Entanglement and tensor network states

Jens Eisert
Freie Universität Berlin

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Quantum lattice models

- **Quantum lattice models**: Models for strongly correlated quantum many-body systems

- Ubiquitous in **condensed-matter context** and for **cold atoms in optical lattices**
Many natural quantum lattice models have ground states that are little, in fact very little, entangled in a precise sense. This shows that `nature is lurking in some small corner of Hilbert space', one that can be essentially efficiently parametrized. This basic yet fundamental insight allows for a plethora of new methods for the numerical simulation of quantum lattice models using tensor network states, as well as a novel toolbox to analytically study such systems.

**This lecture:** Find out what that means

Is "double" with subsequent lecture by Uli Schollwoeck

On slides, will avoid all references (sincere apologies!): For script and references, see http://arxiv.org/abs/1308.3318
Correlations in quantum many-body systems
Quantum lattice models

- **Quantum lattice models**: Some lattice $G = (V,E)$, with quantum degree of freedom per vertex: Bosonic, fermionic, spin degree of freedom.
Quantum lattice models

- **Quantum lattice models**: Some lattice \( G = (V, E) \), with **quantum degree of freedom** per vertex: Bosonic, fermionic, spin degree of freedom

- **Distance in lattice**: \( \text{dist}(A, B) \)
Local Hamiltonians

- **Local Hamiltonian** \( H = \sum_{j \in V} h_j \), with each \( h_j \) supported only on finite neighboring sites, reflecting finite-ranged interactions.

\[ h_j \]
Local Hamiltonians

- **Example:** XY model

\[
H = -\frac{1}{2} \sum_{\langle j,k \rangle} \left( \frac{1 + \gamma}{4} X^{(j)} X^{(k)} + \frac{1 - \gamma}{4} Y^{(j)} Y^{(k)} \right) - \frac{\lambda}{2} \sum_{j \in V} Z^{(j)},
\]

- **Pauli operators** on site \( j \) called \( X^{(j)}, Y^{(j)}, Z^{(j)} \)

- **External field** \( \lambda \), **anisotropy parameter** \( \gamma \) : Easily exactly solvable in 1d
Ground states and spectral gaps

- **Ground space** $\mathcal{G}$ spanned by vectors minimising $\langle \psi | H | \psi \rangle$

- One-dimensional: Unique, otherwise degenerate

- **Spectral gap:** $\Delta E = \inf_{|\psi\rangle \in \mathcal{H} \setminus \mathcal{G}} \langle \psi | H | \psi \rangle - E_0$
Clustering of correlations in gapped models

- Gapped models have short-ranged correlations
- In fact, they decay, "cluster", exponentially fast

For $\Delta E > 0$

$$\left| \langle O_A O_B \rangle - \langle O_A \rangle \langle O_B \rangle \right| \leq C e^{-\text{dist}(A,B)\Delta E/(2v)} \|O_A\| \|O_B\|$$

where $C, v > 0$

- Here, $\xi := \frac{2v}{\Delta E} > 0$, is the correlation length
Entanglement entropies

- **Gapless** models have **algebraically decaying correlations** (conformal field theory)
- Locality of interactions inherited by something much stronger?
- Yes, by **entanglement** qualifiers!
Entanglement
Entanglement entropies

- Assume the entire system is in **pure state**
- Think of some region $A$ of sites, and consider **reduced state** $\rho_A = \text{tr}_B(\rho)$ where $B = V \setminus A$ is complement of region
- All local expectation values in $A$ can be computed using $\rho_A$ only
- In general, $\rho_A$ will be a **mixed state**, even if $\rho$ is pure!
**Entanglement entropies**

- **Entropy** of $\rho_A$, $S(\rho_A) = -\text{tr}(\rho_A \log \rho_A)$ will be non-vanishing, even if $S(\rho) = 0$

- Can be computed from eigenvalues of reduced state as $S(\rho_A) = -\sum_k \lambda_k \log \lambda_k$

- Reflects **entanglement** of $A$ with respect to complement: "Unique" measure of entanglement for pure states

- How does the (von-Neumann)-entropy **scale** with the size of $A$?

- Like its **volume**, as an **extensive quantity**?
Area laws for the entanglement entropy

- Nope: Entanglement entropies of gapped models generalically scale like the boundary area of the region
  \[ S(\rho_A) = O(|\partial A|) \]
- Entanglement is boundary effect: **Much (!) less** entanglement than there could be
Area laws for the entanglement entropy

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- Proven instances of area laws
  - 1d gapped models
  - Gapped **free bosonic and fermionic** models in **any dimension**
  - For graph states, projected entangled pair states, matrix-product states, see later
  - Any Hamiltonian that is in the **same gapped phase** as a free model

- Evidence that **gapped models satisfy area laws**
Critical models in 1d are known to violate area laws, but only logarithmically

\[ S(\rho_A) = \Theta(\log(|A|)) \]

Conformal field theory, conformal charge \( c \), suggests

\[ S(\rho_A) = \left(\frac{c}{3}\right) \log(l/a) + C \]

Critical higher-dimensional free models: scaling is different for bosons and fermions: Bosons satisfy an area law, while fermions violate it

\[ S(\rho_A) = \Theta(L^{D-1} \log L) \]
Lesson

- Possible entanglement

- Actual entanglement
Other measures of entanglement

- Replace for pure states von-Neumann entropy by **Renyi entropies**, $\alpha > 0$
  \[ S_\alpha(\rho_A) = \frac{1}{1 - \alpha} \log_2 \text{tr}(\rho_A^\alpha) \]

- For mixed states such as thermal states, use **mutual information** or **negativity**

- **Entanglement spectra** heavily studied (but not here :o)

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\( S_\alpha(\rho_A) = \frac{1}{1 - \alpha} \log_2 \text{tr}(\rho_A^\alpha) \)
Hilbert space is a fiction!

- Tiny subset occupied by natural states of local Hamiltonian models
- Not even a **quantum computer** could prepare a large set of states
- Hilbert space is a fiction: We only need to capture natural states: **Tensor network states**
- Hilbert space dimension of spin models: $\dim(\mathcal{H}) = O(d^n)$
Tensors and graphical notation
- **Tensor**: Multi-dimensional array of complex numbers
- Dimensionality of array *is order of tensor*
- Extensive use of **graphical notation**: Tensors are boxes, order: number of edges
Tensors and graphical notation

- This is how a **scalar** looks like

![Scalar](image)
Tensors and graphical notation

- Vectors and dual vectors
Matrices

Contraction of edge: Summation

E.g. matrix product $C_{\alpha, \beta} = \sum_{\gamma=1}^{N} A_{\alpha, \gamma} B_{\gamma, \beta}$
• Trace

• Partial trace

• Scalar product

• An uncontracted index is open index
- **Contraction of a tensor network**: Contraction of all edges not open
Matrix-product states
**Arbitrary state vector** $|\psi\rangle \in (\mathbb{C}^d)^\otimes n$

$$|\psi\rangle = \sum_{j_1,\ldots,j_n=1}^{d} c_{j_1,\ldots,j_n} |j_1, \ldots, j_n\rangle$$

graphically

"Physical edges"
Matrix-product states

- **Matrix-product state (MPS)** vector of "bond dimension" $D$

$$|\psi\rangle = \sum_{j_1, \ldots, j_n=1}^d c_{j_1, \ldots, j_n} |j_1, \ldots, j_n\rangle$$

graphically

where

$$c_{j_1, \ldots, j_n} = \sum_{\alpha, \beta, \ldots, \omega=1}^D A^{(1)}_{\alpha, \beta; j_1} A^{(2)}_{\beta, \gamma; i_2} \cdots A^{(n)}_{\omega, \alpha; j_n} = \text{tr}(A^{(1)}_{j_1} A^{(2)}_{j_2} \cdots A^{(n)}_{j_n})$$
Matrix-product states

- **Matrix-product state (MPS)** vector of "bond dimension" $D$

$$|\psi\rangle = \sum_{j_1, \ldots, j_n = 1}^{d} c_{j_1, \ldots, j_n} |j_1, \ldots, j_n\rangle$$

graphically

where

$$c_{j_1, \ldots, j_n} = \sum_{\alpha, \beta, \ldots, \omega = 1}^{D} A^{(1)}_{\alpha, \beta; j_1} A^{(2)}_{\beta, \gamma; i_2} \cdots A^{(n)}_{j_{n-1}, j_n}$$

- Each tensor
Bond dimensions

- What is $D$? A **refinement parameter**
  - How many parameters for arbitrary pure state?
    \[ O(d^n) \]
  - How many parameters for MPS?
    \[ O(ndD^2) \]

- Linear in $n$, not exponential!
- The larger $D$, the larger the set of states that can be represented
- Gutzwiller mean field $D = 1$, all states can be represented for exponentially large $D$
Area laws and approximations with area laws

- Ground states of local Hamiltonians
- MPS with bond dimension 2, 3, 4, ...
Area laws and approximations with area laws

- Easy to see: For each subset $A$ of consecutive sites,
  \[ S(\rho_A) = O(\log(D)) \]

- MPS satisfy area laws

- But the converse is also true!

- **1d states satisfying area laws can be well approximated by MPS**

**Fine print:** If for a family of state vectors $|\psi_n\rangle$ there exist constants $c, C' > 0$ such that for all $0 < \alpha < 1$ the Renyi entropies of the reduced state of any subsystem $A$ of the one-dimensional system satisfy

\[ S_\alpha(\rho_A) \leq c \log(n) + C' \]

then it can be efficiently approximated by an MPS (the bond dimension will have to grow polynomially with $n$, the system size, and $1/\epsilon$, where $\epsilon > 0$ is the approximation error)
Projected entangled pair state (PEPS) picture of MPS

- Start from **maximally entangled states in 'virtual space'**

\[ |\omega\rangle = \sum_{j=1}^{D} |j, j\rangle \]

\[ P^{(j)} = \sum_{k=1}^{d} \sum_{\alpha, \beta=1}^{D} A_{\alpha, \beta; k}^{(j)} |k\rangle \langle \alpha, \beta| \]

\[ |\psi\rangle = (P^{(1)} \otimes \ldots \otimes P^{(n)}) |\omega\rangle \otimes (n-1) \]

- Generates MPS

- **Two more ways of generating MPS**: Sequential generation and successive SVD
Translationally invariant MPS

- Take for periodic boundary conditions $A_{\alpha,\beta;k}^{(j)} = A_{\alpha,\beta;k}$

- Make a lot of sense in analytical considerations, specifically in thermodynamic limit
- Numerically, advisable to break symmetry, see Uli's lecture
Computation of expectation values
Computation of expectation values

- We want to compute $\langle \psi | O | \psi \rangle$ for local observables $O$

- **Reasons to get worried:** Fact that MPS is described by poly many parameters alone does not mean that we can efficiently compute it (permanents in \#P)

- **In fact:** In a naive way, we need exponentially many steps

- But we can do better!
Computation of expectation values

- Assume $O$ is only supported on sites $l$ and $l + 1$
- Graphically

\[
\begin{align*}
\bar{A}^{(1)} & \quad \bar{A}^{(2)} & \quad \bar{A}^{(l-1)} & \quad \bar{A}^{(l)} & \quad \bar{A}^{(l+1)} & \quad \bar{A}^{(n)} \\
A^{(1)} & \quad A^{(2)} & \quad A^{(l-1)} & \quad A^{(l)} & \quad A^{(l+1)} & \quad A^{(n)}
\end{align*}
\]

- Left boundary

\[
L_{\alpha,\beta} := \sum_{j=1}^{d} A_{\alpha;j}^{(1)} \bar{A}_{\beta;j}^{(1)}
\]
Computation of expectation values

- Assume $O$ is only supported on sites $l$ and $l + 1$

- Graphically

\[ \mathcal{A}^{(1)} \quad \mathcal{A}^{(2)} \quad \mathcal{A}^{(l-1)} \quad \mathcal{A}^{(l)} \quad \mathcal{A}^{(l+1)} \quad \mathcal{A}^{(n)} \]

\[ \mathcal{A}^{(1)} \quad \mathcal{A}^{(2)} \quad \mathcal{A}^{(l-1)} \quad \mathcal{A}^{(l)} \quad \mathcal{A}^{(l+1)} \quad \mathcal{A}^{(n)} \]

- Transfer operator

\[ (E_{\parallel}^{(k)})_{\alpha,\beta;\gamma,\delta} = \sum_{j=1}^{d} A^{(k)}_{\alpha,\beta;j} \mathcal{A}^{(k)}_{\gamma,\delta;j} \]
Computation of expectation values

- Assume $O$ is only supported on sites $l$ and $l+1$

- Graphically
Computation of expectation values

- Assume $O$ is only supported on sites $l$ and $l + 1$

- Graphically

$$R_{\alpha, \beta} = \sum_{j=1}^{d} A^{(n)}_{\alpha; j} \bar{A}^{(n)}_{\beta; j}$$
Computation of expectation values

- Assume \( O \) is only supported on sites \( l \) and \( l + 1 \)

- Graphically

- Can be efficiently computed!

- There are yet smarter ways, see Uli's lecture
Decay of correlations

- Stick for simplicity to infinite translationally invariant MPS
- Transfer operator $E_{\Pi} = \sum_{j=1}^{d} (A_j \otimes \bar{A}_j)$, graphically

$$E_{\Pi} = \sum_{j=1}^{d} (A_j \otimes \bar{A}_j)$$

and $E_{O_A} = \sum_{j,k=1}^{d} \langle k | O_A | j \rangle (A_j \otimes \bar{A}_k)$, graphically

$$E_{O_A} = \sum_{j,k=1}^{d} \langle k | O_A | j \rangle (A_j \otimes \bar{A}_k)$$

- Correlation function

$$\langle O_A O_B \rangle = \frac{\text{tr}(E_{O_A} E_{\Pi}^{\text{dist}(A,B)-1} E_{\Pi}^{n-\text{dist}(A,B)-1})}{\text{tr}(E_{\Pi}^{n})}$$
• Interested in $n \to \infty$

• Find $E^{k}_I = |r_1\rangle \langle l_1| + \sum_{j=2}^{D^2} \lambda_{j}^{k} |r_j\rangle \langle l_j|$, so $\langle OA OB \rangle = \langle l_1| E_{OA} E^{\text{dist}(A,B)-1}_I E_{OB} |r_1\rangle$

becomes

$$\langle OA OB \rangle = \langle l_1| E_{OA} |r_1\rangle \langle l_1| E_{OB} |l_1\rangle + \sum_{j=2}^{D^2} \lambda_{j}^{\text{dist}(A,B)-1} \langle l_1| E_{OA} |r_j\rangle \langle l_j| E_{OB} |l_1\rangle$$

$$= \langle OA \rangle \langle OB \rangle$$

• So $| \langle OA OB \rangle - \langle OA \rangle \langle OB \rangle |$ decays exponentially in the distance and correlation length is given by ratio of the second largest $\lambda_2$ to the largest $\lambda_1 = 1$ (taken to be unity) eigenvalue of $E_I$,

$$\xi^{-1} = - \log |\lambda_2|$$
- Powerful numerical techniques, matrix-product operators, time-evolution:

  See next lecture
Matrix-product states as ground states
Exact MPS ground states

- Are there any Hamiltonians models that have exact MPS ground states?
- Take physical dimension \( d = 3 \), a spin-1 model, and bond dimension \( D = 2 \)
- In the PEPS picture take \( P = \Pi_{S=1}(\mathbb{1} \otimes iY) \), where \( \Pi_{S=1} \) is projection onto the spin-1 subspace of two sites
- Surely gives rise to valid MPS \( |\psi\rangle \)

\[ S = 0 \]

Reduced state orthogonal to \( S=2 \)

Now \( h_j = \Pi_{S=2} \), then \( h_j |\psi\rangle = 0 \)
But all $h_j$ are positive, so $\langle \psi | H | \psi \rangle = \langle \psi | \sum_j h_j | \psi \rangle \geq 0$

That is, $|\psi\rangle$ must be a **ground state vector**!

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That is, $|\psi\rangle$ must be a ground state vector!

Famous AKLT-model (Affleck, Kennedy, Lieb, Tasaki)

$$h_j = \frac{1}{2} S^{(j)} \cdot S^{(j+1)} + \frac{1}{6} (S^{(j)} \cdot S^{(j+1)})^2 + \frac{1}{3}$$

Resembles Spin-1 Heisenberg model
Gauge freedom in MPS

- An MPS is uniquely defined by the matrices defining it, but the converse is not true

\[ A^{(k)}_{jk} A^{(k+1)}_{jk+1} = A^{(k)}_{jk} XX^{-1} A^{(k+1)}_{jk+1} \]

for every \( X \in \text{Gl}(D, \mathbb{C}) \)

- Hence, can pick a suitable **gauge** in which matrices take simple form

\[
\begin{align*}
\sum_j (A^{(k)}_{j})^\dagger \Lambda^{(k-1)} A^{(k)}_{j} &= \sum_j (A^{(k)}_{j})^\dagger \Lambda^{(k)} A^{(k)}_{j} = \Lambda^{(k)} \\
\text{and } \Lambda^{(0)} &= \Lambda^{(n)} = 1
\end{align*}
\]

where each \( \Lambda^{(k)} \in \mathbb{C}^{D \times D} \) for \( k = 1, \ldots, n - 1 \) is diagonal, positive, has full rank and unit trace
Applications in quantum information theory and quantum state tomography
• Matrix-product states can be used in metrology, say, the **GHZ-state**

\[ |\psi\rangle = \left( |0, \ldots, 0\rangle + |1, \ldots, 1\rangle \right)/\sqrt{2} \]

is MPS with \( D = 2 \) and \( A_1 = |0\rangle\langle 0| \) and \( A_2 = |1\rangle\langle 1| \)

• **Other MPS** are better suited under noise
MPS in measurement-based quantum computing

- Quantum computing based on measurements only
• One-dimensional cluster states

• Start from

$|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$
MPS in measurement-based quantum computing

- One-dimensional cluster states
- Start from

\[ |j, k\rangle \leftrightarrow |j, k\rangle (-1)^{\delta_{j,1}\delta_{k,1}} \]
MPS in measurement-based quantum computing

- One-dimensional cluster states

- Is MPS - and this picture explains how the principle works!
MPS in quantum state tomography

- Measure unknown quantum state of single spin
- Requires 3 measurement settings
MPS in quantum state tomography

- Measure unknown quantum state of 3 spins
- Requires 63 measurement settings
- Measure unknown quantum state of 8 spins
- Requires 65535 measurement settings
MPS in quantum state tomography

- Measure unknown quantum state of 20 spins
- Requires 1099511627775 measurement settings
- Use matrix-product states (or compressed sensing)
Higher-dimensional tensor network states
For a cubic lattice $V = L^D$ for $D = 2$

All tensors $A^{(k)}_{\alpha,\beta,\gamma,\delta; j}$ can be taken differently per site $k \in V, j = 1, \ldots, d$ and $\alpha, \beta, \gamma, \delta = 1, \ldots, D$
PEPS in higher dimensions

**PEPS construction**

\[ P^{(k)} = \sum_{\alpha, \beta, \gamma, \delta = 1}^{D} \sum_{j = 1}^{d} A^{(k)}_{\alpha, \beta, \gamma, \delta; j} |j\rangle \langle \alpha, \beta, \gamma, \delta | \]
Properties of PEPS

- PEPS satisfy an **area law**: The entanglement entropy is bounded from above by $O(L \log \mathcal{D})$ for $\mathcal{D} = 2$

- Again, if the bond dimension is large enough one can write every state as a PEPS

- Again, one can again have exponentially clustering correlations

- Interestingly, as a difference to MPS, one can construct PEPS that have algebraically decaying correlations in $\text{dist}(A, B)$
PEPS contraction

- Transfer operator

- Tricky: Can only *approximately* contract, not *exactly*!

- Exact contraction is in #P
Cluster states in measurement-based computing

Toric code Hamiltonian defined on edges (!) of a cubic lattice

\[ H = -J_a \sum_{s} A_s - J_b \sum_{p} B_p \]

where \( \{ A_s \} \) and \( \{ B_p \} \) are the star and plaquette operators, defined as

\[ A_s = \prod_{j \in s} X^{(j)} \]
\[ B_p = \prod_{j \in p} Z^{(j)} \]
More general tensor networks

- Checklist
  - the tensor network should be described by polynomially many parameters,
  - it should be efficiently contractible, either exactly or approximately, and
  - the corresponding class of quantum states should be able to grasp the natural entanglement or correlation structure
• Take $n = 2^T$, and think of "temporal" layers $t = 1, \ldots, T$
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Multi-scale entanglement renormalisation

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$U \in U(d^2_j)$
Multi-scale entanglement renormalisation

- Causal cone leads to efficient contraction
Multi-scale entanglement renormalisation

- This idea works in **any dimension**
- It also works for **fermions**
- Nice connection to **AdS-cft**
- Can be proven to be efficiently contractible PEPS
Lessons
Lessons

- Exciting field of research!
- Good for **numerical** and **analytical** studies
- For two dimensions, full potential is yet to be explored
- Again :)

Many natural quantum lattice models have ground states that are little, in fact very little, entangled in a precise sense. This shows that `nature is lurking in some small corner of Hilbert space`, one that can be essentially efficiently parametrized. This basic yet fundamental insight allows for a plethora of new methods for the numerical simulation of quantum lattice models using tensor network states, as well as a novel toolbox to analytically study such systems.
