\bigcirc\overset{1}{\text{——}}\bigcirc\overset{1}{\text{——}}\bigcirc = \exp -\beta H(\bigcirc\text{——}\bigcirc\text{——}\bigcirc) - \bigcirc\text{——}\bigcirc\text{——}\bigcirc \tag{9}$$

General idea



(9)

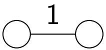
1D: Variant A



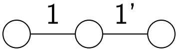
(10a)
(10b)
(10c)
(10d)
(10e)

1D: Variant E

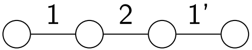

(11a)



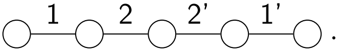
(11b)



(11c)



(11d)



(11e)

1D: Variant F

$$\bigcirc \tag{12a}$$

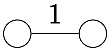
$$\bigcirc \overset{1'}{-\!\!-\!\!-} \bigcirc + \bigcirc \overset{1}{-\!\!-\!\!-} \bigcirc \tag{12b}$$

$$\bigcirc \overset{1}{-\!\!-\!\!-} \bigcirc \overset{1}{-\!\!-\!\!-} \bigcirc \tag{12c}$$

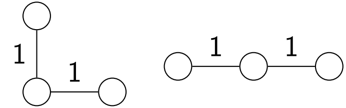
$$\begin{aligned} &\bigcirc \overset{1}{-\!\!-\!\!-} \bigcirc \overset{2}{-\!\!-\!\!-} \bigcirc \overset{1}{-\!\!-\!\!-} \bigcirc + \\ &\bigcirc \overset{1}{-\!\!-\!\!-} \bigcirc \overset{2'}{-\!\!-\!\!-} \bigcirc \overset{1}{-\!\!-\!\!-} \bigcirc \end{aligned} \tag{12d}$$

$$\bigcirc \overset{1}{-\!\!-\!\!-} \bigcirc \overset{2}{-\!\!-\!\!-} \bigcirc \overset{2}{-\!\!-\!\!-} \bigcirc \overset{1}{-\!\!-\!\!-} \bigcirc\,. \tag{12e}$$

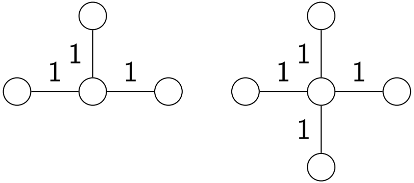
2D: Linear Blocks



(13a)

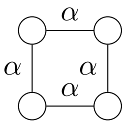


(13b)

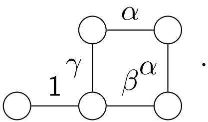


(13c)

2D: Nonlinear Blocks



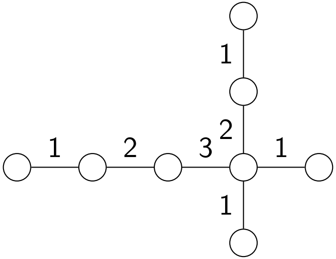
(14)



(15)

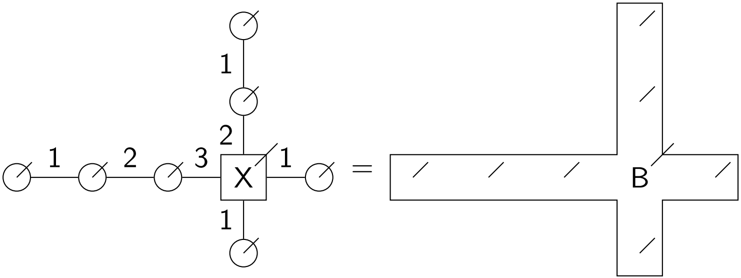
Solvers

Linear Solver: Standard Form



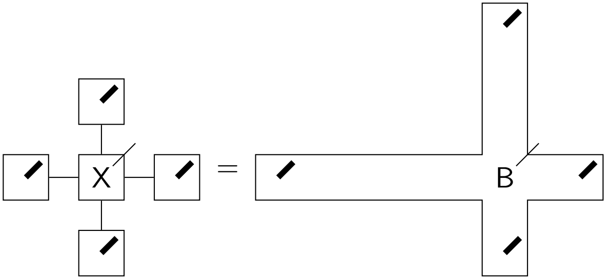
(16)

Linear Solver: Standard Form



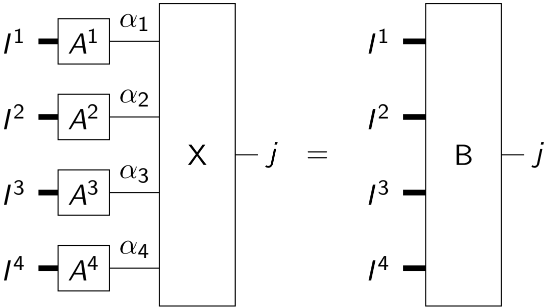
(16)

Linear Solver: Standard Form



(16)

Linear Solver: Standard Form



(16)

Linear Solver: Inversion Scheme

- Invert A^i separately
  - Fast
  - Numerically unstable

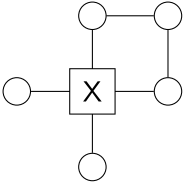
Linear Solver: Inversion Scheme

- Invert A^i separately
- Full inversion $A = A^1 \otimes A^2 \cdots \otimes A^m$
  - Slow
  - Stable for pseudoinverse

Linear Solver: Inversion Scheme

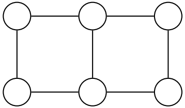
- Invert A^i separately
- Full inversion $A = A^1 \otimes A^2 \cdots \otimes A^m$
- Sparse full inversion
  - $A^i = U \Sigma V^\dagger$
  - $S = S^1 \otimes S^2 \cdots \otimes S^m$

Linear Solver: Applicability

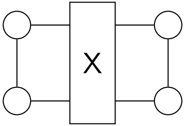


(17)

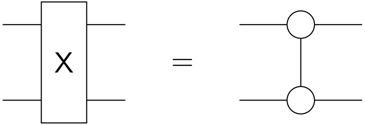
Linear Solver: Applicability



(18)



(19a)



(19b)

Nonlinear Solver

- Nonlinear least squares
- Jacobian
- Permutations

Sequential Linear Solver

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

Results

1D: Transverse Field Ising

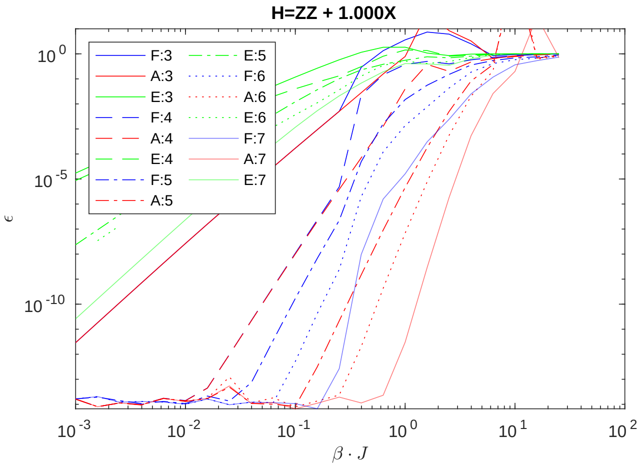
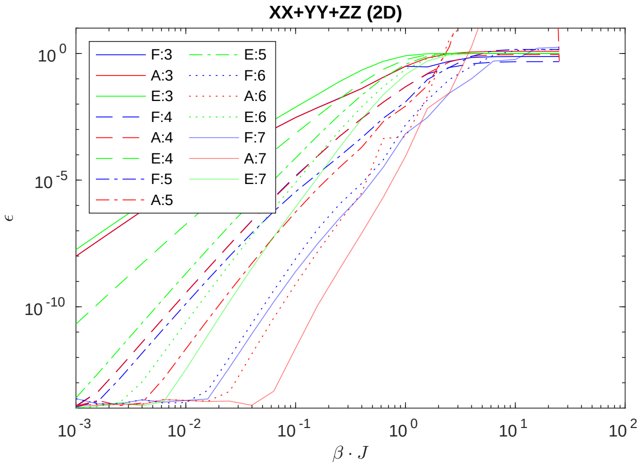


Table: χ

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

1D: Heisenberg XXX



2D: TFI

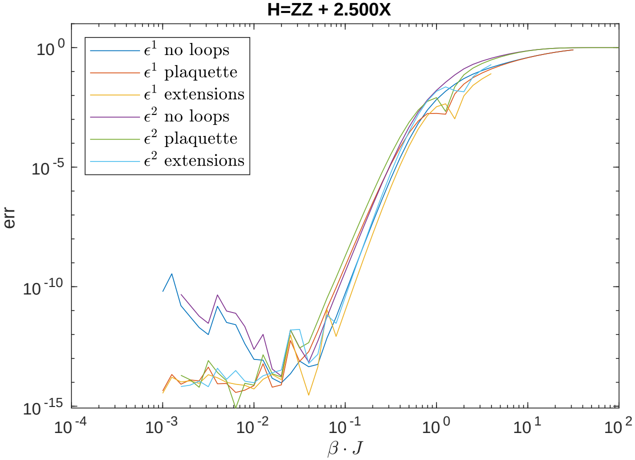


Table: χ

no loops	21
loops	27
extensions	43

2D: TFI

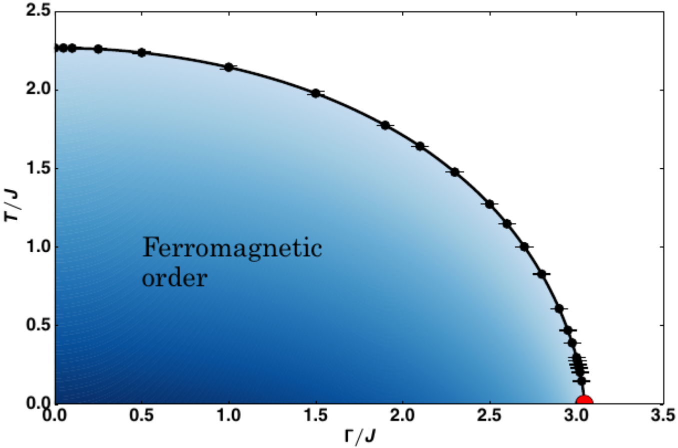
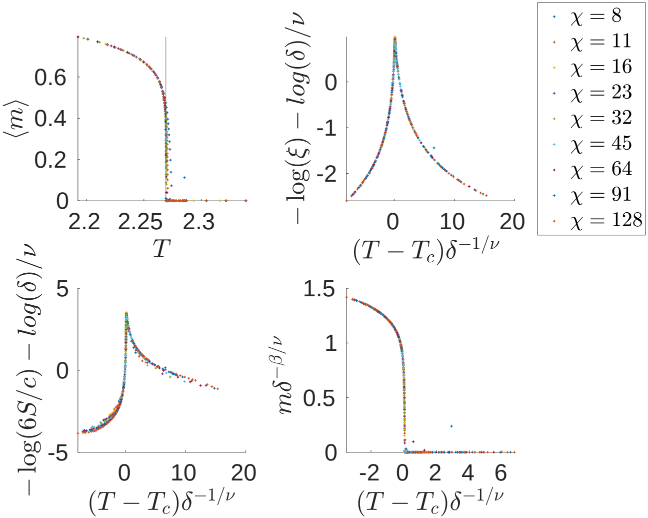


Figure: Figure taken from [2]

2D: Classical Ising



	T_c
Fit	2.691(9)
Exact	2.691853

2D: TFI $g = 2.5$

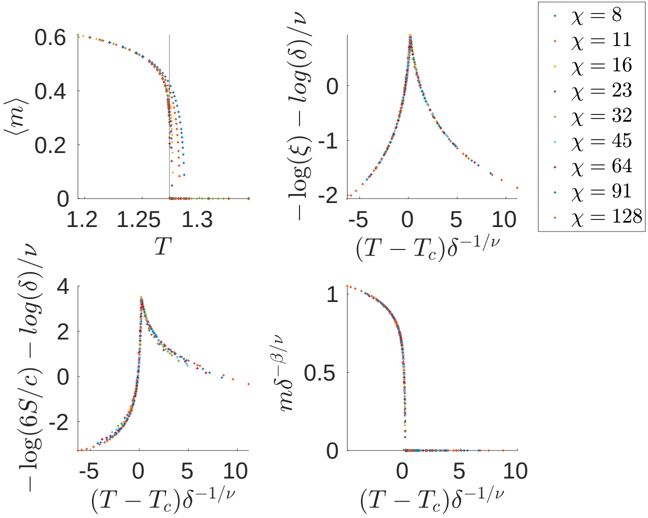


Table: Data from [3]

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

Conclusion

References I

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References II

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