Entanglement in Featureless Mott Insulators

Brayden Ware

September 18th 2014

Outline

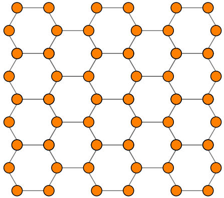
Outline

1. Motivation
   - Featureless Insulators
   - Lieb-Schultz-Mattis Theorem
   - Magnetization Plateaus
2. Distinguishing Featureless Insulators by Entanglement
   - Matrix Product States
3. Featureless Boson Mott Insulators
   - Honeycomb Featureless Insulator Proposal
   - Tensor Network Construction
   - Entanglement Spectra Results
   - Identifying CFTs by Spectra

Featureless Insulators

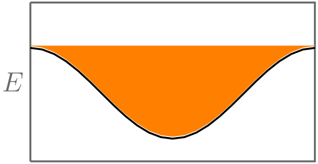
Definition of 'Featureless Insulator'

- Gapped
- Symmetric
- No (bulk) fractionalization
- Unique ground state on torus

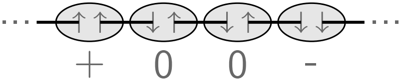


Bosonic Mott insulator with integer filling

Examples:



Band Insulator



Haldane phase of spin-1 Chain (AKLT)

Lieb-Schultz-Mattis Theorem

Featured states are

- either gapless
- or spontaneously break spin symmetry
- or spontaneously break translational symmetry
- or topologically ordered
- but always have (nearly) degenerate states when placed in periodic boundary conditions.

States with fractional charge per unit cell cannot be featureless.

Theorem: Lieb, Schultz, Mattis (1961)

A spin $1/2$ chain with $SU(2)$ and translational symmetry has a ground state that is either gapless or breaks symmetry.

Lieb-Schultz-Mattis Theorem

Featured states are

- either gapless
- or spontaneously break spin symmetry
- or spontaneously break translational symmetry
- or topologically ordered
- but always have (nearly) degenerate states when placed in periodic boundary conditions.

States with fractional charge per unit cell cannot be featureless.

Extension: Oshikawa (1999)

A particle-number conserving system with a fractional number of particles per unit cell cannot have a fixed energy gap on a torus. The same holds for a $U(1)$-symmetric spin system with total spin j per unit cell and magnetization m per unit cell, with $j - m$ not integer.

Lieb-Schultz-Mattis Theorem

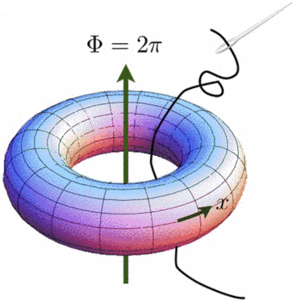
Featured states are

- either gapless
- or spontaneously break spin symmetry
- or spontaneously break translational symmetry
- or topologically ordered
- but always have (nearly) degenerate states when placed in periodic boundary conditions.

States with fractional charge per unit cell cannot be featureless.

Proof:

The Lieb-Schultz-Mattis-Laughlin-Bonesteel-Affleck-Yamanaka-Oshikawa flux-threading argument



Application of LSM

Spin-$1/2$ XXZ chain

$$H_{XY} = J \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)$$

Jordan-Wigner transformation maps to half-filled free-fermion band. Remains gapless under small $U(1)$ perserving pertubations:

- hS^z - gapless until $m = \pm 1/2$
- $J_z S_i^z S_{i+1}^z$ - gapless until AFM/FM order
- $J_2 \vec{S}_i \cdot \vec{S}_{i+2}$ - gapless until SSB of translation, unit cell doubles

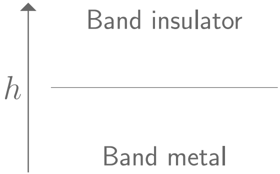
Application of LSM

Spin-$1/2$ XXZ chain

$$H_{XY} = J \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \frac{h}{J} S_i^z)$$

Jordan-Wigner transformation maps to half-filled free-fermion band. Remains gapless under small $U(1)$ perserving pertubations:

- hS^z - gapless until $m = \pm 1/2$
- $J_z S_i^z S_{i+1}^z$ - gapless until AFM/FM order
- $J_2 \vec{S}_i \cdot \vec{S}_{i+2}$ - gapless until SSB of translation, unit cell doubles



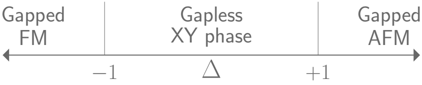
Application of LSM

Spin-$1/2$ XXZ chain

$$H_{XXZ} = J \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z)$$

Jordan-Wigner transformation maps to half-filled free-fermion band. Remains gapless under small $U(1)$ perserving pertubations:

- hS^z - gapless until $m = \pm 1/2$
- $J_z S_i^z S_{i+1}^z$ - gapless until AFM/FM order
- $J_2 \vec{S}_i \cdot \vec{S}_{i+2}$ - gapless until SSB of translation, unit cell doubles



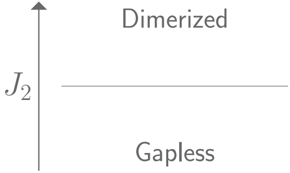
Application of LSM

Spin-$1/2$ XXZ chain

$$H_{XXZ} = J \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z + \frac{J_2}{J} \vec{S}_i \cdot \vec{S}_{i+1})$$

Jordan-Wigner transformation maps to half-filled free-fermion band. Remains gapless under small $U(1)$ perserving pertubations:

- hS^z - gapless until $m = \pm 1/2$
- $J_z S_i^z S_{i+1}^z$ - gapless until AFM/FM order
- $J_2 \vec{S}_i \cdot \vec{S}_{i+2}$ - gapless until SSB of translation, unit cell doubles

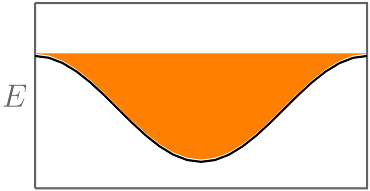


Magnetization/Density Plateaus

Stable featureless insulators form magnetization or density plateaus
Example Hamiltonians and phase diagrams:

Band Insulators

$$H_{FF} = \sum_{<ij>} -t_{ij} c_i^\dagger c_j - \mu \sum_i N_i$$



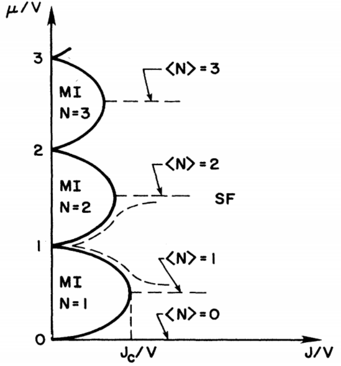
- Symmetry protected band touchings can constrain existence of a band insulator
- Topological invariants can distinguish different types of band insulators
- Some invariants only make sense in the presence of additional symmetries $(\mathcal{T}, \mathcal{C}, \mathcal{I})$

Magnetization/Density Plateaus

Stable featureless insulators form magnetization or density plateaus
Example Hamiltonians and phase diagrams:

Bose-Hubbard model

$$H_{BH} = -J \sum_{<ij>} b_i^\dagger b_j - \mu \sum_i N_i + \frac{1}{2} V \sum_i N_i(N_i - 1)$$



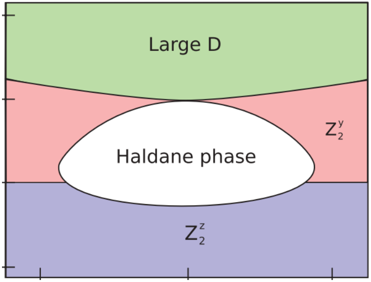
- Interactions are always needed to stop Bose condensation
- Unlike free-fermions, not obvious how to construct fractional site filling insulators
- Tensor network states give us access to needed construction and to interacting invariants.

Magnetization/Density Plateaus

Stable featureless insulators form magnetization or density plateaus
Example Hamiltonians and phase diagrams:

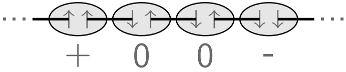
Haldane Phase for Spin-1 chains $(j = 1, m = 0)$

$$H_{AKLT} = \sum_i J\vec{S}_i \cdot \vec{S}_{i+1} + J'(\vec{S}_i \cdot \vec{S}_{i+1})^2 + D(S_i^z)^2 + BS^x$$



Two distinct featureless insulators:

- Large-D phase
  - Contains product state wavefunction $|\psi\rangle = |000...\rangle$
- Haldane phase
  - Contains AKLT wavefunction $|\psi\rangle = \Sigma| + 00 - 0 + ...\rangle$



Motivating Questions

Are there general principles for distinguishing potential featureless insulator ground states of Hamiltonians?

The theory of *symmetry protected topological phases* (SPTs) is a general framework for distinguishing different featureless insulators.

- *Topological* - some discrete invariant that won't change under continuous (adiabatic) changes in Hamiltonian
- Invariants should be defined for interacting systems that obey certain symmetries
- Often features edge fractionalization and degeneracy in open boundary conditions
- In 1D, universally distinguished by entanglement spectra

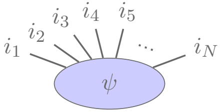
Are there additional constraints on the existence of featureless insulators in interacting systems?

Outline

What is entanglement?

When a wavefunction in a product Hilbert space cannot be written as a product state, it is **entangled**.

$$|\psi\rangle = |\psi_L\rangle \otimes |\psi_R\rangle ?$$

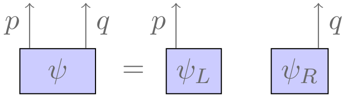


$$|\psi\rangle = \sum \psi_{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle$$

What is entanglement?

When a wavefunction in a product Hilbert space cannot be written as a product state, it is **entangled**.

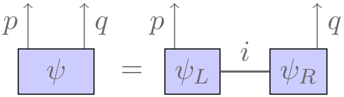
$$|\psi\rangle = |\psi_L\rangle \otimes |\psi_R\rangle?$$



What is entanglement?

When a wavefunction in a product Hilbert space cannot be written as a product state, it is **entangled**.

$$|\psi\rangle = \sum_i |\psi_L^i\rangle \otimes |\psi_R^i\rangle$$

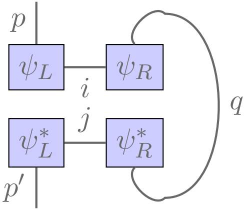


Calculate reduced density matrices

$$\rho_L = Tr_R |\psi\rangle\langle\psi|$$

Diagonalize

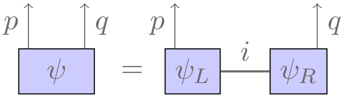
$$\rho_L = \sum_\alpha \rho_\alpha |\psi_L^\alpha\rangle\langle\psi_L^\alpha|$$



What is entanglement?

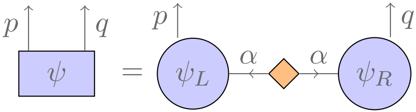
When a wavefunction in a product Hilbert space cannot be written as a product state, it is **entangled**.

$$|\psi\rangle = \sum_i |\psi_L^i\rangle \otimes |\psi_R^i\rangle$$



Diagonalize and form the Schmidt decomposition

$$|\psi\rangle = \sum_\alpha \sqrt{\rho_\alpha}|\psi_L^\alpha\rangle \otimes |\psi_R^\alpha\rangle$$



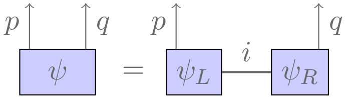
Quantitative measures of entanglement - rank

$$S_A^0 = \sum_\alpha \rho_\alpha^0 = \#\{\rho_\alpha \neq 0\}$$

What is entanglement?

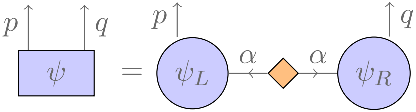
When a wavefunction in a product Hilbert space cannot be written as a product state, it is **entangled**.

$$|\psi\rangle = \sum_i |\psi_L^i\rangle \otimes |\psi_R^i\rangle$$



Diagonalize and form the Schmidt decomposition

$$|\psi\rangle = \sum_\alpha \sqrt{\rho_\alpha} |\psi_L^\alpha\rangle \otimes |\psi_R^\alpha\rangle$$

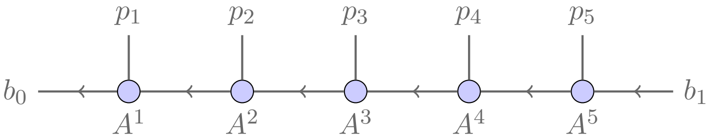


Quantitative measures of entanglement - entropy

$$S_A = -\sum_\alpha \rho_\alpha \log \rho_\alpha$$

What is a matrix product state?

Matrix product states provide a parameterization of the space of wavefunctions of a 1D or quasi-1D system.

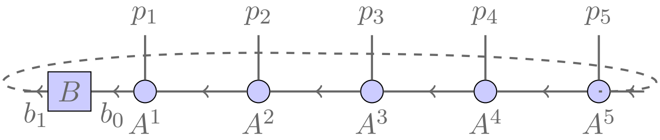


$$|\psi^{b_0 b_1}\rangle = \sum_{p_1 \ldots p_5} (b_0| \, A_1^{p_1} \ldots A_5^{p_5} \, |b_1) \, |p_1 \ldots p_5\rangle$$

Coefficients of the wavefunction are calculated via a product of matrices, one per site. The matrix at each site depends on the physical state at that site.

What is a matrix product state?

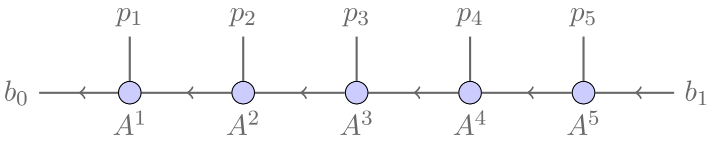
Matrix product states provide a parameterization of the space of wavefunctions of a 1D or quasi-1D system.



$$|\psi\rangle = \sum_{p_1 \dots p_5} Tr(BA_1^{p_1} \dots A_5^{p_5})|p_1 \dots p_5\rangle$$

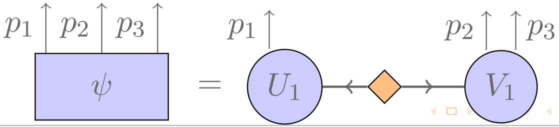
What is a matrix product state?

Matrix product states provide a parameterization of the space of wavefunctions of a 1D or quasi-1D system.



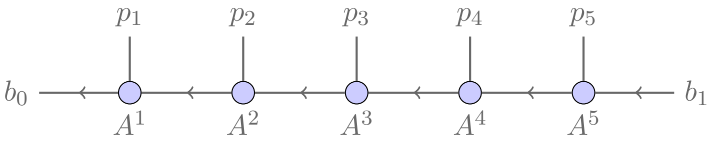
Coefficients of the wavefunction are calculated via a product of matrices, one per site. The matrix at each site depends on the physical state at that site.

Every state has a matrix product state representation formed through the process of repeated SVD.

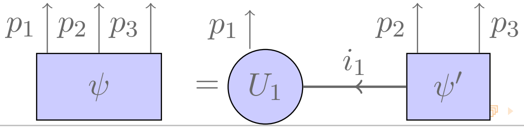


What is a matrix product state?

Matrix product states provide a parameterization of the space of wavefunctions of a 1D or quasi-1D system.

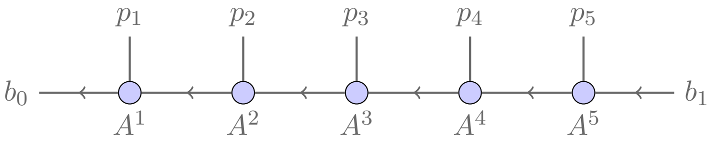


Coefficients of the wavefunction are calculated via a product of matrices, one per site. The matrix at each site depends on the physical state at that site.
Every state has a matrix product state representation formed through the process of repeated SVD.



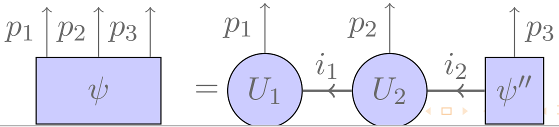
What is a matrix product state?

Matrix product states provide a parameterization of the space of wavefunctions of a 1D or quasi-1D system.



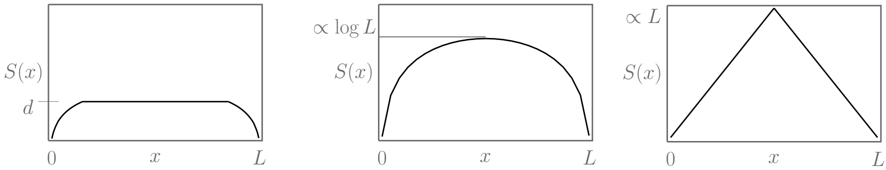
Coefficients of the wavefunction are calculated via a product of matrices, one per site. The matrix at each site depends on the physical state at that site.

Every state has a matrix product state representation formed through the process of repeated SVD.



Properties of matrix product states

- Representing every wavefunction with perfect accuracy requires exponentially big bond dimensions
- Ground states of gapped quantum Hamiltonians satisfy (rigorously in 1D) an area law: $S_A \approx d \cdot (\partial A)$.
- With a fixed truncation error ϵ, bond dimension needed to represent the wavefunction levels off to a constant $d(\epsilon)$.
- MPS representation is efficient - only needs $d^2 L$ parameters



Gapped ground state | Gapless ground state | Generic State

Computing Correlation Functions in MPS

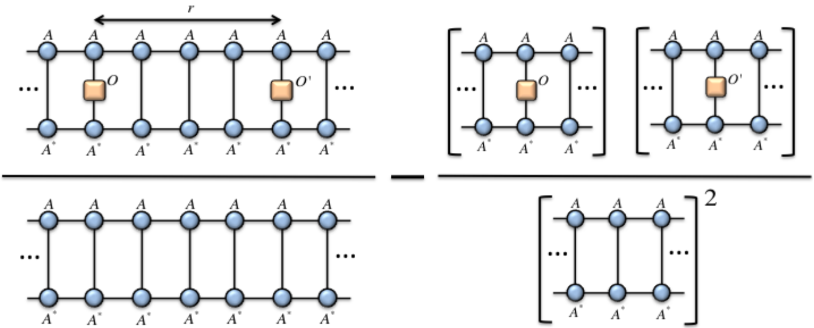
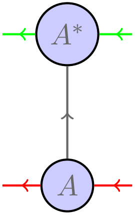
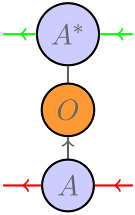


Diagram for $C_{OO'}(r) = \langle O_i O'_{i+r} \rangle - \langle O_i \rangle \langle O'_{i+r} \rangle$

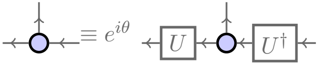
Computing Correlation Functions in MPS



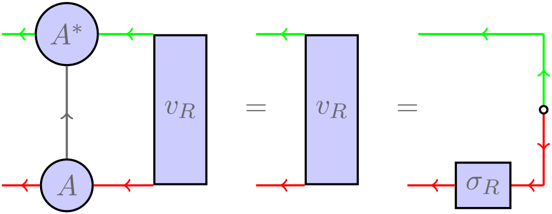
Transfer Matrix $\mathbb{E}_I$



Operator Insertion $\mathbb{E}_O$



MPS gauge redundancy



Computing Correlation Functions in MPS

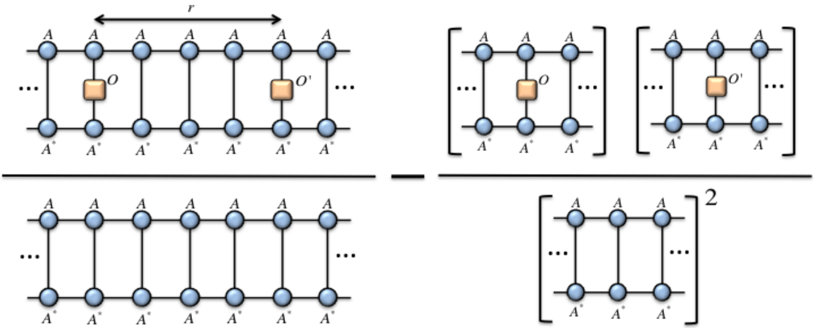


Diagram for $C_{OO'}(r) = \langle O_i O'_{i+r} \rangle - \langle O_i \rangle \langle O'_{i+r} \rangle$

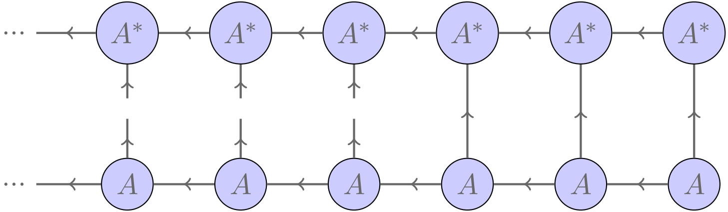
$$\langle O_i O'_{i+r} \rangle = (v_L | \mathbb{E}_O \mathbb{E}_I^r \mathbb{E}_{O'} | v_R)$$

$$\lim_{r \to \infty} \langle O_i O'_{i+r} \rangle = (v_L | \mathbb{E}_O | v_R) \, (v_L | \mathbb{E}_{O'} | v_R)$$

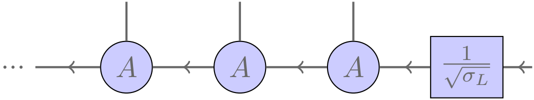
$$C_{OO'}(r) \approx const. \times \lambda_2^r$$

Computing Entanglement in MPS

To compute the spectrum of the reduced density matrix

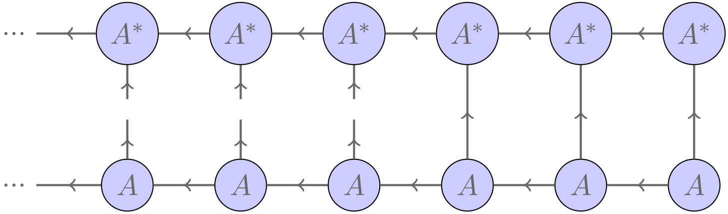


Step 1. Show that the following matrix $\mathcal{U}$ is isometric.



Computing Entanglement in MPS

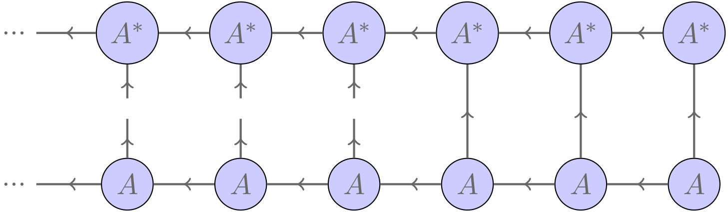
To compute the spectrum of the reduced density matrix



Step 2. Insert identity...

Computing Entanglement in MPS

To compute the spectrum of the reduced density matrix



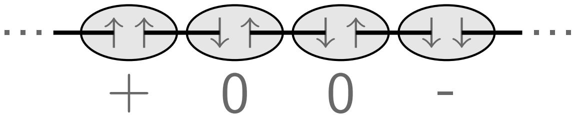
Result:

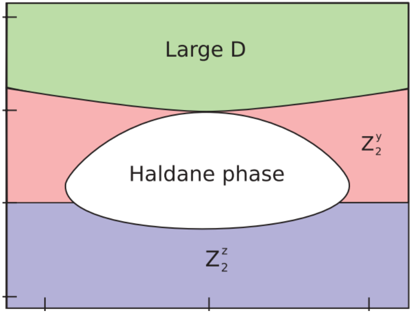
$$\rho_L = \mathcal{U}\sqrt{\sigma_L}\sigma_R\sqrt{\sigma_L}\mathcal{U}^\dagger$$

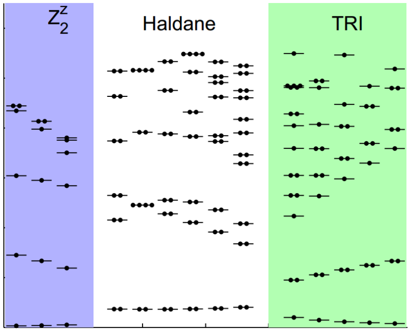
To get the spectrum, we only need to compute the much smaller matrix

$$\tilde{\rho}_L = \sqrt{\sigma_L}\sigma_R\sqrt{\sigma_L}$$

MPS Example: AKLT State





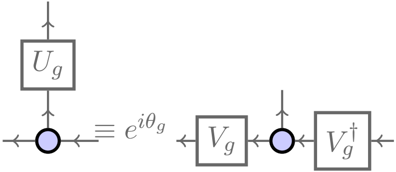


Haldane phase distinguished by exact double degeneracy in entire entanglement spectrum.

Properties of Featureless MPS

MPS for featureless 1D or quasi-1D systems have non-degenerate transfer matrices and are called simple. Simple MPS can be proved to have:

- Correlations are insensitive to boundary conditions
- Can construct a featureless 'parent Hamiltonian'
- Two simple MPS with equal wavefunctions are (uniquely) gauge equivalent
- Corollary: Edges can be labeled with a (possibly projective) representation of the group of physical symmetries.



- Bonus: we can determine V_g by diagonalizing the transfer matrix with the insertion U_g.

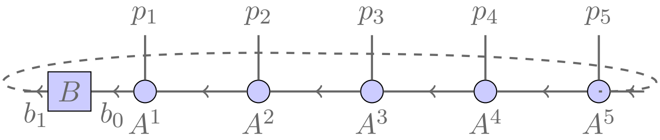
Symmetry Protected Entanglement

- These edge symmetries V_g commute with the 'reduced density matrix' $\tilde{\rho}_L$ of the system and thus only act non-trivially on degenerate entanglement spectra eigenvalues.
- Because the classes of projective symmetry groups are discrete, you can't change the action on the edge continuously between classes (without going through a phase transition.)

symmetry	string order	edge states	degeneracy
D_2 ($=Z_2 \times Z_2$)	yes	yes	yes
time reversal	no	yes	yes
inversion	no	no	yes

Flux-Threading Arguments for SPTs?

Recall that the boundary conditions in a MPS are set by a matrix at the edge.



Inserting the group operation V_g on a single link in a periodic chain is the same as changing the boundary conditions. This is an operational procedure for 'threading a flux' that works in interacting theories or even with then symmetry is inversion or time-reversal.

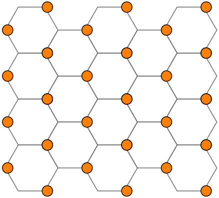
The edge action can be interpreted as a 'composition of fluxes' $V_g V_h = \exp i\omega(g,h) V_{gh}$.

Outline

Existence of Featureless Insulators

Given a (non-Bravais) lattice and an integer particle number per unit cell, is there always a featureless insulator?

Naive constructions don't work on the honeycomb lattice because you can't pick a symmetric unit cell. For fermion band insulators, filling orbitals in a non-symmetric unit cell can still lead to symmetric wave functions to the antisymmetrization of fermions.

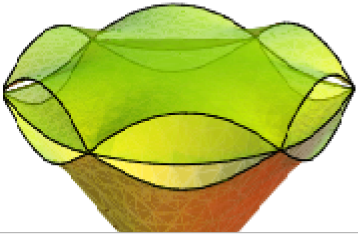


Does there exist a bosonic featureless Mott insulator with half-integer site filling?

Existence of Featureless Insulators

Status of existence question:

- On *non-symmorphic* lattices, not all integer particle-numbers can be realized.
  - Flux removal doesn't commute with glide-reflections or screw-axes where the the translation vector is not a lattice translation.
- On Kagome lattice, boson insulator with 1/3 site filling constructed by filling Wannier orbitals of the lowest band of a fermion band insulator.



Existence of Featureless Insulators

On honeycomb lattice, no such band insulator.

- Proposed wavefunction:

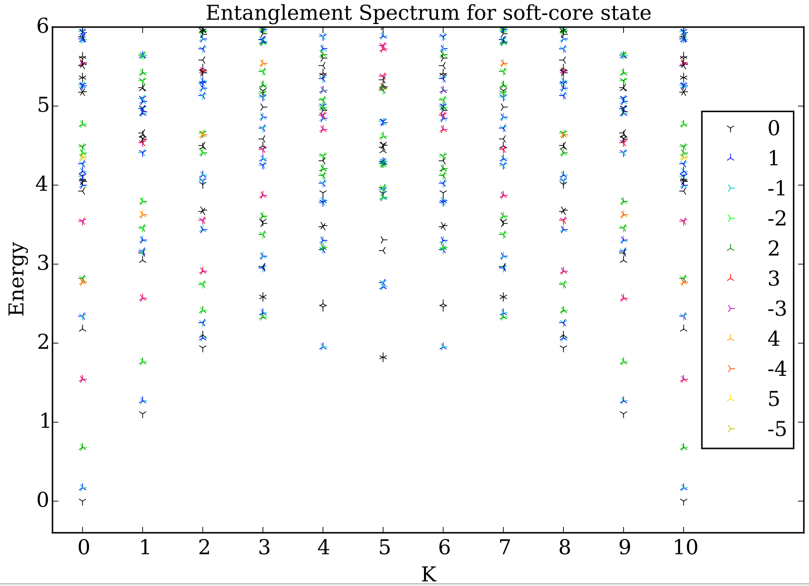
$$|\psi\rangle = \prod_R \sum_{i \in R} b_i^\dagger |\vec{0}\rangle$$

- Goals:
  - Rule out spontaneous symmetry breaking by computing correlations
  - Rule out topological order by computing topological entanglement entropy
  - Distinguish from other featureless phases using edge entanglement

Tensor Network Construction of FBI

A wavefunction written as a product of local operators acting on a product state can simply be turned into a tensor network.

Entanglement Spectra

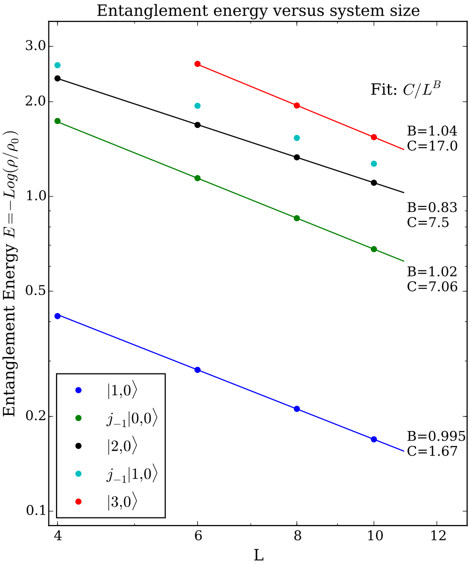


Finite Size Analysis of Spectra

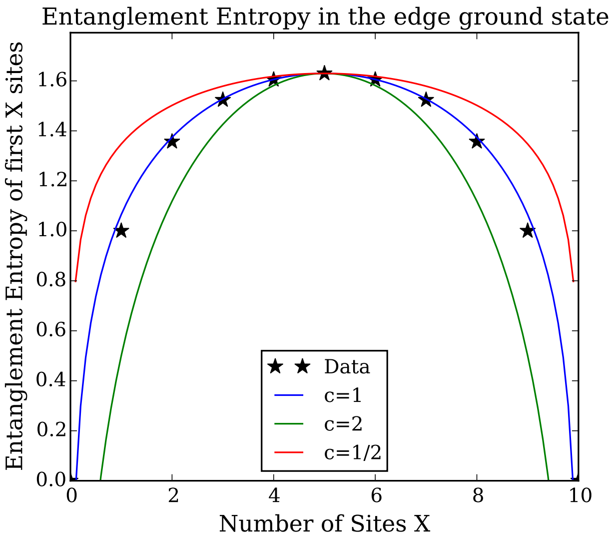
- Topological entanglement entropy is 0
- Low energy modes show gapless $1/L$ behavior

Finite Size Analysis of Spectra

- Topological entanglement entropy is 0
- Low energy modes show gapless $1/L$ behavior



Identifying CFTs: Measuring c



Level identification in CFT spectra

To make a precise comparison with the free-boson CFT, we'll need to solve for (or look up) the solution of this model.
The free-boson CFT is created from the Lagrangian

$$\mathfrak{L} = \frac{g}{2} \int dt \int_0^L dx \left(\frac{1}{v^2}(\partial_t \phi)^2 - (\partial_x \phi)^2\right)$$

and with the compatified field identification

$$\phi \equiv \phi + 2\pi R$$

and placed on the circle of circumference L with periodic boundary conditions

$$\phi(x) \equiv \phi(x + L).$$

Level identification in CFT spectra

$\mathbf{L_0}$	$2\pi g(\frac{e}{4\pi g R} + \frac{mR}{2})^2 + n$
$\mathbf{\bar{L}_0}$	$2\pi g(\frac{e}{4\pi g R} - \frac{mR}{2})^2 + \bar{n}$
$\mathbf{P} = \frac{2\pi v}{L}(\mathbf{L_0} - \mathbf{\bar{L}_0})$	$\frac{2\pi v}{L}(em + n - \bar{n})$
$\mathbf{H} = \frac{2\pi v}{L}(\mathbf{L_0} + \mathbf{\bar{L}_0})$	$\frac{2\pi v}{L}(\frac{e^2}{4\pi g R^2} + \pi g m^2 R^2 + n + \bar{n})$
$\tilde{\mathbf{H}} = \frac{L}{2\pi v \kappa}\mathbf{H}$	$e^2 + \frac{m^2}{4\kappa^2} + \frac{1}{\kappa}(n + \bar{n})$

Eigenvalues of states $|e, m\rangle_{n,\bar{n}}$. The rescaled Hamiltonian $\tilde{\mathbf{H}}$ has eigenvalues that depend on only one free-parameter, $\kappa = 1/(4\pi g R^2)$.(Note: A common convention is to set $g = 1/4\pi$ and describe the system using $R = \sqrt{1/\kappa}$.)

Level identification in CFT spectra