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The spectral gap.

Existence and Implications

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Outline

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The Spectral Gap – Definition

Let $H = H^*$ on a Hilbert space $\mathcal{H}$ be such that $0 = \inf \operatorname{spec} H$ is an eigenvalue. The corresponding eigenspace, $\ker H$ is then the space of the ground states of H.
E.g., H can be the Hamiltonian of a finite system or it could be the GNS Hamiltonian H_ω of a ground state of a C^*-dynamical system $(\mathcal{A}, \tau)$.

We then have $\operatorname{spec} H \subset [0, \infty)$. Define

$$\gamma = \sup\{\eta > 0 \mid (0, \eta) \cap \operatorname{spec} H = \emptyset\},$$

with the convention that $\gamma = 0$ if the set is empty.
γ is called the spectral gap (above the ground state).
If 0 is a simple eigenvalue, γ is a lower bound for the gap iff

$$\omega(A^*[H, A]) \geq \gamma\omega(A^*A), \ A \in \mathrm{Dom}([H, \cdot]), \omega(A) = 0.$$

The Goldstone Theorem

Consider a quantum spin system (QSS) on a lattice with a translation invariant ground state, and with a dynamics that has a local continuous symmetry. For concreteness, let $\Gamma = \mathbb{Z}^\nu$, $\mathcal{H}_x = \mathbb{C}^d$. Let α_x denote the automorphism of translation by x in $\mathcal{A}_\Gamma$: $\alpha_x(\mathcal{A}_y) = \mathcal{A}_{x+y}$, $x, y \in \Gamma$.
A state ω on $\mathcal{A}_\Gamma$ is translation invariant if $\omega(\alpha_x(A)) = \omega(A)$, for all $x \in \Gamma, A \in \mathcal{A}_\Gamma$.

A local symmetry is described by an automorphism σ of the form

$$\sigma(A) = (\bigotimes_{x \in X} U^*) A (\bigotimes_{x \in X} U), \quad A \in \mathcal{A}_X$$

for a unitary $U \in M_d$.

If $\theta \mapsto U_\theta = e^{i\theta S}$, with $S = S^* \in M_d$, we can define a strongly continuous one-parameter group of automorphisms σ_θ , $\theta \in \mathbb{R}$ or $\theta \in [0, 2\pi]$.
σ_θ is a continuous symmetry and we say that the model has this symmetry if

$$\tau_t \circ \sigma_\theta = \sigma_\theta \circ \tau_t, \quad \theta, t \in \mathbb{R}.$$

A sufficient condition for τ_t to commute with σ_θ, is that $\sigma_\theta(\Phi(X)) = \Phi(X)$, for $X \in \mathcal{P}_0(\Gamma)$, which is equivalent to

$$[\sum_{x \in X} S_x, \Phi(X)] = 0.$$

The Goldstone Theorem for ground states in statistical mechanics (as opposed quantum field theory) is the following.

Theorem (Landau-Perez-Wreszinski, 1981)

Let $\Phi \in \mathcal{B}_F(\mathbb{Z}^\nu)$ such that the corresponding dynamics $\{\tau_t = E^{it\delta}\}_t$ commutes with a continuous symmetry $\{\sigma_\theta\}_\theta$. If ω is a translation invariant ground state for which there exists $\gamma > 0$ such that

$$\omega(A^*\delta(A) \geq \gamma\omega(A^*A), \quad A \in \mathcal{A}_{\rm loc}, \ \textit{s.t.} \ \omega(A) = 0.$$

Then $\omega \circ \sigma_\theta = \omega$, for all θ.

In particular, this theorem implies that if there is a spontaneously broken continuous symmetry, then $\gamma = 0$, i.e., the system is gapless in the representation of any translation invariant symmetry broken ground state (that is unique in its GNS representation).

The Exponential Clustering Theorem

This theorem can be proved for any system (the local Hilbert spaces may be infinite-dimensional) on any Γ (no translation invariance is needed) as long as the interactions are of sufficiently short range.

It is easy to see that for any F-function for Γ, $F_a(r) = e^{-ar}F(r)$ defines an F-function for all $a \geq 0$. It is convenient to use an F_a of this form to express the exponential decay of the interactions.

For a system with interaction $\Phi \in \mathcal{B}_{F_a}(\Gamma)$, with $a > 0$, let $\mathcal{H}$ be the GNS space and $H \geq 0$ be the GNS Hamiltonian of a ground state Ω, $H\Omega = 0$, with a spectral gap $\gamma > 0$. Let P_0 denote the orthogonal projection onto $\ker H$. Local observables are of the form $A \in \pi(\mathcal{A}_X) \subset \mathcal{B}(\mathcal{H})$.

Theorem (N-Sims, Koma-Hastings, 2006)

Let $X, Y \in \mathcal{P}_0(\Gamma), X \cap Y = \emptyset$, $A \in \pi(\mathcal{A}_X)$ *and* $B \in \pi(\mathcal{A}_Y)$ *such that* $P_0 B\Omega = P_0 B^*\Omega = 0$. *Then*

$$|\langle \Omega, A\tau_{ib}(B)\Omega\rangle| \;\leq\; C(A,B,\gamma)\, e^{-\mu d(X,Y)\left(1+\frac{\gamma^2 b^2}{4\mu^2 d(X,Y)^2}\right)}$$

for all non-negative b satisfying $0 \leq b\gamma \leq 2\mu d(X,Y)$, *and with*

$$\mu \;=\; \frac{a\,\gamma}{4\|\Phi\|_a C_a \,+\, \gamma},$$

and

$$\frac{C(A,B,\gamma)}{\|A\|\|B\|} = 1 + \sqrt{\frac{1}{\mu d(X,Y)}} + \frac{2\|F_0\|}{\pi C_a}\, \min\left(|\partial_\Phi X|, |\partial_\Phi Y|\right).$$

$$\partial_\Phi X = \{x \in X \mid \exists Z, x \in Z, Z \cap X^c \neq \emptyset, \Phi(Z) \neq 0\}$$

Note that in the case of a non-degenerate ground state, the condition on B is equivalent to $\langle \Omega, B\Omega \rangle = 0$. In this case, the theorem with $b = 0$ becomes

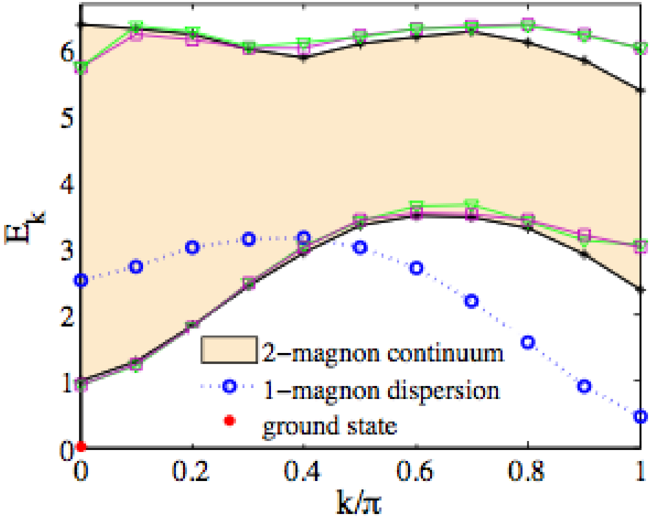
$$|\langle \Omega, AB\Omega \rangle - \langle \Omega, A\Omega \rangle \langle \Omega, B\Omega \rangle| \leq C(A, B, \gamma)\, e^{-\mu d(X,Y)},$$

which is the standard (equal-time) correlation function. Recall that non-degeneracy of the ground state in a given representation does not imply uniqueness of the ground state of the model. There may be other representations.

Quasi-particle Nature of Excited States The current interest in gapped ground state phases is motivated by the potential applications of topologically ordered phases to quantum information processing, in particular the nature of elementary excitations (anyons) in systems with topological order. Structure of ground state is revealed in the structure of excited states.

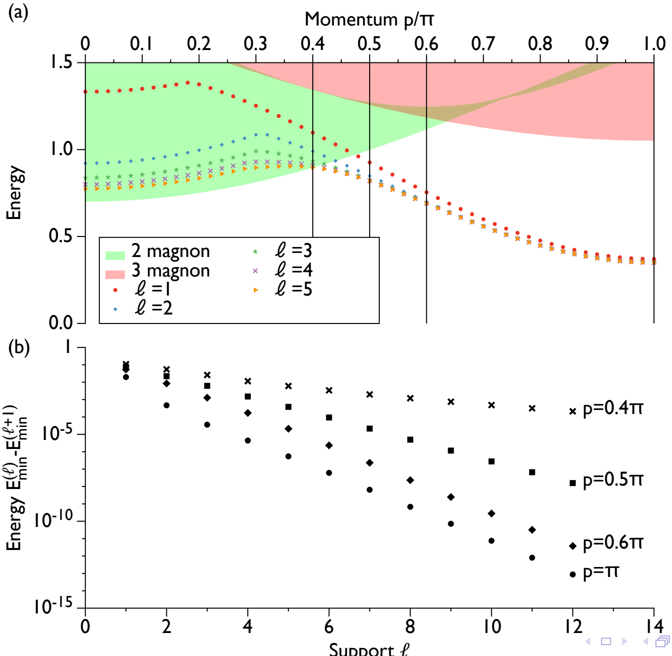
As a first step, we looked at the localized nature of the excitations corresponding to isolated branches in the spectrum ('particles'), of any lattice model with short range interactions.

Such excitations occur, e.g., the spin-1 Heisenberg antiferromagnetic chain.



AF Heisenberg chain spectrum. From: Zheng-Xin Liu, Yi Zhou, Tai-Kai Ng, arXiv:1307.4958

Spectrum of the AKLT chain



Assume that at quasi-momentum p we have a gap $\geq \delta > 0$ between E_p and the higher eigenvalues of the Hamiltonian and the same quasi-momentum, uniformly in the size of the system.

Then, under a technical condition (not satisfied for topological anyons!), the eigenvectors belonging E_p, are of the form

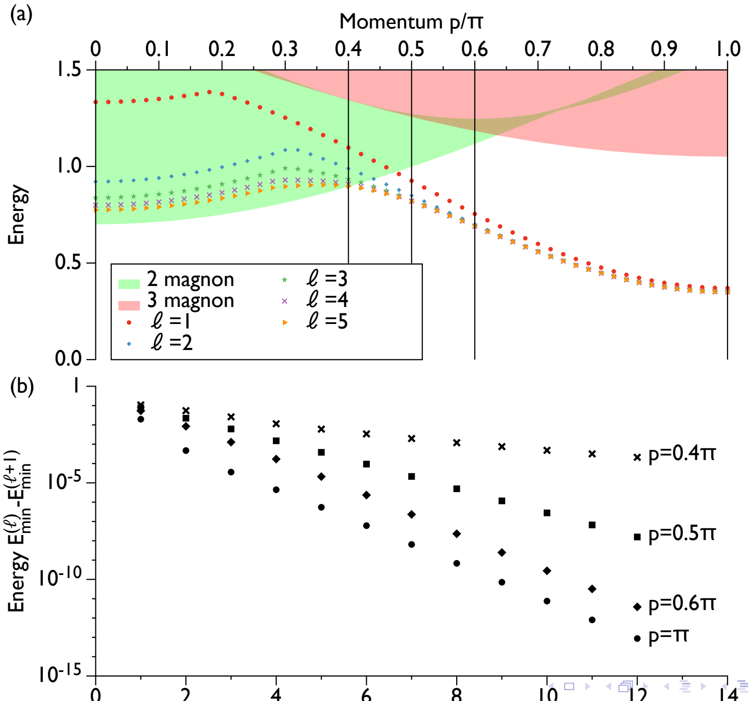
$$\psi_p = \psi(A_p) = \sum_x e^{ipx} T_x(A_p)\Omega$$

where Ω is the ground state, T_x denotes translation by x and A_p is a quasi-local observable. More precisely:

Theorem (Haegeman-M-N-Osborne-Schuch-Verstraete, 2013)

There exists a constants $v > 0$ and $n \geq 1$, such that for $\ell \geq \ell_0$, there exists $A_p^{(\ell)} \in \mathcal{A}_{B_\ell}$ such that

$$|\langle \psi_p, \psi(A_p^{(\ell)})\rangle| \geq 1 - c\ell^n e^{-\delta\ell/v}.$$


(a)
Momentum p/π
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.5
1.0
0.5
0.0
Energy
2 magnon
3 magnon
ℓ =1
ℓ =2
ℓ =3
ℓ =4
ℓ =5
(b)
1
10-5
10-10
10-15
Energy E(ℓ)min-E(ℓ+1)min
p=0.4π
p=0.5π
p=0.6π
p=π
0
2
4
6
8
10
12
14

Given that particle-like excitations exist, it is natural to ask whether there is a scattering theory for them.

Under reasonable assumptions on the shape of the joint spectrum of H and translations, Bachmann-Dybalski-Naaijkens (2014), showed that this can be done in close analogy with standard scattering theory.

Spectral Gap for chains with Matrix Product Ground States – The Martingale Method

How does one prove that quantum spin/qubit model is gapped?

No general method exists, but for frustration-free models there is a method that works particularly well in one dimension. One can also show stability under perturbations around frustration-free models with a gap.

Under a natural condition on the Hamiltonian, the method applies to chains with with a unique matrix product ground state.

Matrix Product States aka Finitely Correlated States

The model defined by Φ is Frustration-Free if for all finite $\Lambda \subset \mathbb{Z}^\nu$

$$\inf \mathrm{spec}\, H_\Lambda = \sum_{X \subset \Lambda} \inf \mathrm{spec}\, \Phi(X).$$

Equivalently, there is a ground state of H_Λ that is simultaneously a ground state of all $\Phi(X)$, for $X \subset H_\Lambda$.

Product structure of frustration-free ground states in $d = 1$

For simlicity, consider FF translation invariant nearest neighbor model. For each $x \in \mathbb{Z}$, $\mathcal{H}_x = \mathbb{C}^d$.

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

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

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

Frustration free means that $\ker H_{[1,L]} \neq \{0\}$ for all $L \geq 2$.

Operator product representation

(Bratteli-Jørgensen-Kishimoto-Werner, 2000; FNW in preparation)

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 $h_{x,x+1}, x \geq 1$.

Any such pure 'zero-energy state' ω has an unique 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

$$\widehat{\mathbb{E}}(X) = \sum_{\alpha=1}^{d} V_\alpha^* X V_\alpha$$

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

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

When $\dim \mathcal{K} < \infty$, the states are referred to as Matrix Product States, aka as purely generated Finitely Correlated States **(FNW, 1992)**.

The spectral gap for FF spin chains

In FNW 1992 it was shown that when ω is a pure zero-energy state for a chain with interaction h, such that $\dim \mathcal{K} < \infty$ (MPS case) and such that for some n

$$\mathcal{G}_{[1,n]} \equiv \text{support of } \omega|_{\mathcal{A}_{[1,n]}} = \ker H_{[1,n]},$$

then the model is gapped. The support property is sometimes referred to by saying that H_Λ is a parent Hamiltonian for the MPS state ω. In general

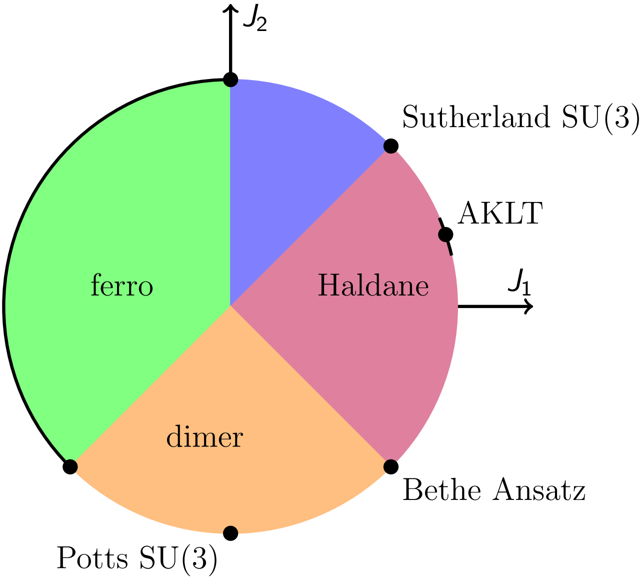
$$\text{support of } \omega|_{\mathcal{A}_{[1,n]}} \subset \ker H_{[1,n]},$$

If there is no equality, H_Λ is sometimes referred to a as an uncle Hamiltoninan, which may not have a gap.

2. The AKLT model **(Affleck-Kennedy-Lieb-Tasaki, 1987-88)**. $\Lambda \subset \mathbb{Z}$, $\mathcal{H}_x = \mathbb{C}^3$;

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

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). Ground state is frustration free (Valence Bond Solid state (VBS), aka Matrix Product State (MPS), aka Finitely Correlated State (FCS)).



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

The Martingale Method (CMP 1996)

The following conditions must hold for one and the same value of $\ell \geq 2$, e.g., for $\Lambda_n = [1, n]$.

(1) There exists a constant d_ℓ for which the local Hamiltonians satisfy

$$0 \leq \sum_{n=\ell}^{N} H_{\Lambda_n \setminus \Lambda_{n-\ell}} \leq d_\ell H_{\Lambda_N}.$$

(2) The local Hamiltonians H_{Λ_n} have a non-trivial kernel $\mathcal{G}_{\Lambda_n} \subseteq \mathcal{H}_{\Lambda_n}$. Furthermore, there is a nonvanishing spectral gap $\gamma_\ell > 0$ such that:

$$H_{\Lambda_n \setminus \Lambda_{n-\ell}} \geq \gamma_\ell (\mathbb{I} - G_{\Lambda_n \setminus \Lambda_{n-\ell}})$$

for all $n \geq n_\ell$ where G_{Λ_n} is the orthogonal projection onto $\mathcal{G}_{\Lambda_n}$.

(3) There exists a constant $\epsilon_\ell < \frac{1}{\sqrt{\ell}}$ and some n_ℓ such that for all $n \geq n_\ell$,

$$\| G_{\Lambda_{n+1} \setminus \Lambda_{n-\ell}} E_n \| \leq \epsilon_\ell$$

where $E_n = G_{\Lambda_n} - G_{\Lambda_{n+1}}$.

Theorem

Assume that conditions (1)-(3) are satisfied for the same integer $\ell \geq 2$. *Then for any* N *and any* $\psi \in \mathcal{H}_{\Lambda_N}$ *such that* $G_{\Lambda_N}\psi = 0$, *one has*

$$\langle \psi, \, H_{\Lambda_N}\psi \rangle \geq \frac{\gamma_\ell}{2d_\ell}(1 - \epsilon_\ell\sqrt{\ell})^2 \|\psi\|^2$$