Yerevan, September 4, 2012

On the classification of gapped ground state phases[1]

Bruno Nachtergaele
(UC Davis)

based on joint work with

Sven Bachmann, Spyridon Michalakis, Robert Sims

[1]Based on work supported by the U.S. National Science Foundation under grants # DMS-0757581, DMS-0757424, and DMS-1009502.

Outline

- Quantum spin systems. Thermodynamic limits.
- Automorphic equivalence within a gapped phase
- Product Vacua with Boundary States (PVBS)
- The AKLT model and quantum phase transitions
- Concluding remarks

Notations

- 'Lattice' Γ, usually infinite set such as $\mathbb{Z}^\nu$;
- finite-dimensional Hilbert space of states $\mathcal{H}_x$ for each $x \in \Gamma$;
- For each finite $\Lambda \subset \Gamma$,

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

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

- The algebra of observables of the system in the finite volume Λ:

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

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

$$\mathcal{A} = \overline{\bigcup_\Lambda \mathcal{A}_\Lambda}^{\|\cdot\|}$$

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 (sometimes several 'small eigenvalues').

Thermodynamic Limits

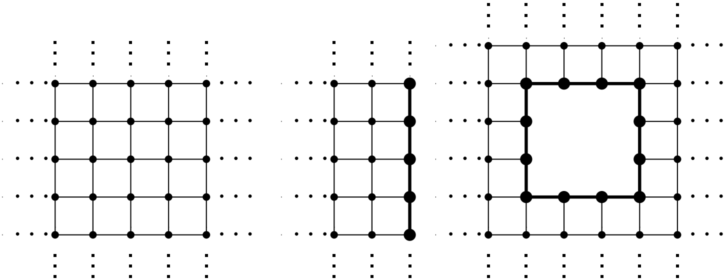
Behavior at the boundaries and dependence on topology of the lattice when classifying the qualitative behavior of the ground states of a given model is important (cfr. Graf's talk).

Therefore, consider them as a family of models defined by interactions Φ^g on lattices Γ^g, which are identical in the bulk, i.e., away from boundaries and on a scale too short to detect the topology, which is labeled by $g \in G$ (e.g., genus g). In order to classify not only the bulk phases, but also boundary and topological phases, one needs to consider a variety of thermodynamic limits leading to infinite systems The different topologies of interest are represented by $\{\Gamma^g\}_{g\in G}$.

Take thermodynamic limit along $\Lambda_n \uparrow \Gamma^g$.

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

The bold site denotes a boundary. A classification of one-dimensional models with gapped ground states The simplest examples in two dimensions are:



etc.

What is a quantum ground state phase?

By phase, here we mean a set of models with qualitatively similar behavior. E.g., a g.s. ψ_0 of one model could evolve to a g.s. ψ_1 of another model in the same phase by some physically acceptable dynamics and in finite time. For finite systems such a dynamics is provided by a quasi-local unitary U_Λ.

When we take the thermodynamic limit

$$\lim_{\Lambda\uparrow\Gamma} U_\Lambda^* A U_\Lambda = \alpha(A), \quad A \in \mathcal{A}_{\Lambda_0},$$

this dynamics converges to an automorphism of the algebra of observables. The quasi-locality property is expressed as follows: there exists a rapidly decreasing function $F(d)$, and balls, B_d, of radius d, and $A_d \in \mathcal{A}_{B_d}$ such that

$$\|\alpha(A) - A_d\| \leq F(d)$$

Suppose Φ_0^g and Φ_1^g are two interactions for two models on lattices Γ^g, $g \in G$.

Each has its set $\mathcal{S}_i^g$, $i = 0, 1$, of ground states in the thermodynamic limit. I.e., for $\omega \in \mathcal{S}_0^g$, there exists

$$\psi_{\Lambda_n} \text{ g.s. of } H_{\Lambda_n} = \sum_{X \subset \Lambda_n} \Phi_0^g(X),$$

for a sequence of $\Lambda_n \in \Gamma^g$ such that

$$\omega(A) = \lim_{n \to \infty} \langle \psi_{\Lambda_n}, A\psi_{\Lambda_n} \rangle.$$

If the two models are in the same phase, for all $g \in G$, we have a suitably local automorphism α^g such that

$$\mathcal{S}_1^g = \mathcal{S}_0^g \circ \alpha^g$$

This means that for any state $\omega_1 \in \mathcal{S}_1^g$, there exists a state $\omega_0 \in \mathcal{S}_0^g$, such that the expectation value of any observable A in ω_1 can be obtained by computing the expectation of $\alpha^g(A)$ in ω_0:

$$\omega_1(A) = \omega_0(\alpha^g(A)).$$

The quasi-local character of α^g guarantees that the support of $\alpha^g(A)$ need not be much larger than the support of A in order to have this identity with small error.

In examples α^g is constructed as the dynamics for a fictitious short-range interaction (Bachmann, Michalakis, N, Sims, CMP 2012).

E.g., if Φ_0 and Φ_1 are interactions for there exists a smooth interpolation $\Phi_s, s \in [0,1]$, and such that there is a spectral gap $\geq \gamma > 0$ above the ground state for all $s \in [0,1]$, then there are automorphisms α_s such that $\mathcal{S}(s) = \mathcal{S}(0) \circ \alpha_s$.

α_s can be constructed as the thermodynamic limit of the s-dependent "time" evolution for an interaction $\Omega(X,s)$.

Concretely, the action of α_s on observables is given by

$$\alpha_s(A) = \lim_{n \to \infty} V_n^*(s) A V_n(s)$$

where $V_n(s)$ solves a Schrödinger equation:

$$\frac{d}{ds} V_n(s) = i D_n(s) V_n(s), \quad V_n(0) = \mathbb{1},$$

with $D_n(s) = \sum_{X \subset \Lambda_n} \Omega(X,s)$.

Product Vacua with Boundary States (PVBS)

(joint work with Sven Bachmann, PRB 2012)
We consider a quantum spin chain with $n+1$ states at each site that we interpret as n distinguishable particles labeled $i = 1, \dots, n$, and an empty state denoted by 0.
The Hamiltonian for a chain of L spins is given by

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

where each $h_{x,x+1}$ is a sum of 'hopping' terms (each normalized to be an orthogonal projection) and projections that penalize particles of the same type to be nearest neighbors.

$$h = \sum_{i=1}^{n} |\hat{\phi}_i\rangle\langle\hat{\phi}_i| + \sum_{1\le i\le j\le n}^{n} |\hat{\phi}_{ij}\rangle\langle\hat{\phi}_{ij}|,$$

The $\phi_{ij} \in \mathbb{C}^{n+1} \otimes \mathbb{C}^{n+1}$ are given by

$$\phi_i = |i,0\rangle - e^{-\theta_{i0}}\lambda_i^{-1}|0,i\rangle\,, \phi_{ij} = |i,j\rangle - e^{-\theta_{ij}}\lambda_i^{-1}\lambda_j|j,i\rangle\,, \phi_{ii} = |i,i\rangle$$

for $i = 1, \dots, n$ and $i \neq j = 1, \dots, n$.
The parameters satisfy: $\theta_{ij} \in \mathbb{R}$, $\theta_{ij} = -\theta_{ji}$, and $\lambda_i > 0$, for $0 \le i, j \le n$, and $\lambda_0 = 1$.

There exist $n+1$ $2^n \times 2^n$ matrices $v_0, v_1, \ldots, v_n$, satisfying the following commutation relations:

$$\begin{aligned} v_i v_j &= e^{i\theta_{ij}} \lambda_i \lambda_j^{-1} v_j v_i, \quad i \neq j \qquad (2) \\ v_i^2 &= 0, \quad i \neq 0 \qquad (3) \end{aligned}$$

Then, for B an arbitrary $2^n \times 2^n$ matrix,

$$\psi(B) = \sum_{i_1,\ldots,i_L=0}^{n} \mathrm{Tr}(B v_{i_L} \cdots v_{i_1}) |i_1, \ldots, i_L\rangle \qquad (4)$$

is a ground state of the model (MPS vector). In fact, they are all the ground states. E.g., one can pick B such that

$$\psi(B) = \sum_{x=1}^{L} \left(e^{i\theta_{i0}} \lambda_i\right)^x |0, \ldots, 0, i, 0, \ldots, 0\rangle$$

If we add the assumption that $\lambda_i \neq 1$, for $i = 1, \ldots, n$, we will have n_L particles having $\lambda_i < 1$ that bind to the left edge, and $n_R = n - n_L$ particles with $\lambda_i > 1$, which, when present, bind to the right edge. The bulk ground state is the vacuum state

$$\Omega = |0, \ldots, 0\rangle \, .$$

All other ground states differ from Ω only near the edges. We can prove that the energy of the first excited state is bounded below by a positive constant, independently of the length of the chain. As at most one particle of each type can bind to the edge, any second particle of that type must be in a scattering state. The dispersion relation is

$$\epsilon_i(k) = 1 - \frac{2\lambda_i}{1+\lambda_i^2} \cos(k + \theta_{i0}) \, .$$

We conjecture that the *exact* gap of the infinite chain is

$$\gamma = \min \left\{ \frac{(1-\lambda_i)^2}{1+\lambda_i^2} \,\middle|\, i = 1, \ldots, n \right\} \, .$$

Automorphic equivalence of PVBS models

Two PVBS models belong to the same equivalence class if and only if they have the same n_L and n_R.

(i) Since equivalent phases are related by an automorphism, a unique bulk ground state can only be mapped to another unique bulk state. Similarly, the ground state space dimensions of the half-infinite chains, 2^{n_L} and 2^{n_R}, are also preserved by an automorphism. Hence, if two PVBS models belong to the same phase, they must have equal n_L and n_R.

(ii) Conversely, if two PVBS models have the same values of n_L and n_R but each with their own sets of parameters $\{\lambda_i(s) \mid 1 \leq i \leq n_L + n_R\}$ and $\{\theta_{ij}(s) \mid 1 \leq i, j \leq n_L + n_R\}$, for $s = 0, 1$, first, perform a change of basis in spin space such that both sets of PVBS states are expressed in the same spin basis and such that $\lambda_i(s) < 1$ for $1 \leq i \leq n_L$ and $\lambda_i(s) > 1$ for $n_L + 1 \leq i \leq n_L + n_R$, for $s = 0$ and $s = 1$.

Next, deform the parameters by simple linear interpolation:

$$\lambda_i(s) = (1-s)\lambda_i(0) + s\lambda_i(1) \quad (5)$$

$$\theta_{ij}(s) = (1-s)\theta_{ij}(0) + s\theta_{ij}(1) \quad (6)$$

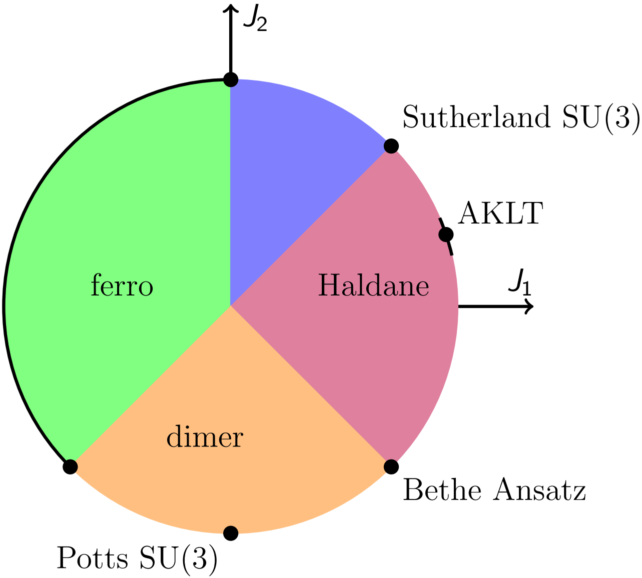
This yields a smooth family of vectors $\phi_{ij}(s)$ and thereby a smooth family of nearest neighbor interactions $h(s)$. The gap remains open because $\lambda_i(s) \neq 1$ for all $i = 1, \ldots, n$ and $s \in [0, 1]$. By our general result this implies the quasi-local automorphic equivalence of the two models.
If one uses the same type of interpolation to connect models with different values of n_L and n_R, the gap necessarily closes along the path and there is a quantum phase transition.

The AKLT model (Affleck-Kennedy-Lieb-Tasaki, 1987)

Antiferromagnetic spin-1 chain: $[1, L] \subset \mathbb{Z}$, $\mathcal{H}_x = \mathbb{C}^3$,

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

The ground state space of $H_{[1,L]}$ is 4-dimensional for all $L \geq 2$. 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)).



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

Theorem (Bachmann-N)

The AKLT model belongs to the same equivalence class as the PVBS models with $n_L = n_R = 1$.

The 4 ground states of the a finite chain are usually described in terms of a spin $1/2$ particle attached to the two ends of the chain. We constructed a smooth gapped path of nearest neighbor interactions connecting the AKLT model with a PBVS model with $n_L = n_R = 1$, i.e., with one particle for each boundary.

and proved that the spectral gap does not close along the path.

Hence, the AKLT model is in the same gapped quantum phase as the PVBS model with $n_L = n_R = 1$.

In particular, the sets of ground states of these models are automorphically equivalent for the finite, half-infinite and infinite chains, where they are isomorphic to a pair of qubits, a single qubit, and a unique pure state, respectively.

In the bulk the unique ground state is equivalent to a translation invariant product state.

Contrast with Kennedy-Tasaki unitary, which reveals the hidden symmetry in the AKLT ground state, but is non-local and maps the AKLT ground state into 4 translation invariant product states. The quasi-locality requirement matters.
In the same way, the integer spin chains with $SO(2J+1)$ symmetry, introduced by Tu, Zhang, and Xiang, Phys. Rev. B 78, 094404 (2008), can be connected by a smooth curve of models with a gap to the PVBS models with $n_L = n_R = J$. (Bachmann-N, arXiv:1112.4097)

Concluding comments

- There is a message in the boundary.
- The PVBS Hamiltonians are just toy models, but we conjecture that a generalization of this class describes a complete classification of gapped ground state phases in one dimension.
- By requiring that a given set of symmetries are preserved along the interpolating path one obtains automorphisms that commute with these symmetries, which leads to a finer classification.
- We are close to a comprehensive picture in one dimension, but in two (and more) dimensions many questions remain open.