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

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based on joint work with

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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 quantum 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 $\operatorname{diam} X \geq R$.
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.

Examples

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

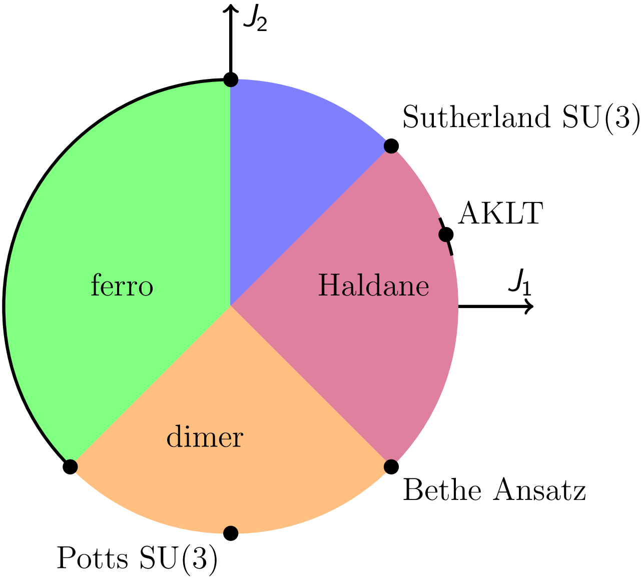
$$H_\Lambda = \sum_{x \in \Lambda} B S_x^3 + \sum_{|x-y|=1} J_{xy} \mathbf{S}_x \cdot \mathbf{S}_y$$

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).
$\Lambda \subset \mathbb{Z}$, $\mathcal{H}_x = \mathbb{C}^3$;

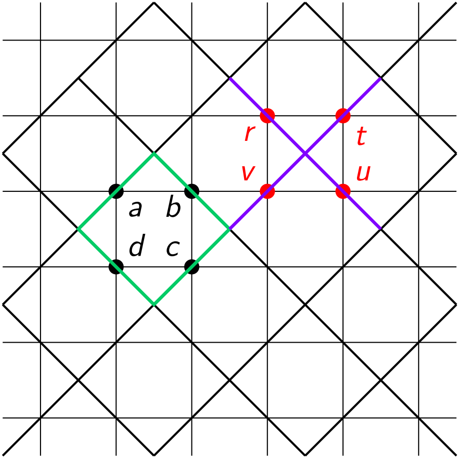
$$H_{[1,L]} = \sum_{x=1}^{L} \left(\frac{1}{3} \mathbb{1} + \frac{1}{2} \mathbf{S}_x \cdot \mathbf{S}_{x+1} + \frac{1}{6} (\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2 \right) = \sum_{x=1}^{L} P^{(2)}_{x,x+1}$$

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). $\Lambda \subset \mathbb{Z}^2$, $\mathcal{H}_x = \mathbb{C}^2$.



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

$$h_p = \sigma^3_a \sigma^3_b \sigma^3_c \sigma^3_d$$

$$h_s = \sigma^1_r \sigma^1_t \sigma^1_u \sigma^1_v$$

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)

Any pure zero-energy state ω 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

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

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 $V_1, \dots V_d \in \mathcal{B}(\mathcal{K})$ 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, $\alpha = 1, \ldots r$, 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 $\widehat{\mathbb{E}}$. Amanda Young worked out a few important cases in an REU project this past summer.

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*

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

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.

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).

But how should one define "type"?

When are two gapped ground states representing the same "gapped 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)

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 recently proved a 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).

Theorem

Let Φ_0 and Φ_1 be two exponentially interactions for a quantum spin system on $\mathbb{Z}^\nu$, and suppose we have an interpolating $\Phi(s)$, such that for all s, $H_{\Lambda_n}(s)$ has a gap $\geq \gamma > 0$ above the ground states for all $s \in [0,1]$ and all Λ_n in a nice sequence of $\Lambda_n \uparrow \mathbb{Z}^\nu$. Let $\mathcal{S}(s)$ be the set of thermodynamic limits of ground states of $H_{\Lambda_n}(s)$.
Then, there exist automorphisms α_s of the quasi-local algebra

$$\mathcal{A} = \overline{\bigcup_{\Lambda \subset \mathbb{Z}^\nu} \mathcal{A}_\Lambda}$$

such that $\mathcal{S}(s) = \mathcal{S}(0) \circ \alpha_s$, for $s \in [0,1]$.

The automorphism α is constructed as the thermodynamic limit of the "time" evolution at $s = 1$ for an interaction $\Omega(X, s)$, which decays almost exponentially.