Entanglement in Featureless Mott Insulators

Brayden Ware

September 26th 2014

Outline

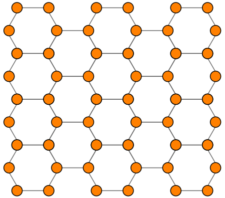
Motivation

Featureless Insulators

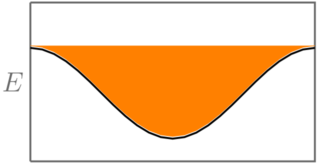
Definition of 'Featureless Insulator'

- Gapped
- Symmetric
- No topological order
- Integer charge per unit cell
- Unique ground state with P.B.C.

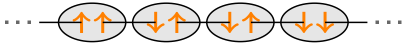
Examples:



Bosonic Mott insulator with integer filling



Band Insulator



Heisenberg AF Spin-1 chain

Free Fermion Band Insulators

- Crystalline, 0T insulators (including semiconductors)
- Tight-binding Hamiltonian

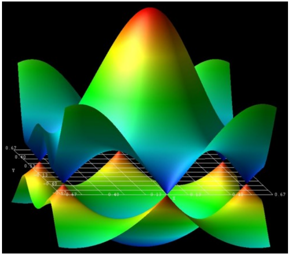
$$\mathcal{H}_{FF} = \sum_{<ij>} \sum_{\alpha,\beta} -t_{\alpha,\beta} c_i^{\alpha\dagger} c_j^{\beta} - \mu \sum_{i,\alpha} N_i^{\alpha}$$

- Bloch wavefunctions $|u_{\mathbf{k}}^{\alpha}\rangle$
- Massive Dirac Hamiltonian

$$\mathcal{H}_D(\mathbf{k}) = \mathbf{k}_x \sigma_x + \mathbf{k}_y \sigma_y + m_* \sigma_z$$

- Atomic-insulating like Wannier basis
- Density plateau

Semiconductor GaN



Band Theory

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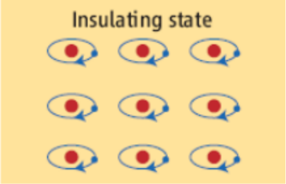

Atomic Insulator

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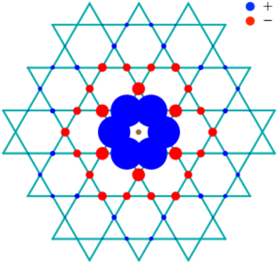
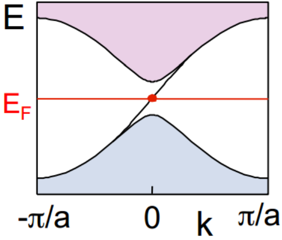


Wannier Function

Topological Band Insulators

Topological bands discovered in Integer Quantum Hall Effect (IQHE) (1984)

- Bulk conductance drops to 0
- Integer filling of Landau levels
- Robust chiral edge modes
- Quantized Hall conductivity $\sigma_H = n\frac{e^2}{\hbar}$
- No longer an atomic insulator
- Topological invariant Chern number (a.k.a. TKNN)



Chiral Edge [1]

[1] (Hasan and Kane, 2010)

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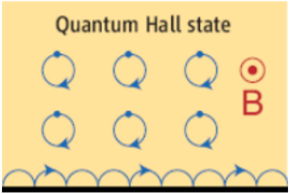

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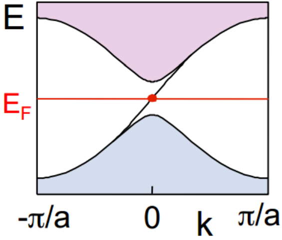

Chiral Edge [1]

$$n^\alpha = \frac{i}{2\pi}\int_{B.Z.} d^2\mathbf{k}\langle\partial_{\mathbf{k}_x}u^\alpha_{\mathbf{k}}||\partial_{\mathbf{k}_y}u^\alpha_{\mathbf{k}}\rangle - \langle\partial_{\mathbf{k}_y}u^\alpha_{\mathbf{k}}||\partial_{\mathbf{k}_x}u^\alpha_{\mathbf{k}}\rangle$$

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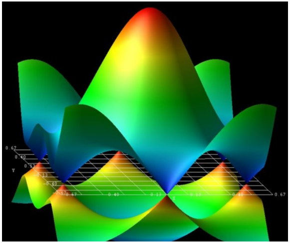
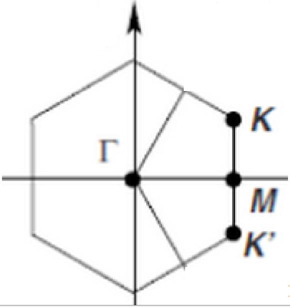
$\mathcal{T}$-Symmetric Honeycomb Band Insulators

From considerations of graphene, a tight-binding honeycomb lattice model of fermions:

- A spinless fermion has protected Dirac points
  - with $\mathcal{I}$ and $\mathcal{T}$ symmetry
  - NO featureless insulators at filling 1 on the honeycomb lattice with $\mathcal{T}$
- Breaking $\mathcal{T}$ leads to non-zero Chern number - $\mathbb{Z}$ invariant, QAHE
- Spinful fermions with spin-orbit couplings have two bands, with Chern numbers ± 1.
- $\mathbb{Z}_2$ topological invariant





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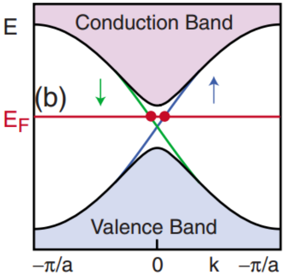

Helical Edge [2]

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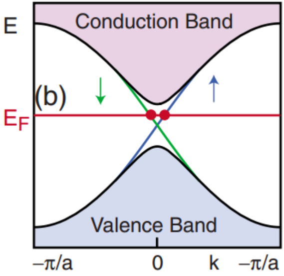

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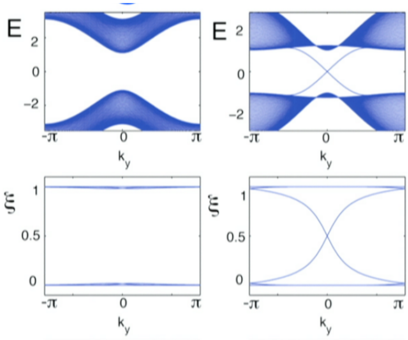
Free Fermion Edge Classification

By partitioning the wavefunction, we can glimpse the edge



Top: Physical spectrum with boundary. Bottom: 'Single particle entanglement spectrum'

- $G_{ij} = \langle c_i^\dagger c_j \rangle$
- G_{ij}^L is G restricted to left half of cylinder
- Spectrum of G^L shown.
- 'Gapless entanglement mode' protected by $\mathcal{T}$
- Bulk wavefunction E.S. shown to capture edge physics
- Bulk wavefunction shown to be distinct from atomic insulator

Free Fermion Edge Classification

Results for free fermions without lattice symmetries:

IQHE

p+ip wave SC

polyacetylene

3He B

TMTSF

Z2 topological insulator

AZ\ d	0	1	2	3	4	5	6	7	8	9
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	$\cdots$
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\cdots$
AI	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	$\cdots$
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\cdots$
D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\cdots$
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\cdots$
AII	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	$\cdots$
CII	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\cdots$
C	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\cdots$
CI	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	$\cdots$

QSHE

d+id wave SC

Free-fermion classification (ten-fold way) for $\mathcal{T}, \mathcal{C}$

[5] (Ryu et al., 2009)

Motivating Questions

Existence

Fix a lattice Λ, symmetry group G, and integer filling number m
Do there exist any featureless insulators at all?

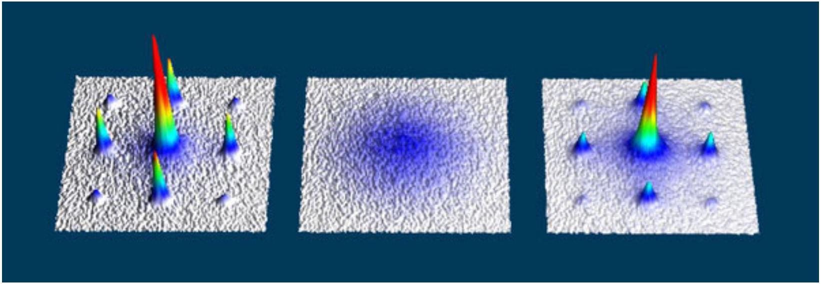
- Find **obstruction** to existence
- or **construct** a reference featureless insulator

Characterization

Given a quantum wavefunction, is it a featureless insulator? Is it distinguishable from atomic insulator in the presence of a symmetry group G? What is G?

- Show non-trivial protected physical or entanglement edge modes
- Find a topological invariant that distinguishes it

Bosonic Mott Insulators



Mott insulator with cold atoms in optical lattice[3]

Bose-Hubbard model

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

[3](Greiner et al., 2002)

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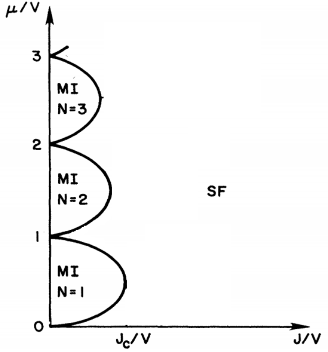
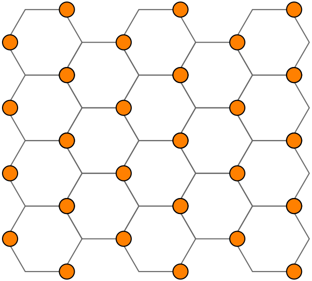


- Form an atomic insulator with N bosons to minimize $-\mu N + VN(N-1)/2$
- Gap to particle/hole excitations
- Bosons free to hop will instantly condense into superfluid with any J
- Number conserving - so no superfluid phase coherence

[4] (Fisher et al., 1989)

Honeycomb Bosonic Mott Insulators

Does there exist a featureless bosonic insulator with filling m=1 on the honeycomb?



Breaks point group symmetry D_6 to D_3

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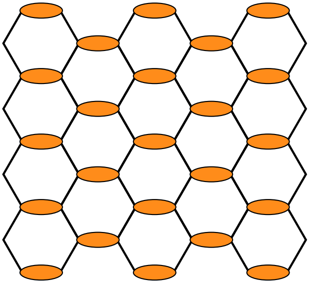

Breaks rotational symmetry

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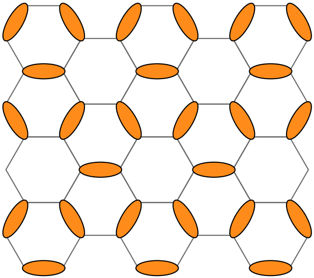


Breaks translationally symmetry, unit cell is 3 times larger

Can we use ‘band bosons‘?

Band fermions have atomic insulator picture using Wannier functions.

$$W_R^\alpha(x) = \int_{B.Z.} d\mathbf{k} e^{-iR\cdot\mathbf{k}} \psi_{\mathbf{k}}^\alpha(x)$$

$$d_R^{\alpha\dagger} = \sum_x W_R^\alpha(x) c_x^\dagger$$

$$|\psi\rangle = \prod_R d_R^{\alpha\dagger} |\mathbf{0}\rangle$$

Wannier functions are not unique and often don’t respect lattice symmetries depending on choice of phase for original basis functions.

But the resulting 'Slater determinant' wavefunction is symmetric regardless.

Can we use ‘band bosons‘?

‘Band bosons’ a.k.a. Boson Permanent

A boson permanent wavefunction created from filling an orbital ϕ_{R+x} for each unit cell R with a boson

Analogous to the Slater determinant for fermions except:

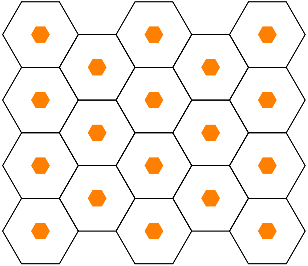
- $|\psi\rangle$ respects lattice symmetries only if ϕ does
- H needs repulsive interactions to stop Bose condensation
  - e.g. H_{BH} with
$$d_R^\dagger = \sum_i \phi_i b_i^\dagger$$
- Orbitals will need to be localized and orthogonal for H_{BH} to be a parent Hamiltonian

Honeycomb Mott Insulators

Proposed Wavefunction

Key insight[3]: 'Center of charge' must lie at symmetric point

$$|\psi\rangle = \prod_{\hexagon} \left(\sum_{i \in \hexagon} b_i^\dagger \right) |\mathbf{0}\rangle$$



[3](Kimchi et al., 2012)

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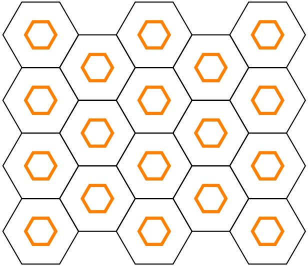

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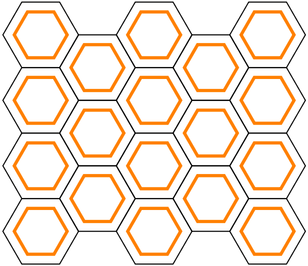

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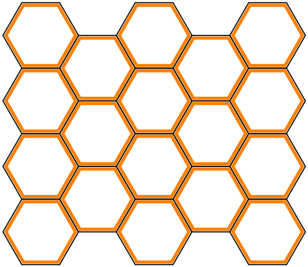
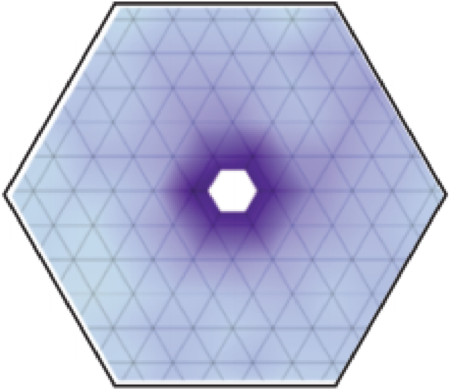


Overlapping orbitals NOT orthogonal

Goals for Honeycomb Mott Insulator

- Build a tensor network representation for doing computations
- Verify that no spontaneous symmetry breaking occurs



Exponentially decaying rotationally symmetric correlations computed using Monte Carlo sampling, (Kimchi et al., 2012)

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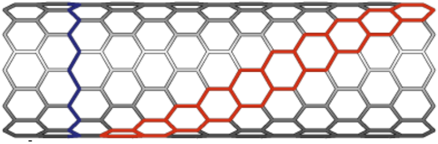

- Rule out topological order
- Compute entanglement spectrum to check for nontrivial entanglement
- Understand the role of symmetries in protecting entanglement in interacting quasi-1D and 2D theories
- Find distinguishing topological invariant and/or physical signatures
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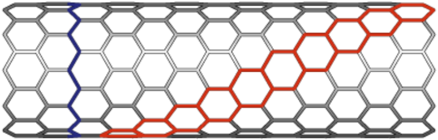

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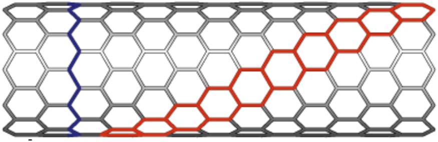

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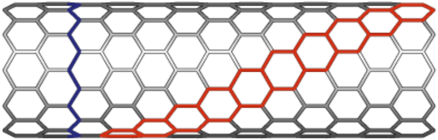

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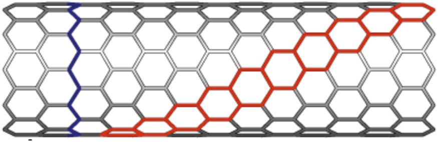

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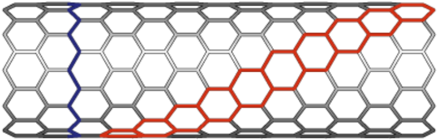

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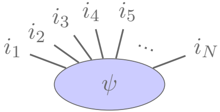
Entanglement

What is entanglement?

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

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



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

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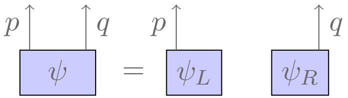

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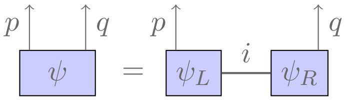
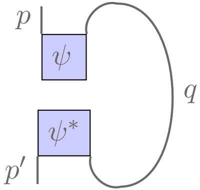


Calculate reduced density matrices

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

Diagonalize

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



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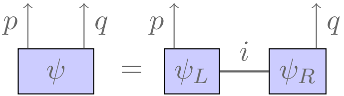
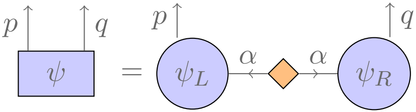


Diagonalize and form the Schmidt decomposition

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



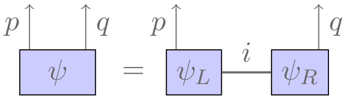
Quantitative measures of entanglement - rank

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

What is entanglement?

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

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



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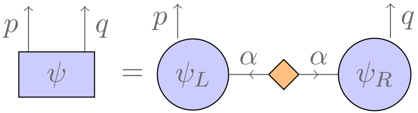


Quantitative measures of entanglement - entropy

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

Entanglement Entropy Area Law

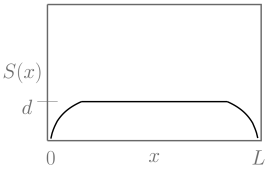
Ground states of gapped quantum Hamiltonians satisfy an area law:

$$S_V \lesssim d \cdot (\partial V) - \gamma$$

γ is universal and detects presence of topological order

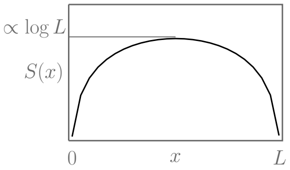
In 1D:

$S(x) \lesssim d$



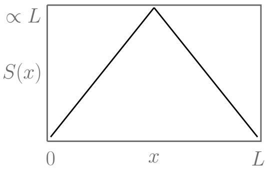
Gapped ground state

$S(x) \lesssim c \log x$



Gapless ground state

$S(x) \propto x$



Generic State

Symmetry Protected Topological Phases

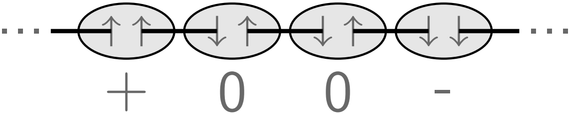
Entanglement measures the obstruction from writing a single wavefunction as an atomic insulator. Protected entanglement is entanglement that can't be removed by adiabatic changes in the Hamiltonian.

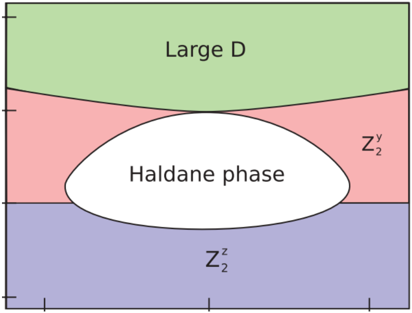
SPT phase

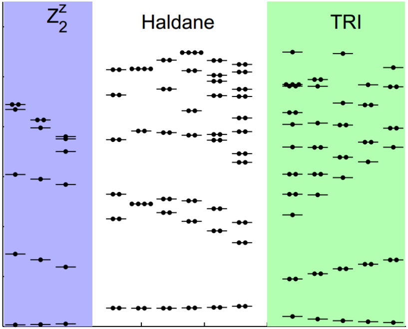
A phase of matter that cannot be connected adiabatically to an atomic insulator, using G-symmetric Hamiltonians, is called a *symmetry protected topological* or SPT phase.

- No symmetry group needed, then topological ordered - not SPT.
- Featureless but feature featured edges.
  - Physical or entanglement edge, when cut respects G
  - Look for these patterns in entanglement spectra!

Haldane Phase of Spin-1 Chain

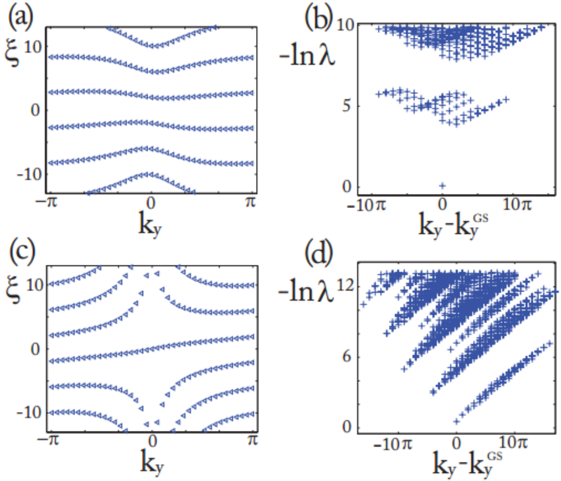






Haldane phase distinguished by exact double degeneracy in entire entanglement spectrum.
Plotted using $E_\alpha = -\log \rho_\alpha$ or $\rho = e^{-H}$

2D SPT Example: Chern Insulator

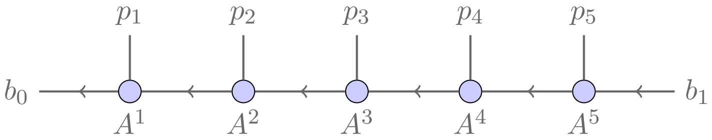


- Start with 'single particle entanglement spectra' of restricted correlation matrix C_{ij}
- Transform the eigenvalues using $\log \frac{C}{1-C}$
- Fill up to 'zero'
- Result: Entanglement spectra

Tensor Networks

What is a Matrix Product State?

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

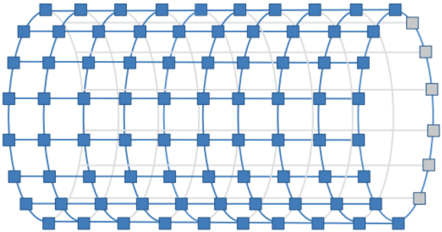


$$|\psi^{b_0 b_1}\rangle = \sum_{p_1 \ldots p_5} (b_0| \, A_1^{p_1} \ldots A_5^{p_5} \, |b_1) \, |p_1 \ldots p_5\rangle$$

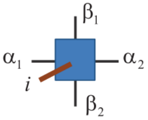
Each coefficient of the w.f. computed via a product of matrices
With a fixed bond dimension d, you have $d^2 * p * L$ parameters

Tensor Network States

- MPS and the generalization to PEPS automatically satisfy area law.
- Entanglement rank and entropy bounded by total bond dimension across any cut.
- Can view PEPS on cylinder as a MPS.

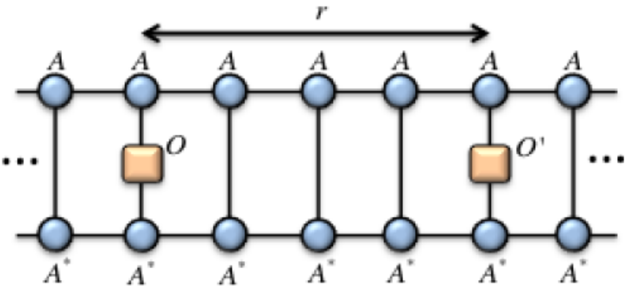


Translationally symmetric PEPS on a cylinder



Close-up of site-tensor in PEPS

Computing Correlation Functions in MPS/PEPS



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

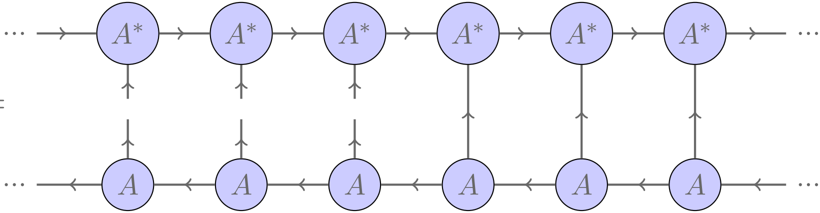
$$\lim_{r\to\infty} \langle O_i O'_{i+r} \rangle = (v_L | \mathbb{E}_O | v_R)\,(v_L | \mathbb{E}_{O'} | v_R)$$

$$\langle O_i O'_{i+r} \rangle \approx const. \times \lambda_2^r$$

Computing Entanglement in MPS/PEPS

To compute the spectrum of the reduced density matrix

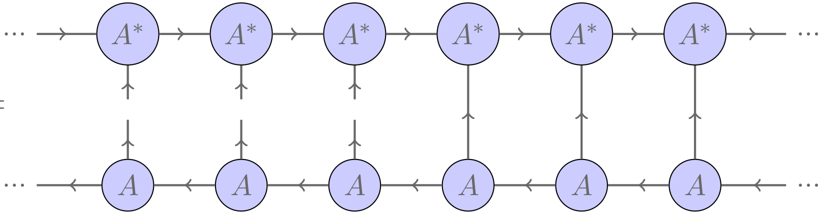
$\rho =$



Computing Entanglement in MPS/PEPS

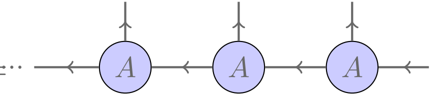
To compute the spectrum of the reduced density matrix

$\rho =$



A valid simplified case is when the contraction

$\mathcal{U} =$

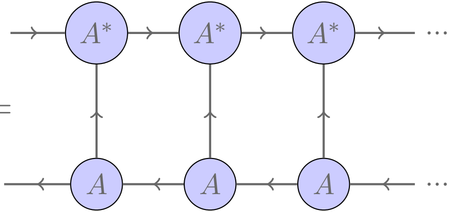


is isometric. We can always get into this canonical form.

Computing Entanglement in MPS/PEPS

To compute the spectrum of the reduced density matrix

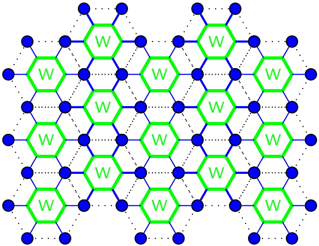
$\widetilde{\rho} =$



- $\rho = \mathcal{U} \cdot \widetilde{\rho} \cdot \mathcal{U}^\dagger$
- $\widetilde{\rho}$ is isometric to real ρ - same spectrum, many less 0s.

PEPS Construction of Honeycomb F.B.I.

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

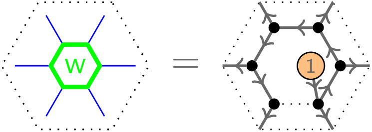


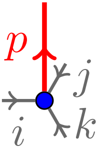
Virtual W-state on each plaquette used to synchronize the creation operators in the sum $\sum_{i \in \hexagon} b_i^\dagger$

$$|W) = |000001) + |000010) + |000100) + |001000) + |010000) + |100000)$$

PEPS Construction of Honeycomb F.B.I.

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



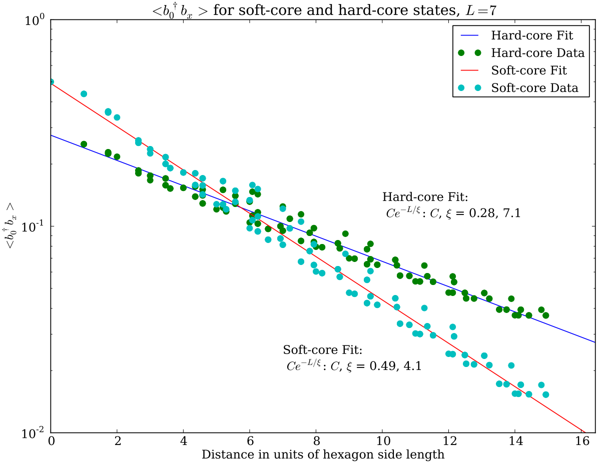


$$|W) = |100...) + ...$$

- W-State can be factored and put on hexagon sites
- Each black directed string has either charge 0 or 1
- Charge conserved

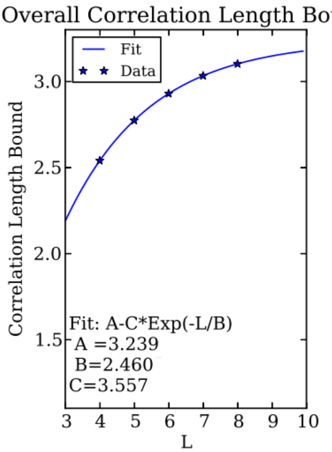
- 'Projects' the three virtual qubits coming into each vertex on to a state in physical Hilbert space
- Physical state is either $|0\rangle, |1\rangle, |2\rangle, |3\rangle$
- Charge conserved

Correlations in Honeycomb F.B.Is



The correlation function $< b_x b_0^\dagger >$ shown on a log-scale F.B.I. and hard-core projected version.

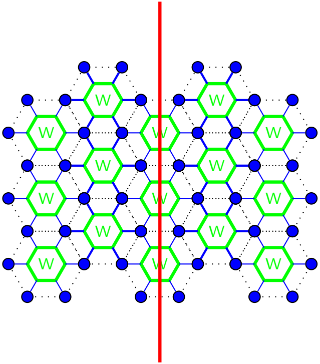
Correlations in Honeycomb F.B.Is



Evidence for energy gap - exponentially decaying correlations in thermodynamic limit

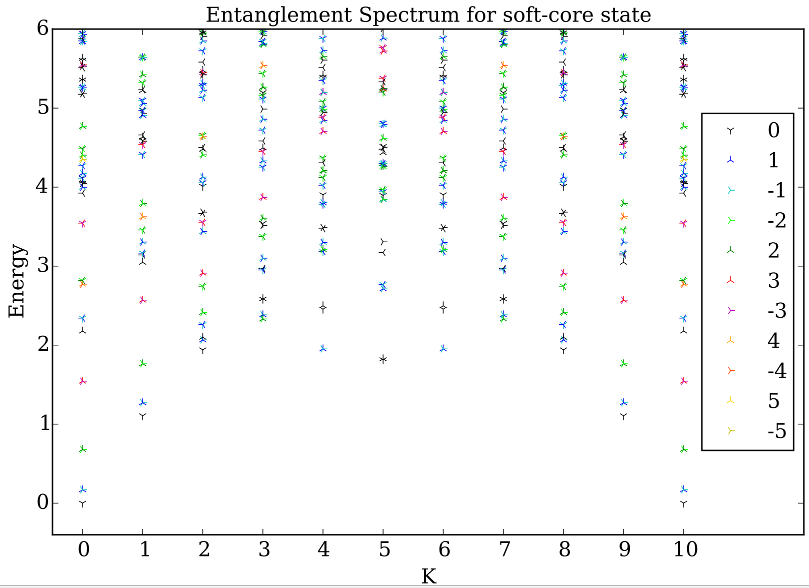
Entanglement Edge of Honeycomb Insulators

Zig-zag Edge Entanglement Cut

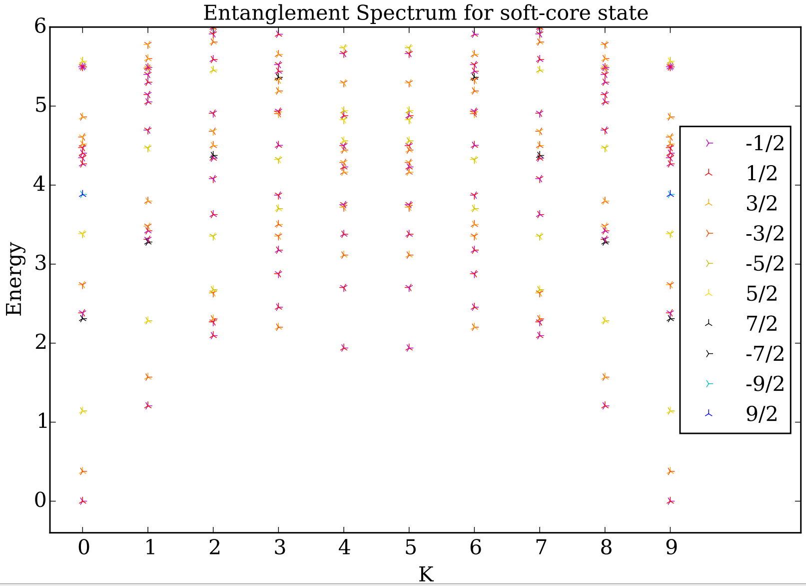


- Cylinder, Circumference L
- Cut crosses L W-strings
- $\widetilde{\rho} = \exp -\widetilde{H}$ is a density matrix on L spin 1/2s

Entanglement Spectra

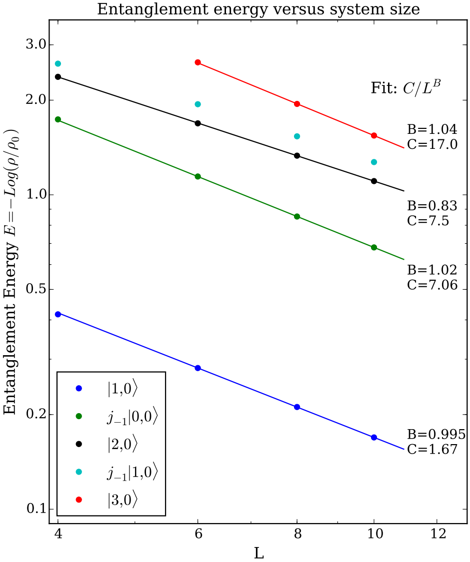


Entanglement Spectra



Finite Size Analysis of Spectra

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



Finite Size Analysis of Spectra

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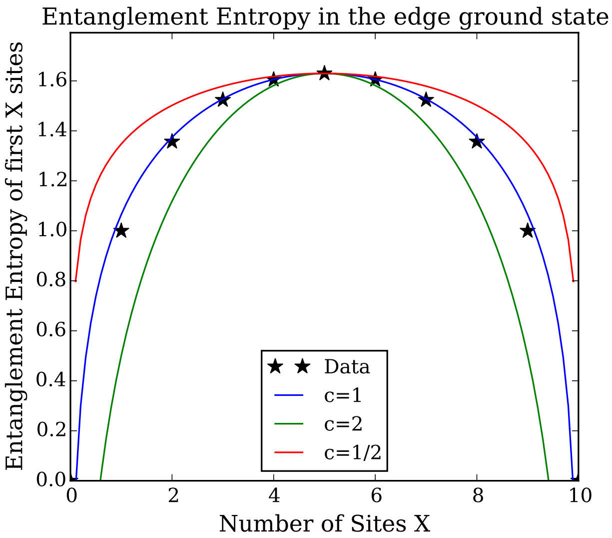
- Topological entanglement entropy is 0

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

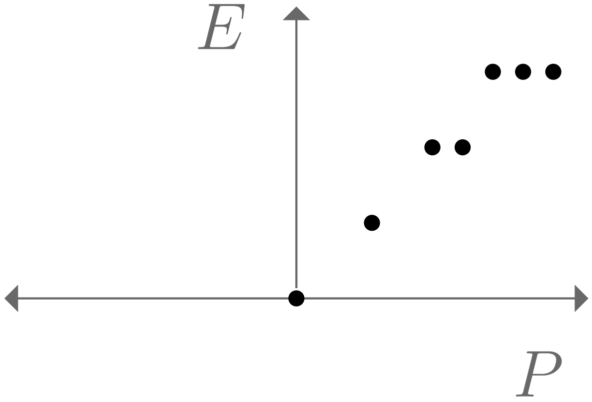
$$\phi \equiv \phi + 2\pi R$$

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

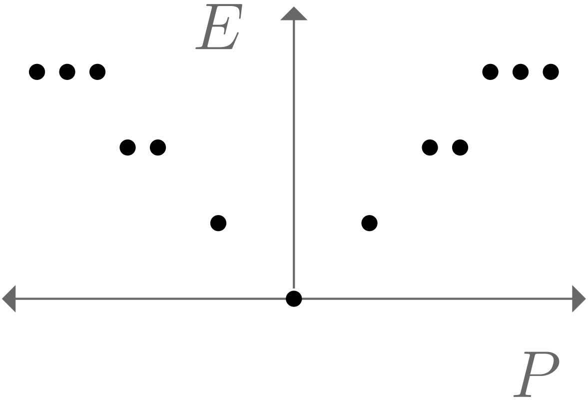
$$\phi(x) \equiv \phi(x+L).$$

Canonically quantize!

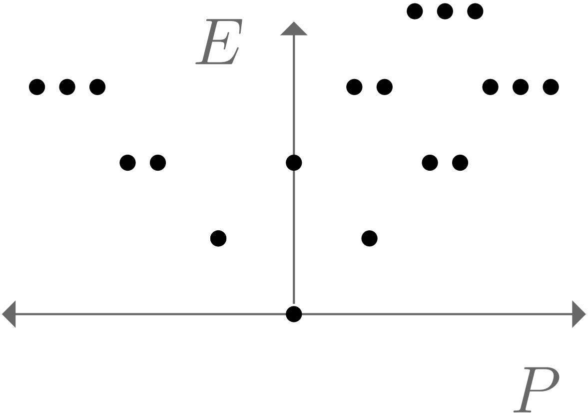
Conformal Tower



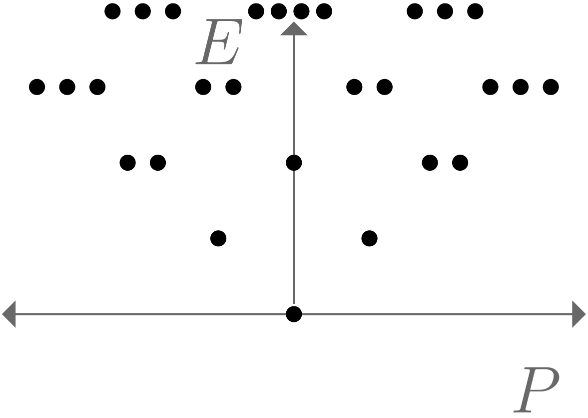
Conformal Tower



Conformal Tower



Conformal Tower



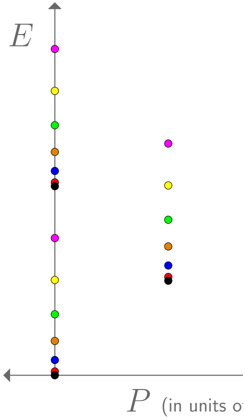
Level identification in CFT spectra

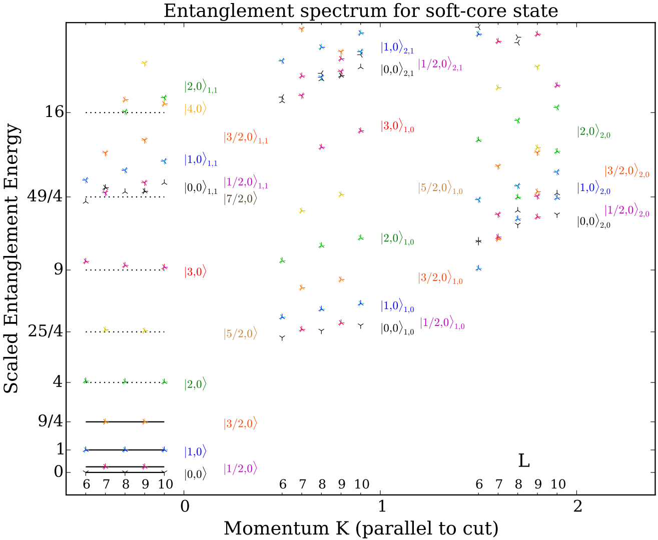
$\mathbf{P} = \frac{2\pi}{L}(\mathbf{L_0} - \mathbf{\bar{L}_0})$	$\frac{2\pi}{L}(em + n - \bar{n})$
$\widetilde{\mathbf{P}}$	$(em + n - \bar{n})$
$\mathbf{H} = \frac{2\pi}{L}(\mathbf{L_0} + \mathbf{\bar{L}_0})$	$\frac{2\pi}{L}(\frac{\kappa e^2}{2} + \frac{m^2}{2\kappa} + \frac{n+\bar{n}}{2})$
$\widetilde{\mathbf{H}}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

Eigenvalues of states $|e, m\rangle_{n,\bar{n}}$.

The rescaled Hamiltonian $\widetilde{\mathbf{H}}$ has eigenvalues that depend on only one free-parameter, $\kappa = 1/(4\pi g R^2)$.

Level identification in CFT spectra





Goals for Honeycomb Mott Insulator

Completed

- Build a tensor network representation for doing computations
- Verify that no spontaneous symmetry breaking occurs
- Rule out topological order
- Compute entanglement spectrum to check for nontrivial entanglement

Not Yet

- Understand the role of symmetries in protecting entanglement in interacting quasi-1D and 2D theories
- Find distinguishing topological invariant and/or physical signatures
- Find a parent Hamiltonian

Open questions and speculation

- Parent Hamiltonian - Construct or obstruction?
- Symmetry group/groups that protect edge?
- Correspondence between bulk perturbations and edge perturbations?
- Nearby phase transitions?
- Is the edge 'anomalous'?
- We can put lots of known SPTs in tensor networks. What should we do next?
- Can we represent transfer matrix as a MPO for efficient contraction?
- Tensor Network RG?

Resources

Alexandradinata, A., Hughes, T. L., and Andrei Bernevig, B. (2011). Trace index and spectral flow in the entanglement spectrum.

Fisher, Weichman, Grinstein, and Fisher (1989). Boson localization and the superfluid-insulator transition. *Physical review. B, Condensed matter*, 40(1):546–570.

Greiner, M., Mandel, O., Esslinger, T., H̀ansch, T. W., and Bloch, I. (2002). Quantum phase transition from a superfluid to a mott insulator in a gas of ultracold atoms. *Nature*, 415(6867):39–44.

Hasan, M. Z. and Kane, C. L. (2010). *Colloquium*: Topological insulators. *Reviews of modern physics*, 82(4):3045–3067.

Kimchi, I., Parameswaran, S. A., Turner, A. M., Wang, F., and Vishwanath, A. (2012). Featureless and non-fractionalized mott insulators on the honeycomb lattice at 1/2 site filling.

Ryu, S., Schnyder, A., Furusaki, A., and Ludwig, A. (2009). Topological insulators and superconductors: ten-fold way and dimensional hierarchy.

Questions?

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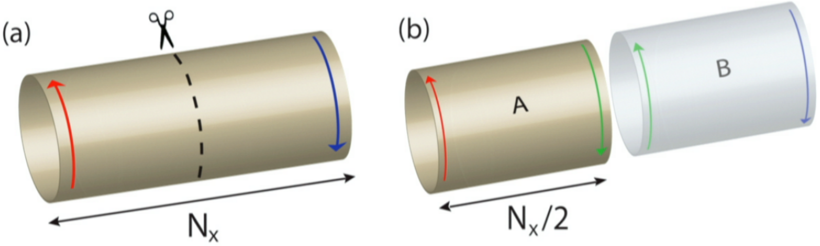
Bonus slides

Bonus slides

Bulk Entanglement and Edges

Bulk ground state contains information about edge physics

- Imagine cutting IQH state in half, forming edge states $|k\rangle_{L,R}$
- Adiabatically tune the coupling back to normal value
- System can lower its energy by coupling the currents
- Entangled eigenstate $\sum |k\rangle_L \otimes |-k\rangle_R$
- Atomic insulator wavefunctions factor trivially - no entanglement.

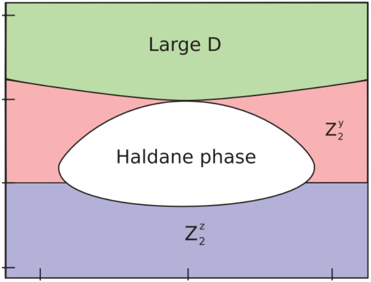


[3] (Alexandradinata et al., 2011)

MPS Example: AKLT State

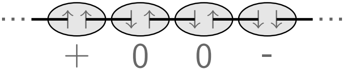
Haldane Phase for Spin-1 chains $(j = 1, m = 0)$

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

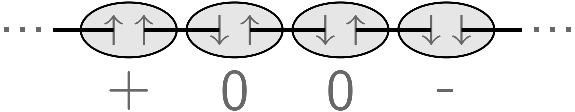


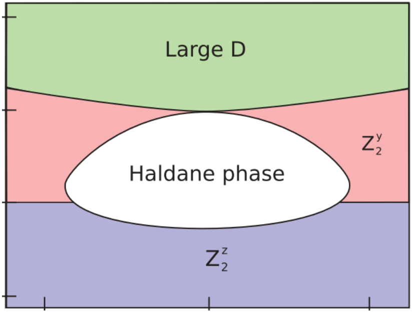
Two distinct featureless insulators:

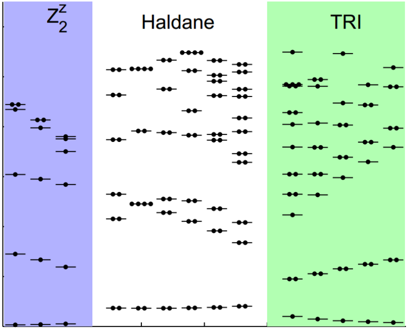
- Large-D phase
  - Contains product state wavefunction $|\psi\rangle = |000...\rangle$
- Haldane phase
  - Contains AKLT wavefunction $|\psi\rangle = \Sigma| + 00 - 0 + ...\rangle$



1D SPT Example: AKLT State







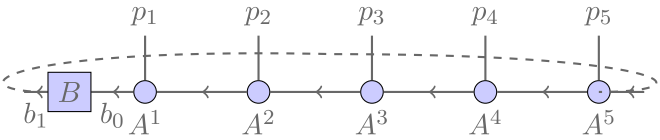
Haldane phase distinguished by exact double degeneracy in entire entanglement spectrum.

1D SPT Example: AKLT State

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

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

Technical Slide: Threading Flux in a MPS

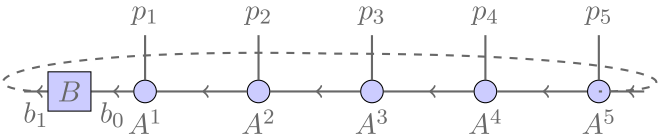


$$|\psi\rangle = \sum_{p_1 \ldots p_5} Tr(BA_1^{p_1} \ldots A_5^{p_5})|p_1 \ldots p_5\rangle$$

Flux threading = twist in boundary conditions Applications of flux threading: Proof of LSM Theorem and extensions Detecting 2D SPT order on a cylinder

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' $V_g V_h = \exp i\omega(g,h) V_{gh}$.

Symmetry Protected Entanglement in 1D

Touch on inversion symmetry?

- 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.)

Properties of Featureless MPS

Make this more brief, move details to end Boil down to we can determine the symmetry properties Show pictures of what it looks like for symmetry to act on the edge of the chain, say what it means for schmidt states

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.