Why study tensor networks? Because tensor networks provide a flexible description of quantum states.

They encode <u>entanglement</u> between subsystems in the <u>bonds</u> linking the tensors of the network.

Course outline:

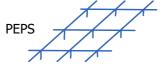
- Tensor network basics
- Matrix product states (MPS): 1d tensor networks

MPS

- Symmetries QSpace
- Density Matrix Renormalization Group (DMRG) for 1d quantum lattices models
- Numerical Renormalization Group (NRG) for quantum impurity models



- Projected Entangled Pair States (PEPS) for 2d quantum lattice models
- Various Tensor Renormalization Group (TRG) approaches



References: consult the bibtex file TensorNetworkLiterature.bib on course website → References

Lecture 01: Tensor networks basics I

- 1. Notation for generic quantum lattice system
- 2. Entanglement and Area Laws
- 3. Tensor network diagrams (graphical conventions)
- 4. Covariant index notation

1. Notation for generic quantum lattice system

TNB-I.1

For concreteness, we introduce some general notation for describing a generic quantum lattice system.

Think of spin- $\frac{1}{2}$ lattice in arbitrary dimensions, with $\frac{1}{2}$ sites, enumerated by an index $\frac{1}{2}$ = $\frac{1}{2}$, ..., $\frac{1}{2}$

16 = /

Local state space of site ℓ :

$$\left| \zeta_{k} \right| \in \left\{ \left| 1 \right\rangle_{k}, \left| 2 \right\rangle_{k}, \dots \left| 2 \right\rangle_{k} \right\} \tag{1}$$

Local state label:

$$6_{R} = 1, 2, ..., 25 + 1$$
 (2)

Local dimension:

$$d = ZS+1 \tag{3}$$

Shorthand:

$$|\sigma_{\ell}\rangle := |\sigma_{\ell}\rangle_{\ell}$$

Index ℓ on state label \P suffices to identify the site Hilbert space

Generic basis state for full system of N sites (convention: add state spaces for new sites from the left):

$$|\mathfrak{G}_{N}\rangle\otimes\ldots\otimes|\mathfrak{G}_{2}\rangle\otimes\ldots|\mathfrak{G}_{2}\rangle\otimes|\mathfrak{G}_{1}\rangle:=|\mathfrak{G}_{1},\mathfrak{G}_{2},\ldots,\mathfrak{G}_{N}\rangle:=|\mathfrak{F}_{N}\rangle\otimes\ldots\otimes|\mathfrak{G}_{2}\rangle\otimes(\mathfrak{G}_{1})$$

Hilbert space for full chain:

$$H^{N} = span \{ | \vec{6} \rangle_{N} \}$$
 (6)

General quantum state:

$$|\psi\rangle_{N} = \sum_{\mathbf{6_{1}}, \dots, \mathbf{6_{N}}} |\mathbf{6_{1}}, \dots, \mathbf{6_{N}}\rangle \subset \mathbf{6_{1}}, \dots, \mathbf{6_{N}} := |\mathbf{6_{1}}\rangle_{N} \subset \mathbf{6_{1}}$$
wavefunction
arbitrary linear combinations

wavefunction
arbitrary linear combinations

Dimension of full Hilbert space %.

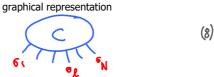
N: d

(# of different configurations of $\stackrel{\frown}{\circ}$)

Specifying $\mathcal{C}^{\overline{\sigma}}$, i.e. d^{N} different complex numbers.

 $C^{\frac{1}{6}} = C^{6_1, \dots, 6_N}$ is a tensor of rank

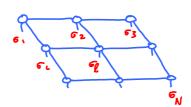
is a tensor of rank N



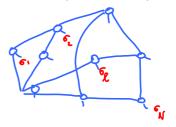
Claim (to be made plausible later): such a rank N tensor can be represented in many different ways:



MPS: matrix product state



PEPS: projected entangled-pair state



arbitrary tensor network

We will see:

- a link between two sites represents entanglement between them
- different representations ⇒ different entanglement book-keeping
- tensor network = entanglement representation of a quantum state

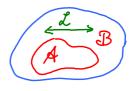
2. EntanglementeEntropy and area laws

TNB-I.2

Consider quantum system in Pure state ψ , with density matrix $\hat{\rho} = \psi \psi$

Divide system into two parts, $extcap{A}$ and $extcap{B}$. Suppose $extcap{A}$ has linear dimension $extcap{L}$.

E.g.
$$W_{3} = span \{ |\vec{\delta}_{3} \rangle \}$$
, $W_{3} = span \{ |\vec{\delta}_{3} \rangle \}$



To obtain reduced density matrix of A (or B), trace out B (or A):

'reduced density matrix' for
$$rac{4}{}$$
:

$$\hat{p}_{A} \equiv T_{T_{A}} \hat{p} \qquad \text{and} \qquad \hat{p}_{B} \equiv T_{T_{A}} \hat{p} \qquad (1)$$

'Entanglement entropy' of
$$A$$
 and B : $S_{A/B} = - T_{A} \hat{S}_{A} \log_2 \hat{S}_{A} = - \sum_{\alpha} w_{\alpha} \log_2 w_{\alpha}$ (2)

Remarkable fact: for Hamiltonians with only local interactions, the ground state entanglement entropy is governed by an 'area law':

$$S = S_{A/S} \sim \text{ (area of boundary of } A) = \partial A$$

$$\sim$$
 \mathcal{L}^2 in 3D for gapped system \sim \mathcal{L} in 2D for gapped system

$$\sim$$
 $\,$ $\,$ in 2D for gapped systen

(4a)

Area law has consequences for the numerical costs required for adequately encoding the entanglement in tensor network descriptions of the ground state. To see this, we review some basic properties of reduced density matrices.

Suppose the two subsystems, A and B, are defined on Hilbert spaces with

with dimensions \bigcirc and \bigcirc' , and orthonormal bases $\{ \mid \alpha \rangle \}$ and $\{ \mid \beta \rangle \}$.

Here α and β enumerate all basis states of Hilbert spaces of A and A, respectively.

General form of pure state on AU :

graphical notation

Density matrix:
$$\hat{\rho} = |\psi\rangle\langle\psi|$$

Reduced density matrix of subsystem 👃 :

$$\hat{\beta}_{A} = \text{Tr}_{g} | \psi \rangle \langle \psi | = \sum_{\vec{\beta}} \langle \vec{\beta} | \beta \rangle_{g} | \alpha \rangle_{g} \psi^{\alpha \beta} \psi^{\dagger}_{\beta \alpha' A} \langle \alpha' | \langle \beta \beta' | \vec{\beta} \rangle_{g}$$

$$= | \alpha \rangle_{A} \langle \rho_{A} \rangle^{\alpha}_{\alpha'} \langle \alpha' |$$

$$= | \alpha \rangle_{A} \langle \rho_{A} \rangle^{\alpha}_{\alpha'} \langle \alpha' |$$

$$= | \alpha \rangle_{g} \langle \rho_{A} \rangle^{\alpha}_{\alpha'} \langle \alpha' |$$

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$$= | \alpha \rangle_{g} \langle \rho_{A} \rangle^{\alpha}_{\alpha'} \langle \rho_{A} \rangle^{\alpha'}_{\alpha'} \langle \rho_{A} \rangle^{\alpha}_{\alpha'} \langle \rho_{A}$$

with

$$(\beta_{A})^{\alpha}_{\alpha'} = \sum_{\overline{B}} \{\overline{\beta} | \beta_{\overline{B}} \} \psi^{\alpha\beta} \psi^{\dagger}_{\beta'\alpha'} \{\overline{\beta}^{\prime} | \overline{\beta} \}_{\underline{B}} = \psi^{\alpha\beta} \psi^{\dagger}_{\beta\alpha'} = (\psi \psi^{\dagger})^{\alpha}_{\alpha'}$$
(6)

Analogously: reduced density matrix of subsystem $\mathcal S$:

$$\hat{\rho}_{\mathcal{B}} = \text{Tr}_{\mathcal{A}} \left(\psi \right) < \psi \right) = \left(\beta \right)_{\mathcal{B}} \left(\beta_{\mathcal{B}} \right)_{\beta_{1}}^{\beta_{2}} \leq \beta^{1} \quad \text{with} \quad \left(\beta_{\mathcal{B}} \right)_{\beta_{1}}^{\beta_{2}} = \left(\psi^{\dagger} \psi \right)_{\beta_{1}}^{\beta_{2}} \qquad (8)$$

Diagrammatic derivation:

Algebraic derivation:

$$(\beta_{\delta})^{\beta}_{\beta'} = \sum_{\alpha} \langle \alpha | \alpha \rangle_{\alpha} \psi^{\alpha\beta} \psi^{\beta}_{\beta'\alpha'} \langle \alpha' | \alpha \rangle_{\alpha} = \psi^{\dagger}_{\beta\alpha} \psi^{\alpha\beta} \equiv (\psi^{\dagger} \psi)_{\beta'}^{\beta}$$

$$(5)$$

Now it is always possible to find bases for the Hilbert spaces of $\rlap/$ and $\rlap/$ in which reduced density matrices are diagonal. (Tool to achieve this: 'singular value decomposition', see Sec. TNB-II.1.)

E.g. for
$$\hat{p}$$
: $(\psi \psi^{\dagger})^{\alpha}_{\alpha} = \delta^{\alpha}_{\alpha} \psi_{\alpha}$ eigenvalues with $\alpha = 1, ... D$

Normalization
$$I = Tr \hat{\rho}_{A} = \sum_{\alpha} v_{\alpha}$$
 (12)

Entanglement entropy:
$$S' = -\sum_{\alpha=1}^{D} w_{\alpha} \log w_{\alpha} \qquad (13a)$$

Maximal if
$$w_{\kappa} = \frac{1}{D}$$
 for all α : $\leq -\sum_{\kappa=1}^{D} \frac{1}{D} \log_2 \frac{1}{D} = \log_2 D$ (134)

Page 4

$$\Rightarrow \qquad z^{S} \leq D \qquad (14)$$

To fully capture entanglement between subsystems ${\color{red} {\cal A}}$ and ${\color{red} {\cal J}}$, the reduced density matrix dimension ${\color{red} {\cal D}}$ must satisfy

1D gapped: D
$$\sim$$
 Z (independent of system size!) (15 α)

1D critical: \sim 2 const + ln L \sim power law in L \sim (15 Δ)

2D gapped:
$$\frac{(3)}{2}$$
 $\frac{2}{2}$ (15c)

3D gapped:
$$\sim 2^{2}$$
 (15d)

Important conclusion: for gapped and gapless systems in 1D, ground state entanglement can be encoded efficiently using limited numerical resources. For 2D or 3D systems, numerical costs grow exponentially.

the entanglement between subsystems $atural \mathbf{A}$ is encoded in the two-index tensor

Quite generally, entanglement between subsystems can be encoded via tensors. For several connected subsystems (e.g. lattice sites), this leads to a description in terms of tensor networks.

Next:

- Tensor network diagrams (graphical conventions)
- Singular value decomposition (needed for finding efficient representations of entanglement)
- Schmidt decomposition (most efficient way of representing entanglement)

3. Tensor network diagrams

[Orus 2014, Sec. 4.1]

TNB-I.3

'tensor' = multi-dimensional array of numbers

'rank of tensor' = number of indices = # of legs

'dimension of leg' = number of values taken by its index,

rank-0: scalar rank-1: vector rank-2: matrix

rank-3: tensor

 $\mathcal{L} = 1, \dots, \mathcal{D}_{\alpha}$ A := A = Atu = = AFa Atpas := Asas a 15 B

[Our conventions for using arrows and distinguishing between super- and subscripts ('covariant notation') will be explained in Sec. TNB-II.1. In short: incoming = upstairs, outgoing = downstairs. Use of covariant notation is not customary in tensor network litertarure - most authors write all indices downstairs, and you may do so too. However, covariant notation does become useful when exploiting non-Abelian symmetries.]

Index contraction: summation over repeated index

$$C^{\alpha}_{\gamma} = \sum_{\beta=1}^{D_{\beta}} A^{\alpha}_{\beta} \beta^{\beta}_{\gamma} \equiv A^{\alpha}_{\beta} \beta^{\beta}_{\gamma} \qquad \frac{C}{\alpha \gamma} = \frac{A}{\alpha} \frac{B}{\beta} \frac{B}{\gamma}$$

graphical representation of matrix product

 D_{β} = 'bond dimension' of index β

(depends on context, can be different for each index; is often/usually not written explicitly)

'open index' = non-contracted index (here ♥ , **Y**)

'tensor network' = set of tensors with some or all indices contracted according to some pattern

Examples:

$$C = A_{\kappa} B^{\kappa}$$

vector · dual vector scalar

Trace of matrix product:

$$\begin{array}{ccc}
C & = & \stackrel{A}{\longrightarrow} & \stackrel{B}{\longrightarrow} & \stackrel{B}{\longrightarrow} & \stackrel{A}{\longrightarrow} & \stackrel{A}{\longrightarrow} & \stackrel{A}{\longrightarrow} & \stackrel{C}{\longrightarrow} & \stackrel{A}{\longrightarrow} & \stackrel{C}{\longrightarrow} & \stackrel{C}{\longrightarrow}$$

$$T = \delta \int_{D}^{A} \frac{B}{\alpha} \beta$$

Cost of computing contractions

Result of contraction does not depend on order in which indices are summed, but numerical cost does!

Example 1: cost of matrix multiplication is $\mathcal{O}(\mathbb{D}^3)$: $\frac{C}{\alpha} = \frac{A}{\alpha} \frac{B}{\beta} = \frac{C}{\gamma}$

For every fixed $\stackrel{\checkmark}{\sim}$ and $\stackrel{\checkmark}{\gamma}$ ($\stackrel{D_{\alpha} \times D_{\gamma}}{\sim}$ combinations), sum over $\stackrel{D_{\beta}}{\supset}$ values of $\stackrel{\checkmark}{\circ}$ Cost = $\stackrel{D}{\supset}$ $\stackrel{\checkmark}{\sim}$ $\stackrel{D}{\supset}$ (simplifies to $\stackrel{D}{\supset}$ if all bond dimensions are = $\stackrel{D}{\supset}$)

First contraction scheme has total cost $\mathcal{O}(\mathcal{D}^{5})$, second has $\mathcal{O}(\mathcal{D}^{4})$!!

Finding optimal contraction order is difficult problem! In practice: rely on experience, trial and error...

independent of <a>
∠ !!

4. Covariant index notation

TNB-I.4

For exposition of covariant index notation, see chapters L2 & L10 of

"Mathematics for Physicists", Altland & von Delft, www.cambridge.org/altland-vondelft

Index and arrow conventions below, adopted throughout this course, are really useful, though not (yet) standard.

Kets (Hilbert space vectors)

For kets, indices sit downstairs. E.g. basis kets:

For components of kets (w.r.t. a basis), indices sit upstairs:

$$|\phi\rangle = |\varphi\rangle A^6 \qquad (1)$$

Repeated indices (always up-down pairs) are summed over, summation \sum is implied.

Linear combinations of kets:

$$|\phi_{\alpha}\rangle = |\varphi_{6}\rangle A^{\sigma}_{\alpha}$$
 (2)

Note: for A^{6}_{α} the index σ identifies components of kets, hence sits upstairs identifies basis kets (vectors), hence sits downstairs

Basis for direct product space:
$$|\varphi_{6}\rangle \equiv |\varphi_{6}\rangle \otimes |\varphi$$

Note ket order: start with first space on very right, successively attach new spaces from the left.

Linear combinations:
$$|\phi_{\beta}\rangle = |\phi_{\sigma_1\sigma_2...\sigma_M}\rangle A^{\sigma_1\sigma_2...\sigma_M} \approx |\phi_{\sigma_2}\rangle A^{\overline{\sigma}}\beta$$
 (4)

Bras (Hilbert space dual vectors)

For bras, indices sit upstairs. E.g. basis bras:

$$\langle \varphi^{\bullet} |$$
 (5)

< + | = A+ < < 4 = | For components of bras (w.r.t. a basis), indices sit downstairs: (6)

Complex conjugation [(6) is dual of (1)]:

$$A^{\dagger}_{\sigma} = \overline{A}^{\sigma} \tag{3}$$

Linear combinations of bras:

$$\langle \phi^{\alpha} | = A^{\dagger \alpha} \langle \psi^{G} |$$
 (8)

Complex conjugation [(8) is dual of (2)]:

$$A^{+\alpha}_{6} = \overline{A^{6}}_{\alpha}$$
 (Hermitian conjugation!)

Note: for $A^{\dagger \alpha}$, the index α identifies basis bras (dual vectors), hence sits upstairs the index 6 identifies components of bras, hence sits downstairs

Basis for direct product space:
$$\langle \psi^{\bullet} | \equiv \langle \psi^{\bullet_1 \bullet_2 \dots \bullet_N} | \equiv \langle \psi^{\bullet_1} | \otimes \langle \psi^{\bullet_N} | \otimes \langle \psi^{\bullet_N} | \rangle$$

Note bra order: opposite to that of kets in (3), so expectation values yield nested bra-ket pairs:

$$\left\langle \varphi^{\varepsilon_{1}\varepsilon_{2}...\varepsilon_{N}} \middle| \hat{O} \middle| \varphi_{\varepsilon_{1}\varepsilon_{2}...\varepsilon_{N}} \right\rangle = \left\langle \varphi^{\varepsilon_{1}} \middle| \otimes \left\langle \varphi^{\varepsilon_{2}} \middle| \otimes ... \otimes \left\langle \varphi^{\varepsilon_{N}} \middle| \hat{O} \middle| \varphi_{\varepsilon_{N}} \right\rangle \otimes ... \otimes \left| \varphi_{\varepsilon_{2}} \middle| \otimes \left| \varphi_{\varepsilon_{1}} \right\rangle$$
(1)

Linear combinations:
$$\langle \phi \rho \rangle = A^{\dagger \rho} \sigma_{\rho} \cdots \sigma_{\sigma} \sigma_{\sigma} = A^{\dagger \rho} \sigma_{\rho} \cdots \sigma_{\sigma} \sigma_{\sigma}$$

(13)

<u>Orthonormality</u>

If
$$\{|\psi_{\bullet}\rangle\}$$
 form orthonormal basis: $\langle \psi^{\bullet}|\psi_{\bullet'}\rangle = \delta^{\bullet}_{\bullet'}$ (14)

If
$$\{|\phi_{\mathbf{K}}\rangle\}$$
 form orthonormal basis, too: $\langle \phi^{\mathbf{K}} | \phi_{\mathbf{K}'} \rangle = \delta^{\mathbf{K}}_{\mathbf{K}'}$ (15)

Combined:
$$\delta^{\alpha}_{\alpha'} = \langle \phi^{\alpha} | \phi_{\alpha'} \rangle = A^{\dagger \alpha}_{\sigma} \langle \sigma | \sigma' \rangle A^{\sigma'}_{\alpha'} = A^{\dagger \alpha}_{\sigma} A^{\sigma}_{\alpha'} = (A^{\dagger} A)^{\alpha}_{\alpha'} \quad (16)$$
Hence A is unitary:
$$1 = A^{\dagger} A \implies A^{-1} = A^{\dagger} \qquad (17)$$

Hence A is unitary:
$$1 = A^{\dagger}A \implies A^{-1} = A^{\dagger}$$

Operators
$$\hat{O} = |\phi_{\vec{e}}\rangle O^{\vec{e}_{\vec{e}'}} \langle \phi^{\vec{e}'}|$$
, $O^{\vec{e}_{\vec{e}'}} = \langle \phi^{\vec{e}}|\hat{O}|\phi_{\vec{e}'}\rangle$ (18)

Simplified notation

It is customary to simplify notational conventions for kets and bras:

In kets, use subscript indices as ket names:
$$|\vec{\sigma}\rangle \equiv |\varphi_{\vec{\sigma}}\rangle \equiv |$$

In bras, use superscript indices as bra names:
$$\langle \vec{\epsilon} \mid \equiv \langle \phi^{\vec{\epsilon}} \mid \equiv \langle \epsilon_{i_1} \epsilon_{i_2} ..., \epsilon_{i_N} \mid \equiv \langle \epsilon_{i_1} \otimes \langle \epsilon_{i_2} \mid \otimes \langle \epsilon_{i_N} \mid \rangle \rangle$$

Now up/down convention for indices is no longer displayed; but it is still implicit!

Linear combination of kets:
$$|v\rangle = |\sigma\rangle A^{\sigma}$$

Coefficient matrix = overlap:
$$A^{\circ}_{\kappa} = \langle e^{\circ}_{\kappa} \rangle$$

$$A_{e}^{\alpha} = \langle e | \alpha \rangle \tag{55}$$

If direct products are involved:
$$|\beta\rangle \stackrel{(4)}{=} |\sigma_2\rangle \otimes |\sigma_1\rangle |$$

$$|\beta\rangle \stackrel{(4)}{=} |\sigma_2\rangle \otimes |\sigma_1\rangle A^{\sigma_1\sigma_2} \beta$$

$$A^{\sigma_1\sigma_2} \beta \stackrel{=}{=} \langle \sigma_1 | \otimes \langle \sigma_2 | \beta \rangle$$

$$6_1$$
 6_2
 (23)

$$\langle \alpha | \stackrel{=}{=} H^{\dagger \alpha} \langle \alpha |$$

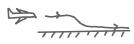
Linear combination of bras:

$$A^{+\alpha}e = \langle \alpha | e \rangle = \langle e | \alpha \rangle = A^{\alpha}$$

$$\mathsf{H}^{\dagger \beta}_{\mathfrak{G}_{2} \mathfrak{G}_{1}} = \langle \beta | \mathfrak{G}_{2} \rangle \otimes | \mathfrak{G}_{1} \rangle = \langle \mathfrak{G}_{1} | \otimes \langle \mathfrak{G}_{2} | \beta \rangle \stackrel{(24)}{=} \mathsf{H}^{\mathfrak{G}_{1} \mathfrak{G}_{2}}$$

$$(28)$$

In all these overlaps (22,24,26,28):



bra indices: written upstairs on A or A^{\dagger} , depicted by incoming arrows ket indices: written downstairs on A or A^{\dagger} , depicted by outgoing arrows

Mnemonic for arrow directions:	'airplane landing':	flying in (up in air), rolling out (down on ground).