# Entanglement in Featureless Mott Insulators

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September 18th 2014

# 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

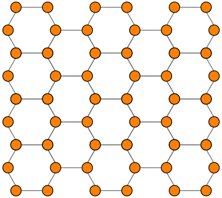
# Outline

# Featureless Insulators

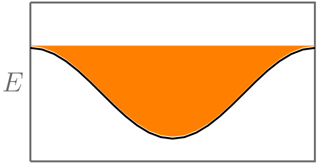
Definition of 'Featureless Insulator'

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

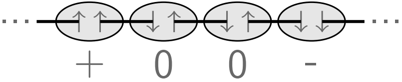
Examples:



Bosonic Mott insulator with integer filling




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

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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

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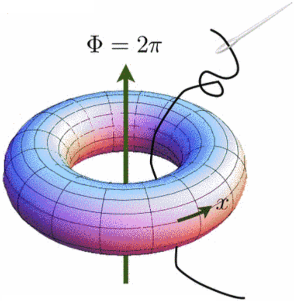
States with fractional charge per unit cell cannot be featureless.

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

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

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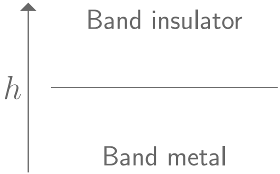

# Application of LSM

## Spin-$1/2$ XXZ chain

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

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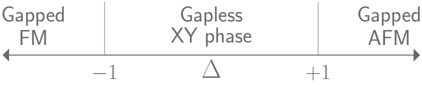

# Application of LSM

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

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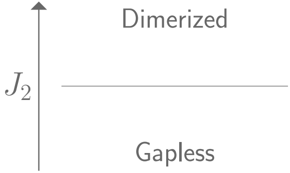
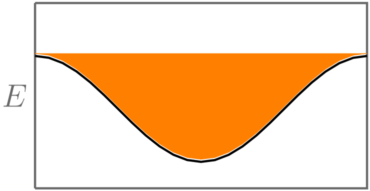


# Magnetization/Density Plateaus

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

## Band Insulators

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



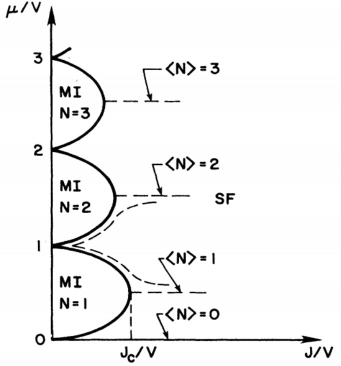

- Symmetry protected band touchings can constrain existence of a band insulator
- Topological invariants can distinguish different types of band insulators
- Some invariants only make sense in the presence of additional symmetries $(\mathcal{T}, \mathcal{C}, \mathcal{I})$

# Magnetization/Density Plateaus

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

### Bose-Hubbard model

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



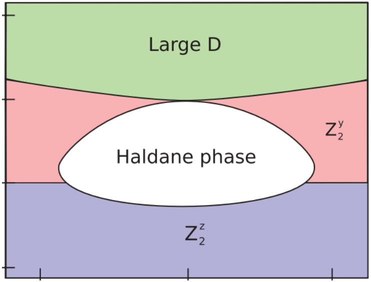

- Interactions are always needed to stop Bose condensation
- Unlike free-fermions, not obvious how to construct fractional site filling insulators
- Tensor network states give us access to needed construction and to interacting invariants.

# Magnetization/Density Plateaus

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

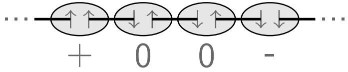
Haldane Phase for Spin-1 chains $(j = 1, m = 0)$

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




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

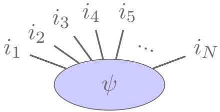
Are there additional constraints on the existence of featureless insulators in interacting systems?

# Outline

# What is entanglement?

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

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




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

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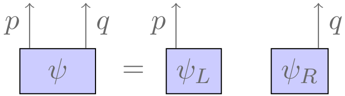

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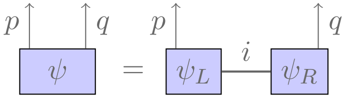
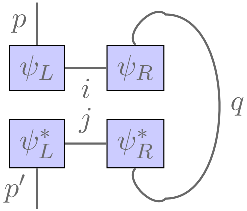



Calculate reduced density matrices

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

Diagonalize

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



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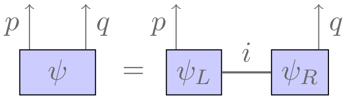
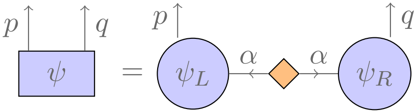



Diagonalize and form the Schmidt decomposition

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




Quantitative measures of entanglement - rank

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

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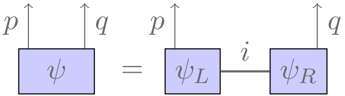


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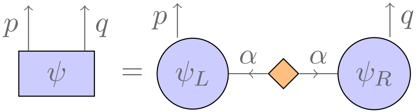
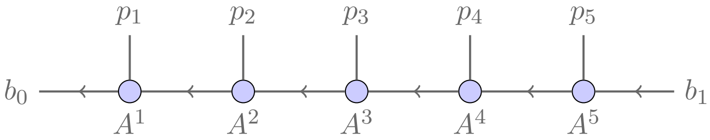



Quantitative measures of entanglement - entropy

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

# 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.

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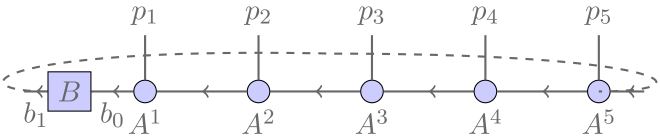


$$|\psi\rangle = \sum_{p_1 \ldots p_5} Tr(BA_1^{p_1} \ldots A_5^{p_5})|p_1 \ldots p_5\rangle$$

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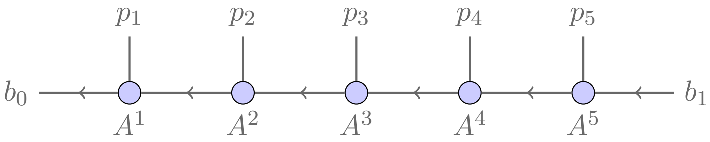
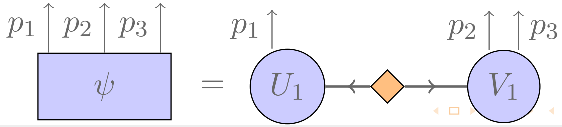



Coefficients of the wavefunction are calculated via a product of matrices, one per site. The matrix at each site depends on the physical state at that site.
Every state has a matrix product state representation formed through the process of repeated SVD.



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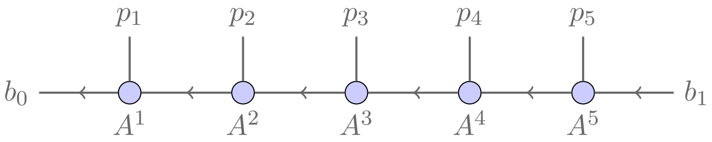


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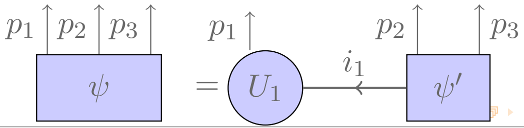

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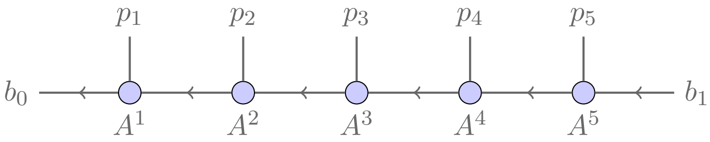


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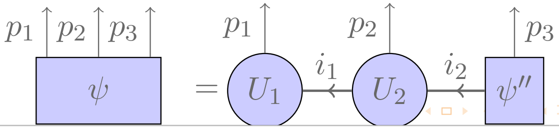
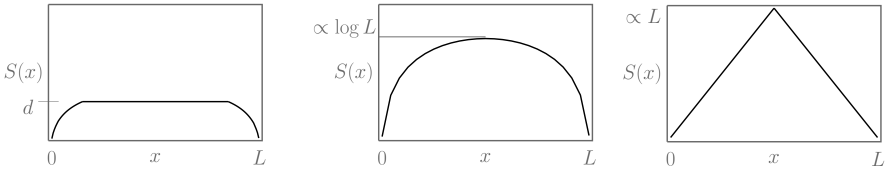


# Properties of matrix product states

- 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 $\epsilon$, 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

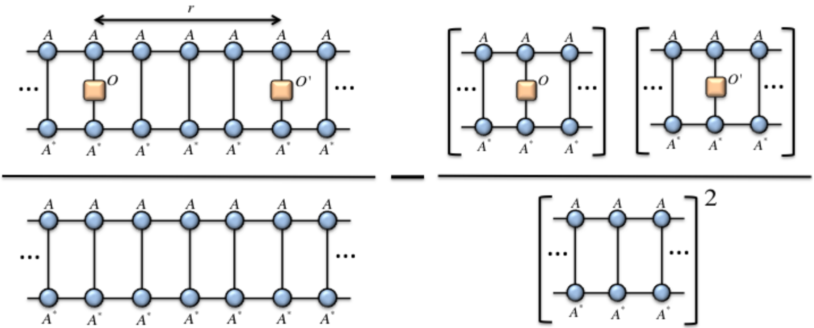
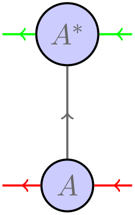
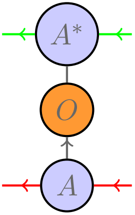



Diagram for $C_{OO'}(r) = \langle O_i O'_{i+r} \rangle - \langle O_i \rangle \langle O'_{i+r} \rangle$

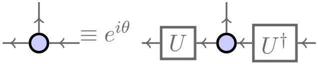
# Computing Correlation Functions in MPS



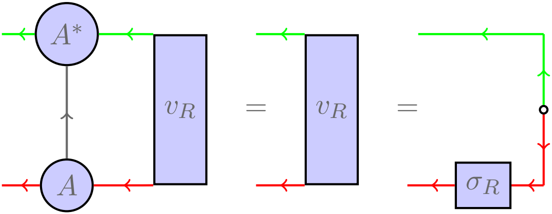

Transfer Matrix $\mathbb{E}_I$




Operator Insertion $\mathbb{E}_O$




MPS gauge redundancy



# Computing Correlation Functions in MPS

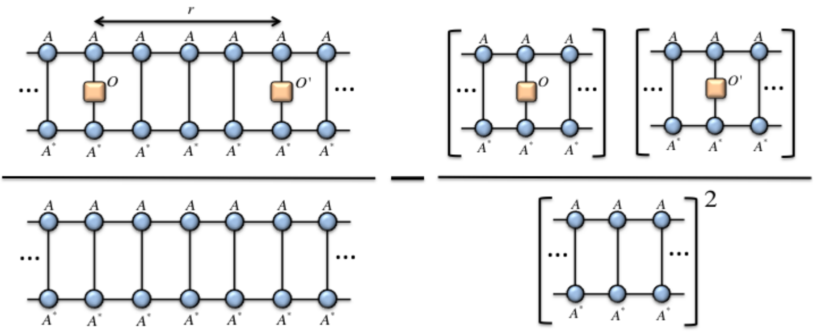



Diagram for $C_{OO'}(r) = \langle O_i O'_{i+r} \rangle - \langle O_i \rangle \langle O'_{i+r} \rangle$

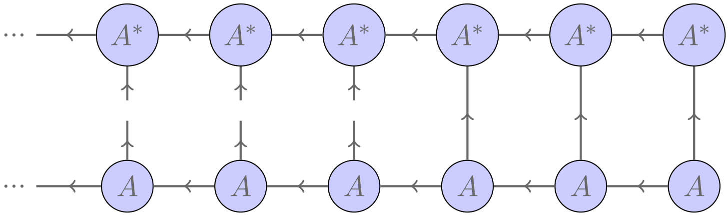
$$\langle O_i O'_{i+r} \rangle = (v_L | \mathbb{E}_O \mathbb{E}_I^r \mathbb{E}_{O'} | v_R)$$

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

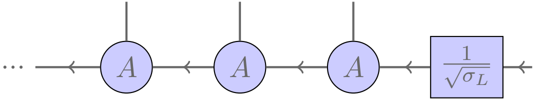
$$C_{OO'}(r) \approx const. \times \lambda_2^r$$

# Computing Entanglement in MPS

To compute the spectrum of the reduced density matrix

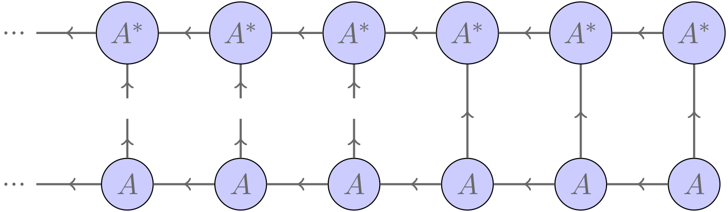



Step 1. Show that the following matrix $\mathcal{U}$ is isometric.



# Computing Entanglement in MPS

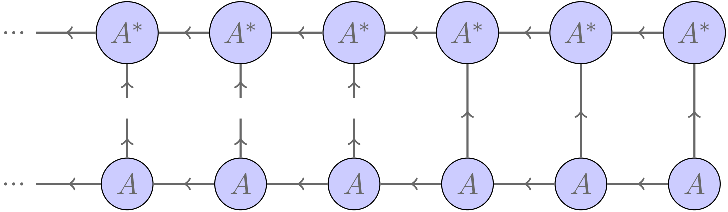
To compute the spectrum of the reduced density matrix




Step 2. Insert identity...

# Computing Entanglement in MPS

To compute the spectrum of the reduced density matrix



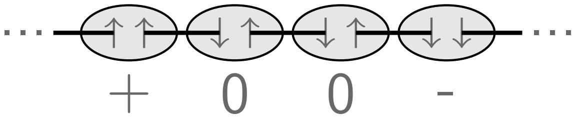

Result:

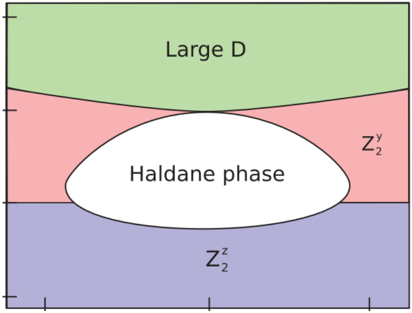
$$\rho_L = \mathcal{U}\sqrt{\sigma_L}\sigma_R\sqrt{\sigma_L}\mathcal{U}^\dagger$$

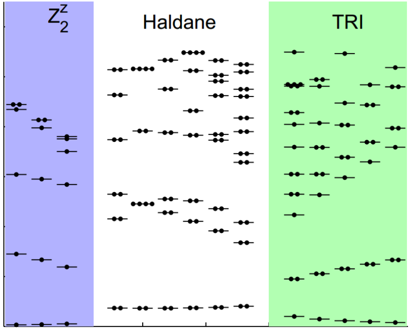
To get the spectrum, we only need to compute the much smaller matrix

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

# MPS Example: AKLT State



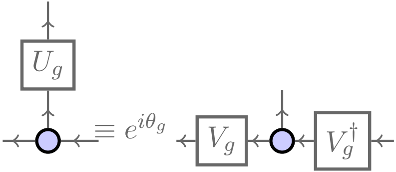




Haldane phase distinguished by exact double degeneracy in entire entanglement spectrum.

# 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 $U_g$.

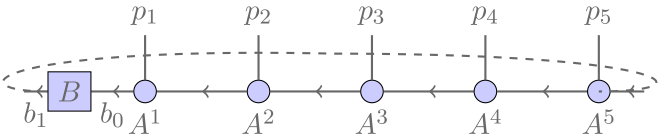
# Symmetry Protected Entanglement

- 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.

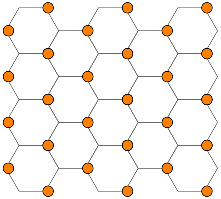
The edge action can be interpreted as a 'composition of fluxes' $V_g V_h = \exp i\omega(g,h) V_{gh}$.

# 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.

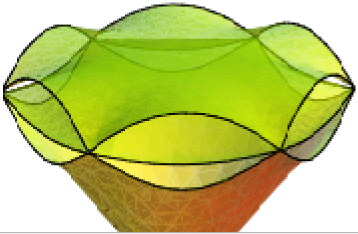


Does there exist a bosonic featureless Mott insulator with half-integer site filling?

# 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:

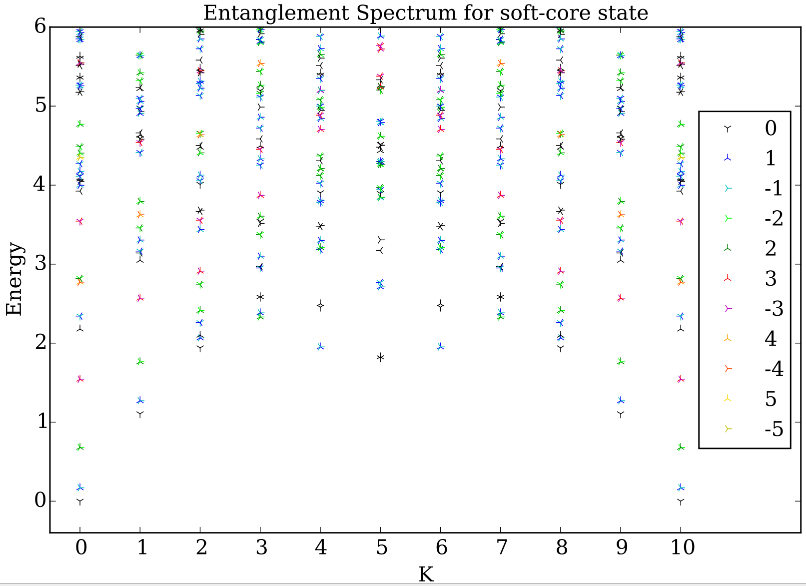
$$|\psi\rangle = \prod_R \sum_{i \in R} b_i^\dagger |\vec{0}\rangle$$

- 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

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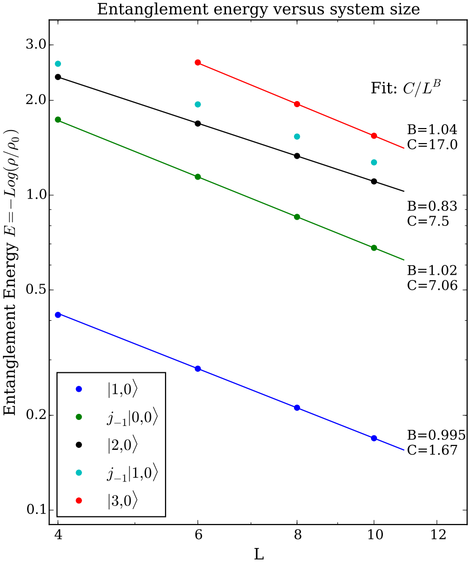
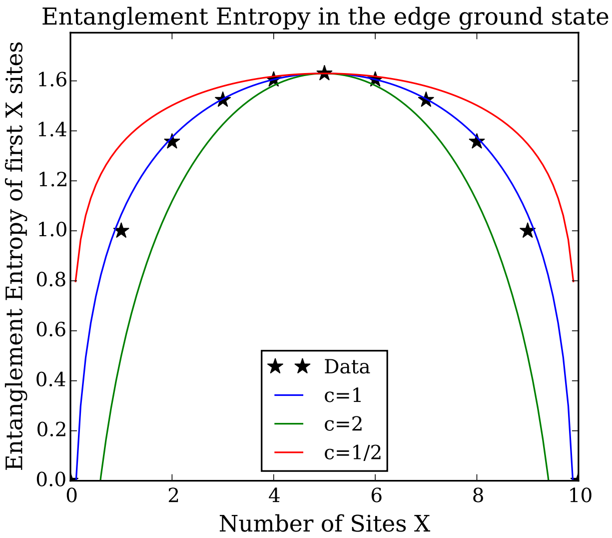


# Identifying CFTs: Measuring c



# 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

| | |
|---|---|
| $\mathbf{L_0}$ | $2\pi g(\frac{e}{4\pi gR} + \frac{mR}{2})^2 + n$ |
| $\bar{\mathbf{L}}_\mathbf{0}$ | $2\pi g(\frac{e}{4\pi gR} - \frac{mR}{2})^2 + \bar{n}$ |
| $\mathbf{P} = \frac{2\pi v}{L}(\mathbf{L_0} - \bar{\mathbf{L}}_\mathbf{0})$ | $\frac{2\pi v}{L}(em + n - \bar{n})$ |
| $\mathbf{H} = \frac{2\pi v}{L}(\mathbf{L_0} + \bar{\mathbf{L}}_\mathbf{0})$ | $\frac{2\pi v}{L}(\frac{e^2}{4\pi gR^2} + \pi g m^2 R^2 + n + \bar{n})$ |
| $\tilde{\mathbf{H}} = \frac{L}{2\pi v\kappa}\mathbf{H}$ | $e^2 + \frac{m^2}{4\kappa^2} + \frac{1}{\kappa}(n + \bar{n})$ |

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