FRG2011, Harvard, May 19, 2011

Frustration-free Ground States of Quantum Spin Systems[1]

Bruno Nachtergaele
(UC Davis)

based on joint work with

Sven Bachmann, Spyridon Michalakis, Robert Sims,
and Reinhard Werner

[1]Based on work supported by the U.S. National Science Foundation under grants # DMS-0757581, DMS-0757424, and DMS-1009502. Work carried out in part during a stay at the Institut Mittag-Leffler, Djursholm, Sweden (Fall 2010) and the Erwin Schrödinger Institute, Vienna, Austria (Spring 2011).

Outline

- Quantum spin models with gapped ground states; examples
- Algebraic approach to models with “frustration-free” ground states; examples
- What is a gapped ground state phase?
- Automorphic equivalence within a gapped phase

Quantum spin models with gapped ground states

By quantum spin system we mean quantum systems of the following type:

- (finite) collection of quantum systems labeled by $x \in \Lambda$, each with a finite-dimensional Hilbert space of states $\mathcal{H}_x$. E.g., a spin of magnitude $S = 1/2, 1, 3/2, \ldots$ would have $\mathcal{H}_x = \mathbb{C}^2, \mathbb{C}^3, \mathbb{C}^4, \ldots$.
- The Hilbert space describing the total system is the tensor product

$$\mathcal{H}_\Lambda = \bigotimes_{x \in \Lambda} \mathcal{H}_x.$$

with a tensor product basis $|\{\alpha_x\}\rangle = \bigotimes_{x\in\Lambda} |\alpha_x\rangle$

We will primarily work in the Heisenberg picture so observables, rather than state vectors, play the lead role:

- The algebra of observables of the composite system is

$$\mathcal{A}_\Lambda = \bigotimes_{x\in\Lambda} \mathcal{B}(\mathcal{H}_x) = \mathcal{B}(\mathcal{H}_\Lambda).$$

  If $X \subset \Lambda$, we have $\mathcal{A}_X \subset \mathcal{A}_\Lambda$, by identifying $A \in \mathcal{A}_X$ with $A \otimes \mathbb{1}_{\Lambda\setminus X} \in \mathcal{A}_\Lambda$. Then

$$\mathcal{A} = \bigcup_X \mathcal{A}_X$$

Our most common choice for Λ will be finite subsets of $\mathbb{Z}^\nu$, e.g., hypercubes of the form $[1, L]^\nu$ or $[-N, N]^\nu$.

Interactions, Dynamics, Ground States

The Hamiltonian $H_\Lambda = H_\Lambda^* \in \mathcal{A}_\Lambda$ is defined in terms of an interaction Φ: for any finite set X, $\Phi(X) = \Phi(X)^* \in \mathcal{A}_X$, and

$$H_\Lambda = \sum_{X \subset \Lambda} \Phi(X)$$

For finite-range interactions, $\Phi(X) = 0$ if $\mathrm{diam}\, X \geq R$.
Heisenberg Dynamics: $A(t) = \tau_t^\Lambda(A)$ is defined by

$$\tau_t^\Lambda(A) = e^{itH_\Lambda} A e^{-itH_\Lambda}$$

For finite systems, ground states are simply eigenvectors of H_Λ belonging to its smallest eigenvalue.

States as expectation functionals, density matrices

States $\psi \in \mathcal{H}_\Lambda$, $\|\psi\| = 1$, allow us to calculate expectation values of observables $A \in \mathcal{A}_\Lambda = \mathcal{B}(\mathcal{H}_\Lambda)$:

$$\omega(A) = \langle \psi, A\psi \rangle : \text{linear, positive, normalized} \tag{1}$$

If $X \subset \Lambda$, $\omega|_{\mathcal{A}_X}$ is also linear, positive, and normalized. We also call such functionals ω states.

If $\dim \mathcal{H}_X < \infty$, and ω is a state on $\mathcal{A}_X$, then there exists a unique density matrix ρ (positive, $\text{Tr}\rho = 1$) such that

$$\omega(A) = \text{Tr}\rho A.$$

(1) is the special case of pure states ($\rho = |\psi\rangle\langle\psi|$).

Examples

1.The spin-1/2 Heisenberg model E.g., $\Lambda \subset \mathbb{Z}^\nu$, $\mathcal{H}_x = \mathbb{C}^2$; the Heisenberg Hamiltonian:

$$H_\Lambda = \sum_{x \in \Lambda} B S_x^3 + \sum_{|x-y|=1} J_{xy} \mathbf{S}_x \cdot \mathbf{S}_y$$

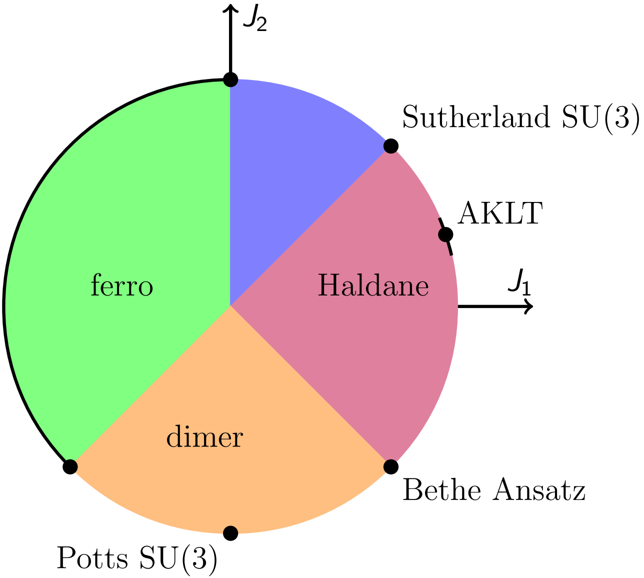
The ground states of the ferromagnetic Heisenberg model ($B = 0, J_{xy} < 0$), are easily found to be the states of maximal spin.

The low-lying excitations are spin waves and in the limit of an infinite lattice the excitation spectrum is gapless.

2. The AKLT model (Affleck-Kennedy-Lieb-Tasaki, 1987).
$\Lambda \subset \mathbb{Z}$, $\mathcal{H}_x = \mathbb{C}^3$;

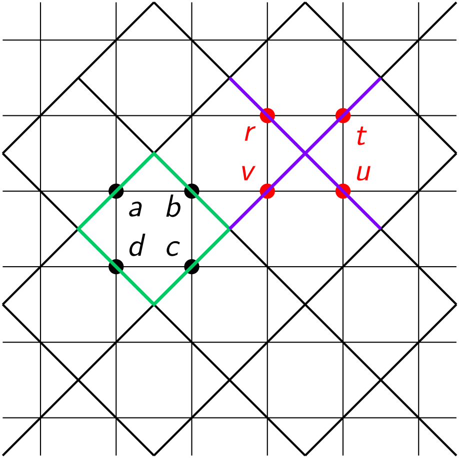
$$H_{[1,L]} = \sum_{x=1}^{L} \left(\frac{1}{3}\mathbb{1} + \frac{1}{2}\mathbf{S}_x \cdot \mathbf{S}_{x+1} + \frac{1}{6}(\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2 \right) = \sum_{x=1}^{L} P^{(2)}_{x,x+1}$$

In the limit of the infinite chain, the ground state is unique, has a finite correlation length, and there is a non-vanishing gap in the spectrum above the ground state (Haldane phase). Exact ground state is "frustration free" (Valence Bond Solid state (VBS), Matrix Product State (MPS), Finitely Correlated State (FCS)).



$$H = \sum_x J_1 \mathbf{S}_x \cdot \mathbf{S}_{x+1} + J_2 (\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2$$

3. Toric Code model (Kitaev, 2003, 2006). $\Lambda \subset \mathbb{Z}^2$, $\mathcal{H}_x = \mathbb{C}^2$.



$$H = -\sum_p h_p - \sum_s h_s$$

$$h_p = \sigma_a^3 \sigma_b^3 \sigma_c^3 \sigma_d^3$$

$$h_s = \sigma_r^1 \sigma_t^1 \sigma_u^1 \sigma_v^1$$

On a surface of genus g, the model has 4^g frustration free ground states.

0-energy / frustration-free ground states

An algebraic approach to existence of frustration free ground states of spin chains. $x \in \mathbb{Z}$, $\mathcal{H}_x = \mathbb{C}^d$.

$$H_{[1,L]} = \sum_{x=1}^{L-1} h_{x,x+1},$$

with $h_{x,x+1} = h \in \mathcal{A}_{[1,2]}$, $h \geq 0$, $\ker h = \mathcal{G} \subset \mathbb{C}^d \otimes \mathbb{C}^d$

$$\ker H_{[1,L]} = \bigcap_{x=1}^{L-1} \underbrace{\mathbb{C}^d \otimes \cdots \mathbb{C}^d}_{x-1} \otimes \mathcal{G} \otimes \underbrace{\mathbb{C}^d \otimes \cdots \mathbb{C}^d}_{L-x-1}$$

For which $\mathcal{G}$ is $\ker H_{[1,L]} \neq \{0\}$ for all $L \geq 2$?

A few easy cases:

- If $h_{1,2}h_{2,3} = h_{2,3}h_{1,2}$, all terms in the Hamiltonian are simultaneously diagonalizable. Just need to check whether there are eigenvectors with common eigenvalue 0. Example: Toric Code model.
- If, for some $0 \neq \phi \in \mathbb{C}^d$, $\phi \otimes \phi \in \mathcal{G}$, then $\underbrace{\phi \otimes \phi \cdots \otimes \phi}_{L} \in \ker H_{[1,L]}$ for all L.
  Example: ferromagnetic Heisenberg model.
- If $\mathcal{G}$ is the antisymmetric subspace of $\mathbb{C}^d \otimes \mathbb{C}^d$, $\ker H_{[1,L]} = \{0\}$ for $L > d$. Example: the Heisenberg antiferromagnetic chain does *not* have a frustration free ground state.

Non-trivial solutions (joint work with RF Werner).

Observation: the existence of 0-eigenvectors of $H_{[1,L]}$ for all finite L is equivalent to the existence of pure states ω of the half-infinite chain with zero expectation of all $h_{x,x+1}, x \geq 1$. Let's call such ω pure zero-energy states.

Each term in the Hamiltonian is minimized individually. Hence the term frustration-free ground states.

Zero-energy states are certainly ground states ($h_{x,x+1} \geq 0$); it is a separate question whether they are all the ground states.

Theorem (Bratteli, Jørgensen, Kishimoto, Werner (2000), N-Werner (2010))

A pure state ω is a zero-energy state iff it has an representation in operator product form: there is a Hilbert space $\mathcal{K}$, bounded linear operators $V_1, \ldots, V_d$ on $\mathcal{K}$, and $\Omega \in \mathcal{K}$, such that
$\mathrm{span}\{V_{\alpha_1} \cdots V_{\alpha_n}\Omega \mid n \geq 0, 1 \leq \alpha_1, \ldots, \alpha_n \leq d\} = \mathcal{K}$

$$\omega(|\alpha_1, \ldots, \alpha_n\rangle\langle\beta_1, \ldots, \beta_n|) = \langle\Omega, V_{\alpha_1}^* \cdots V_{\alpha_n}^* V_{\beta_n} \cdots V_{\beta_1}\Omega\rangle$$

and $\mathbb{1}$ is the only eigenvector with eigenvalue 1 of the operator

$$\widehat{\mathbb{E}} \in \mathcal{B}(\mathcal{B}(\mathcal{K})) : \quad \widehat{\mathbb{E}}(X) = \sum_{\alpha=1}^{d} V_\alpha^* X V_\alpha$$

and for all $\psi \perp \mathcal{G}$, $\psi = \sum_{\alpha,\beta} \psi_{\alpha\beta}|\alpha, \beta\rangle$, we have the relation

$$\sum \overline{\psi_{\alpha\beta}} V_\alpha V_\beta = 0.$$

This theorem is based on a theorem by Bratteli, Jørgensen, Kishimoto, and Werner (J. Operator Theory 2000), about pure states on the Cuntz algebra $\mathcal{O}_d$. States on half-infinite spin chains can be canonically lifted to states on $\mathcal{O}_d$.

In a number of cases we can describe the solutions of these relations.
As a warm-up, consider

$$\mathcal{G} = \{\text{antisymmetric subspace}\} = \{\psi \in \mathbb{C}^d \otimes \mathbb{C}^d \mid F\psi = -\psi\},$$

where F is the operator interchanging the two tensor factors.
E.g., in the case $d = 2$, this is the spin-$1/2$ Heisenberg antiferromagnetic chain.
For a zero-energy state to exist, we would need to have a Hilbert space $\mathcal{K}$ with $V_1, \ldots V_d \in \mathcal{B}(\mathcal{K})$ such that

$$V_\alpha V_\beta = -V_\beta V_\alpha \implies V_\alpha^2 = 0 \implies V_{\alpha_1} \cdots V_{\alpha_r} = 0 \quad (r > d).$$

Hence $\widehat{\mathbb{E}}^r = 0$, for $r > d$, which contradicts $\widehat{\mathbb{E}}(\mathbb{1}) = \mathbb{1}$.

So, there are no solutions with $\mathcal{G} =$ the antisymmetric subspace. This suggests that we next consider

$$\mathcal{G} = \{\text{antisymmetric vectors}\} \oplus \mathbb{C}\psi,$$

where ψ is a symmetric vector. A spanning set for $\mathcal{G}^\perp$ is given by the set $|\alpha, \beta\rangle + |\beta, \alpha\rangle - 2\langle\psi|\alpha, \beta\rangle\psi, \quad 1 \leq \alpha \leq \beta \leq d$. We refer to this situation as "antisymmetric plus one".

The AKLT model is an example: $\mathcal{G} =$ the spin 0 and spin 1 vectors in the tensor product of two spin 1's:

$$D^{(1)} \otimes D^{(1)} \cong D^{(0)} \oplus D^{(1)} \oplus D^{(2)}$$

The irreps are alternatingly symmetric and anti-symmetric, with the maximal spin always symmetric. In this case, $D^{(1)}$ is the antisymmetric subspace and the singlet vector is symmetric:

$$\psi = |1, -1\rangle - |0, 0\rangle + |-1, 1\rangle$$

In general, a standard result of linear algebra (Takagi) gives the existence of an orthonormal basis $\{|\alpha\rangle\}_{1\le\alpha\le d}$ and coefficients $c_1 \ge c_2 \ge \cdots \ge c_d \ge 0$ such that $\psi = \sum_\alpha c_\alpha |\alpha,\alpha\rangle$.
Using this basis, we obtain the following relations for the operators V_α:

$$V_\alpha V_\beta + V_\beta V_\alpha = 2c_\alpha \delta_{\alpha\beta} X, \quad X = \left(\sum_\gamma c_\gamma V_\gamma^2\right).$$

These relations also imply $\widehat{\mathbb{E}}(X) = X$, and therefore $X = x\mathbb{1}$ for a scalar x. Some further algebra gives

$$V_\alpha = v_\alpha Z_\alpha, \text{ with } v_\alpha = \sqrt{\frac{c_\alpha}{\sum_\alpha c_\alpha}}, \quad \text{if } c_\alpha > 0,$$

and $V_\alpha = 0$ is $c_\alpha = 0$. Let r be the number on non-vanishing c_α.

Then, the Z_α, $\alpha = 1, \dots r$, satisfy the standard relations of a Clifford algebra:

$$Z_\alpha Z_\beta + Z_\beta Z_\alpha = 2\delta_{\alpha\beta}\mathbb{1}, \quad 1 \leq \alpha, \beta \leq r.$$

Since the V_α generate $\mathcal{K}$, we must have an irreducible representation of $\mathcal{C}_r$, the Clifford algebra with r generators.
The irreps of the Clifford algebras are well-known:
If r is even, $\mathcal{C}_r \cong M_{2^{r/2}}$, the square matrix algebra of dimension 2^r, which has only one irrep.
If r is odd, $\mathcal{C}_r$ has a non-trivial central element:
$Z_0 = Z_1 \cdots Z_r$, and a decomposition
$\mathcal{C}_r = (\mathbb{1} + Z_0)\mathcal{C}_r \oplus (\mathbb{1} - Z_0)\mathcal{C}_r \cong M_{2^{(r-1)/2}} \oplus M_{2^{(r-1)/2}}$, leading to two, equivalent, irreps.

Conclusion: in the case $\mathcal{G} = \{\text{antisymmetric vectors}\} \oplus \mathbb{C}\psi$, there are always zero-energy states and the operators V_α are (can be chosen to be) finite-dimensional (MPS).
E.g., with the choice

$$\psi = \frac{1}{\sqrt{d}} \sum_{\alpha=1}^{d} |\alpha\alpha\rangle,$$

we find a class of spin chains with $SO(d)$ symmetry recently analyzed in the literature (Tu & Zhang, PRB **78**, 094404 (2008)). These models can be regarded as a new generalization of the AKLT model ($d = 3$). For odd d these models have a unique ground state, for even d they are dimerized (translation invariance is broken to period 2).

The behavior of correlations in these ground states are essentially determined by the spectrum of $\widehat{\mathbb{E}}$.

Lemma

Let $A = \{\alpha_1, \ldots, \alpha_k\} \subset \{1, \ldots, r\}$, *and* $V_A = V_{\alpha_1} \cdots V_{\alpha_k}$.
Then $\widehat{\mathbb{E}}(V_A) = \lambda_A V_A$ *with*

$$\lambda_A = (-1)^{|A|} \Big(1 - 2x \sum_{\alpha \in A} c_\alpha\Big), \tag{2}$$

where $x = \left(\sum_{\alpha=1}^{r} c_\alpha\right)^{-1}$.

Note the eigenvector $V_0 = V_1 \cdots V_r$ with eigenvalue -1 if r is even. This is why dimerization occurs in the $SO(d)$ models with odd d

$\mathcal{G}$ = the symmetric subspace

In this case $\mathcal{G}^{\perp}$ = the anti-symmetric subspace, a basis for which is given $|\alpha, \beta\rangle - |\beta, \alpha\rangle, \alpha < \beta$. The algebraic conditions on the V_α are then

$$V_\alpha V_\beta = V_\beta V_\alpha, \text{ for all } \alpha, \beta$$

Hence, $\widehat{\mathbb{E}}(V_\alpha) = V_\alpha$, and we conclude $V_\alpha = \phi_\alpha \mathbb{1}$, for all α. Therefore, $\mathcal{K}$ is one-dimensional, and the state must be a homogeneous product state. This is the situation of the spin-1/2 Heisenberg ferromagnetic chain.

A small twist with a big effect

Consider $d = 2$ and let $q \in (0, 1)$ and define $\mathcal{G} = \mathrm{span}\{|1,1\rangle, |2,2\rangle, |1,2\rangle + q|2,1\rangle\}$.
Then, $\mathcal{G}^\perp = \mathbb{C}\psi$ with $\psi = q|1,2\rangle - |2,1\rangle$. Hence, the commutation relation of the generators is

$$V_2 V_1 = q V_1 V_2.$$

The corresponding nearest neighbor interaction is $|\psi\rangle\langle\psi|$, which is equivalent to the spin-1/2 XXZ chain with twisted boundary conditions:

$$\begin{aligned} H_{[a,b]} &= -\sum_{x=a}^{b-1} \left(\sigma_x^1 \sigma_{x+1}^1 + \sigma_x^2 \sigma_{x+1}^2 + \frac{2}{q+q^{-1}} (\sigma_x^3 \sigma_{x+1}^3 - \frac{1}{4} \mathbb{1}) \right) \\ &\quad + \frac{1}{2} \frac{1-q^2}{1+q^2} (\sigma_b^3 - \sigma_a^3). \end{aligned}$$

To make a long story short, there is an infinite family of solutions, which can all be derived from a "mother solution" on an infinite-dimensional Hilbert space $\mathcal{K}$, given as follows. Let $\mathcal{K}$ be the separable Hilbert space with orthogonal basis $\{\phi_n\}_{n\geq 0}$ and inner product $\langle \phi_n, \phi_m \rangle = \lambda_n \delta_{n,m}$, with

$$\lambda_0 = 1, \quad \lambda_n = \prod_{m=1}^{n} \frac{q^{2m}}{1 - q^{2m+2}}, n \geq 1.$$

Two bounded operators V_1 and V_2 can then be defined on $\mathcal{K}$ by

$$\begin{aligned} V_1 \phi_n &= q^n \phi_n \\ V_2 \phi_0 &= 0, \quad V_2 \phi_n = q^{n-1} \phi_{n-1}, \text{ for } n \geq 1 \end{aligned}$$

It is then easily seen that $V_1^* = V_1$ and

$$V_2^* \phi_n = \frac{\lambda_n}{\lambda_{n+1}} q^n \phi_{n+1} = (q^{-n} - q^{n+2}) \phi_{n+1}.$$

It is noteworthy that V_1 and V_2 are a concrete representation of $SU_q(2)$, regarded as a compact matrix quantum group in the sense of Woronowicz. This means bounded operators satisfying the relations

$$V_1^* V_1 + V_2^* V_2 = \mathbb{1}, \quad V_2 V_1 = q V_1 V_2$$
$$V_1 V_1^* = V_1^* V_1, \quad V_2 V_1^* = q V_1^* V_2, \quad V_2 V_2^* + q^2 V_1 V_1^* = \mathbb{1}$$

The first two relations in are the normalization condition and the commutation relation we require. The next two relations are trivially satisfied since V_1 is self-adjoint. The last relation is one we did not require but it is straightforward to verify using the definitions of V_1 and V_2.

This model has an infinite family of kink ground states.

What is a quantum ground state phase?

The frustration free models we have discussed, are just a few example of a much larger class. It is believed that any type of gapped ground state is adequately described by a frustration free model (Fannes, N, Werner, 1992 & ff, Schuch, Perez-Garcia, Cirac, arXiv:1010.3732).

But how should one define "type"?

When are two gapped ground states representing the same "gapped phase"?

Clearly, a ground state in which a $\mathbb{Z}_2$ symmetry is spontaneously broken is not the same as one in which the broken symmetry is $\mathbb{Z}_3$. If, e.g., two models have a unique gapped ground state, should they automatically be considered as belonging to the same phase?

Definition of "gapped phase"

(joint work with Bachmann, Michalakis, and Sims)
In arXiv:1004.3835, *Local unitary transformation, long-range quantum entanglement, wave function renormalization, and topological order*, Xie Chen, Zheng-Cheng Gu, Xiao-Gang Wen (Phys. Rev. B 82, 155138 (2010)), give the following definition (paraphrasing):

Two states Ψ_0 and Ψ_1 are in the same phase if there is a family of Hamiltonians $H(s)$, $0 \leq s \leq 1$, such that $H(s)$ has a non-vanishing gap above the ground state for all s and Ψ_i is the ground state of $H(i)$, $i = 0, 1$.

(see also arXiv:1008.3745 by the same authors)

One element of consensus: there can be no phase transition without closing of the gap above the ground state.

In the same paper we also find the statement/conjecture:

Two gapped states Ψ_0 and Ψ_1 belong to the same phase if and only if they are related by a local unitary evolution

We (BMNS) recently obtained a result that allows precise version of this statement using Lieb-Robinson bounds (Lieb & Robinson 1972, N & Sims 2006, Hastings & Koma, 2006) and "quasi-adiabatic continuation" (Hastings 2004, Hastings & Wen, 2005).

Let $\Phi_s, 0, \leq s \leq 1$, be a differentiable family of short-range interactions for a quantum spin system on Γ.
Let $\Lambda_n \subset \Gamma$ be an increasing and absorbing sequence of finite volumes, satisfying suitable regularity conditions.
Suppose there exists $\gamma > 0$, such that the spectral gap above the ground state (or a low-energy interval) of

$$H_{\Lambda_n}(s) = \sum_{X \subset \Lambda_n} \Phi_s(X)$$

$\geq \gamma$.
Let $\mathcal{S}(s)$ be the set of thermodynamic (weak) limits of ground states of $H_{\Lambda_n}(s)$.

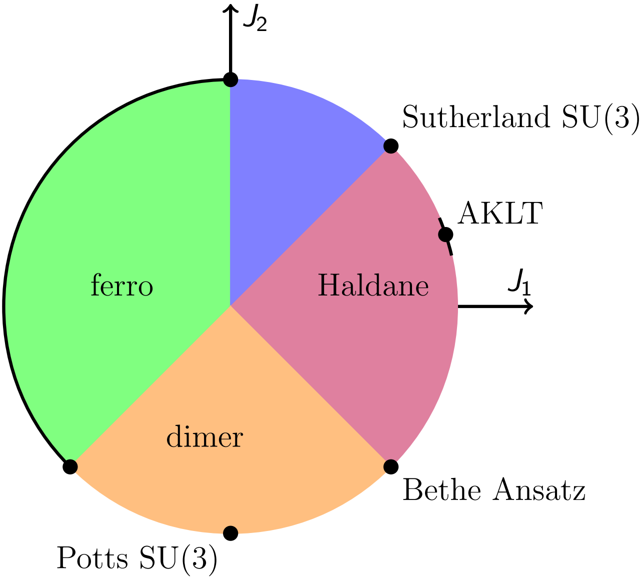
Theorem (Bachmann, Michalakis, N, Sims)

Under the assumptions of above, there exist automorphisms α_s of the quasi-local algebra

$$\mathcal{A} = \overline{\bigcup_{\Lambda_n \subset \Gamma} \mathcal{A}_{\Lambda_n}}$$

such that $\mathcal{S}(s) = \mathcal{S}(0) \circ \alpha_s$, for $s \in [0,1]$.
The automorphisms α_s can be constructed as the thermodynamic limit of the s-dependent "time" evolution for an interaction $\Omega(X,s)$, which decays almost exponentially.

(See Bob Sims's talk for more details.)



$$H = \sum_x J_1 \mathbf{S}_x \cdot \mathbf{S}_{x+1} + J_2 (\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2$$

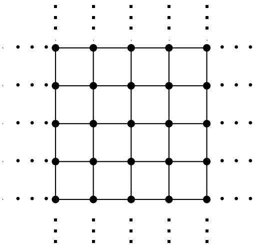
What about the so-called topological phases?

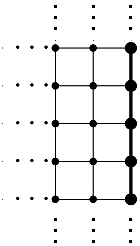
The space of ground states of Kitaev's Toric Code model, and other models introduced depends crucially on the topology of the lattice on which it is defined. Such models are better described as a family of models defined by interactions Φ^α on lattices Γ^α, which are identical in the bulk, i.e., away from boundaries and on a scale too short to detect the topology, but which represent the different topologies of interest. To express the equivalence of members of one "topological phase", we then need to consider paths of interactions Φ_s^α, $0 \leq s \leq 1$, for all α.

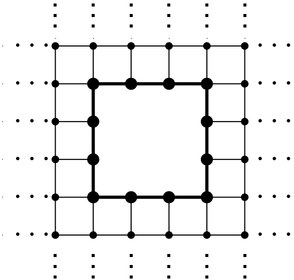
So, in one dimension, we need to consider at least two types of infinite systems:

The bold site denotes a boundary. Other “large” but finite systems can be pieced together from these two. So a classification of one-dimensional gapped phase would involve a bulk phase together with a boundary phase (substituting for a non-trivial topological phase in higher dimensions).
With Bachmann we are working out explicit examples. E.g., for the AKLT model, we can construct a gapped path of frustration free models showing that AKLT is connected to
- a bulk phase that is a unique product state
- a boundary phase with a two-dimensional space of edge states: the product state and an exponentially localized excitation of it.

The simplest examples in two dimensions are:







etc.