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Quantum Entropy in Condensed Matter Physics[1]

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Prologue

1. Quantum Mechanics is both similar to and different from Classical Mechanics:

- similar overall structure of "Hamiltonian dynamics", semiclassical ideas often work (JW, RS);

- but also uncertainty principle, isolated eigenvalues, quantum fluctuations, measurement magic... (RS, JW)

It is important to be aware of both.

2. Entropy can be used as a (one) measure of mixedness of states, which may be entirely due to quantum effects (consequences of non-commutativity).

3. Many interesting phenomena in Condensed Matter Physics are due to quantum effects. Quantum Computing?

Quantum Entropy

For any density matrix ρ on Hilbert space $\mathcal{H}$, define the von Neumann entropy by

$$S(\rho) = -\mathrm{Tr}\rho \log \rho = -\sum_i \rho_i \log \rho_i$$

where ρ_i are the eigenvalues of ρ. $S(\rho) = 0$ iff $\rho = P_\psi = |\psi\rangle\langle\psi|$. If $\dim \mathcal{H} = d < \infty$, S attains its maximum value, $\log d$, in the state $d^{-1}\mathbb{1}$.

Suppose $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, and define

$$\rho_A = \mathrm{Tr}_{\mathcal{H}_B}\rho, \quad \rho_B = \mathrm{Tr}_{\mathcal{H}_A}\rho$$

Then, S is subadditive in the sense that

$$S(\rho) \leq S(\rho_A) + S(\rho_B)$$

Example:

$\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$, $\rho = P_\psi$, with $\psi = (|0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle)/\sqrt{2}$.

$$\rho = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Then $\rho_A = \rho_B = \frac{1}{2}\mathbb{1}$, and we have

$$S(\rho) = 0, \quad S(\rho_A) = S(\rho_B) = \log 2.$$

Therefore subadditivity holds "maximally"!

So, this is very different from entropy in thermodynamics, which is assumed to be additive.

Theme of these lectures

In these lectures I will present some tools to investigate complex quantum states of systems with many components, such as the ones that describe condensed matter at (very) low temperatures.

Such states are also potentially relevant for quantum computation.

One such tool is given by Lieb-Robinson bounds which, in a sense, show that things cannot get too complex too quickly.

Lecture Plan

1. The basic setup. **Lieb-Robinson bounds** for the support of time-evolved observables: (i) lattice systems bounded interactions, (ii) (an)harmomic lattice systems.
2. The **Exponential Clustering Theorem**: spectral gap and correlation length of ground states.
3. **Approximate product structure of gaped ground states**. Matrix Product States. Area Law for the local entropy of a ground with a spectral gap.
4. Local perturbations perturb locally: A **Lieb-Schultz-Mattis Theorem**.

Lecture Notes

(i) Who? A secret collaborator in the audience.

(ii) When?

Setup

- finite collection of quantum systems (spins, qudits, (an)harmonic oscillators, atoms, quantum dots, ...) labeled by $x \in \Lambda$.
- Each system has a Hilbert space $\mathcal{H}_x$. The Hilbert space describing the total system is

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

- Each system has a dynamics described by a s.a. Hamiltonian H_x densely defined on $\mathcal{H}_x$.
- 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 $A \otimes \mathbb{1}_{\Lambda\setminus X} \in \mathcal{A}_\Lambda$.

Interactions

We will primarily consider bounded interactions modeled by map Φ from the set of subsets of Λ to $\mathcal{A}_\Lambda$ such that $\Phi(X) \in \mathcal{A}_X$, and $\Phi(X) = \Phi(X)^*$, for all $X \subset \Lambda$. The full Hamiltonian is

$$H = \sum_{x \in \Lambda} H_x \; + \; \sum_{X \subset \Lambda} \Phi(X).$$

E.g., $\Lambda \subset \mathbb{Z}^d$, $\mathcal{H}_x = \mathbb{C}^2$; the Heisenberg Hamiltonian:

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

The Heisenberg dynamics, $\{\tau_t\}_{t \in \mathbb{R}}$, defined by

$$\tau_t(A) = e^{itH} A e^{-itH}, \quad A \in \mathcal{A}_\Lambda.$$

For systems of oscillators we will consider the standard harmonic interaction and anharmonic perturbations of the following form:
$\Lambda \subset \mathbb{Z}^\nu$, $\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} L^2(\mathbb{R})$, $p_x = -i\frac{d}{dq_x}$, and

$$H_\Lambda = \sum_{x\in\Lambda} p_x^2 + \omega^2 q_x^2 + V(q_x) \quad + \sum_{|x-y|=1} \lambda(q_x - q_y)^2 + \Phi(q_x - q_y)$$

In the cases we will consider we assume the following conditions on V and Φ:
(i) If $\lambda = 0$, it is sufficient that V is such that $p_x^2 + \omega^2 q_x^2 + V(q_x)$ is self-adjoint, and $\Phi \in L^\infty(\mathbb{R})$.
(ii) If $\lambda > 0$, V and Φ have to be C^2, L^1, and such that V'' and $\Phi'' \in L^\infty \cap L^1$.

Ground states, excitations, dynamics

H_Λ: finite system, includes boundary conditions described by additional terms in the Hamiltonian.

Ground state: eigenvector with eigenvalue $E_0 = \inf \operatorname{spec} H_\Lambda$.

Spectral gap above the ground state: if $\dim \mathcal{H}_\Lambda < \infty$, and H_Λ has eigenvalues $E_0 < E_1 < E_2 < \ldots$, we define $\gamma = E_1 - E_0 > 0$. In general

$$\gamma = \sup\{\delta \geq 0 \mid \operatorname{spec} H_\Lambda \cap (E_0, E_0 + \delta) = \emptyset\} \geq 0\,.$$

With some care, this definition can also be applied in the thermodynamic limit.

Excitations: it is often useful to think of excited states as being generated from a ground state by the action of an observable (even in finite systems).

$$\psi = A\Omega, \quad H_\Lambda \Omega = E_0 \Omega$$

Then, one may study the dynamics of ψ, bypassing a full spectral analysis of the Hamiltonian:

$$\psi_t = \tau_t(A)\Omega\,.$$

In these lectures we will focus on model-independent properties, valid for general classes of Hamiltonians that share a few essential properties. But models are of course very important.

Models, types of ground states behavior

(1) Standard Heisenberg model:

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

- Large B: spins align with the field, no correlations, $\gamma \geq c > 0$.

- $B = 0$, $J_{xy} = J < 0$, ferromagnetically ordered g.s., $\gamma \sim C/L^2$ for $\Lambda = [1, L]^d \subset \mathbb{Z}^d$.

- $B = 0$, $J_{xy} = J > 0$, $\Lambda = [1, 2L]^d \subset \mathbb{Z}^d$: unique g.s.. In the limit $L \to \infty$, antiferromagnetically ordered g.s's (proved for $d \geq 3$, and if spin $S \geq 1$, also for $d = 2$, Dyson-Lieb-Simon 1978, and others), and one expects $\gamma \sim C/L$.

- $B = 0$, $J_{xy} = J > 0$, $\Lambda = \mathbb{Z}$: no long-range order. If spin is halfintegral, $\gamma = 0$, power law decay of correlations. If spin is integer, $\gamma > 0$, exponential decay of correlations (Haldane's Conjecture).

Excitations:

- islands of overturned spins aka droplets (Spitzer, Starr)
- spin waves
- domain walls (Contucci, Koma, Michoel, Spitzer)

(2) "Fancy" Heisenberg models:

E.g., $\Lambda \subset \mathbb{Z}^2$, and

$$H_\Lambda = \sum_{x,y\in\Lambda,|x-y|=1} J_1 \mathbf{S}_x \cdot \mathbf{S}_y \quad + \sum_{x,y\in\Lambda,|x-y|=\sqrt{2}} J_2 \mathbf{S}_x \cdot \mathbf{S}_y$$

May have fancy ground states and fancy excitations.

- Dimerized ground states: dimers in a pattern.
- Resonating Valence Bond ground states: dimers without a fixed pattern.
- Spin Liquid: fully disordered.
- Topological Phases, e.g., the Toric Code model on a surface of genus g has 4^g ground states that are locally identical yet globally distinguishable by a topological index.

The support of observables and small commutators

Recall that we can identify $A \in \mathcal{A}_X$ with a unique $A \in \mathcal{A}_Y$, for all Y that contain X.

- The smallest set X such that $A \in \mathcal{A}_X$, is called the support of A, denoted by $\operatorname{supp} A$. I.e., $A \in \mathcal{A}_X$ iff $\operatorname{supp} A \subset X$.
- Even if interactions are between nearest neighbors only, for generic $A \in \mathcal{A}_\Lambda$, $\operatorname{supp} \tau_t(A) = \Lambda$ for all $t \neq 0$,
- This, however, does *not* mean that physical phenomena necessarily require non-local descriptions.

For $X, Y \subset \Lambda$, s.t., $X \cap Y = \emptyset$, $A \in \mathcal{A}_X, B \in \mathcal{A}_Y$, $AB - BA = [A, B] = 0$: observables with disjoint supports commute. Conversely, if $A \in \mathcal{A}_\Lambda$ satisfies

$$[A, B] = 0, \quad \text{for all } B \in \mathcal{A}_Y \tag{1}$$

then $Y \cap \operatorname{supp} A = \emptyset$.

A more general statement is true: if the commutators in (1) are uniformly small, than A is close to $\mathcal{A}_{\Lambda \setminus Y}$.

Lemma

Let $A \in \mathcal{A}_\Lambda$, $\epsilon \geq 0$, *and* $Y \subset \Lambda$ *be such that*

$$\|[A, B]\| \leq \epsilon \|B\|, \quad \textit{for all } B \in \mathcal{A}_Y \tag{2}$$

then there exists $A' \in A_{\Lambda \setminus Y}$ *such that*

$$\|A' \otimes \mathbb{1} - A\| \leq c\epsilon$$

with $c = 1$ *if* $\dim \mathcal{H}_Y < \infty$, *and* $c = 2$ *in general.*

$\Rightarrow$ we can investigate $\operatorname{supp} \tau_t(A)$ by estimating $[\tau_t(A), B]$ for $B \in \mathcal{A}_Y$. This is what Lieb-Robinson bounds are about.

The ϵ will depend on the distance of $Y = \operatorname{supp} B$ to the 'essential support' of B.

Let d be a metric on Λ. Often, Λ is a graph and d is the graph distance: $d(x, y)$ is the length of the shortest path from x to y over edges in the graph.

For $X, Y \subset \Lambda$, we define

$$d(X, Y) = \min\{d(x, y) \mid x \in X, y \in Y\}.$$

The diameter, $\operatorname{diam}(X)$, of a subset $X \subset \Lambda$ is

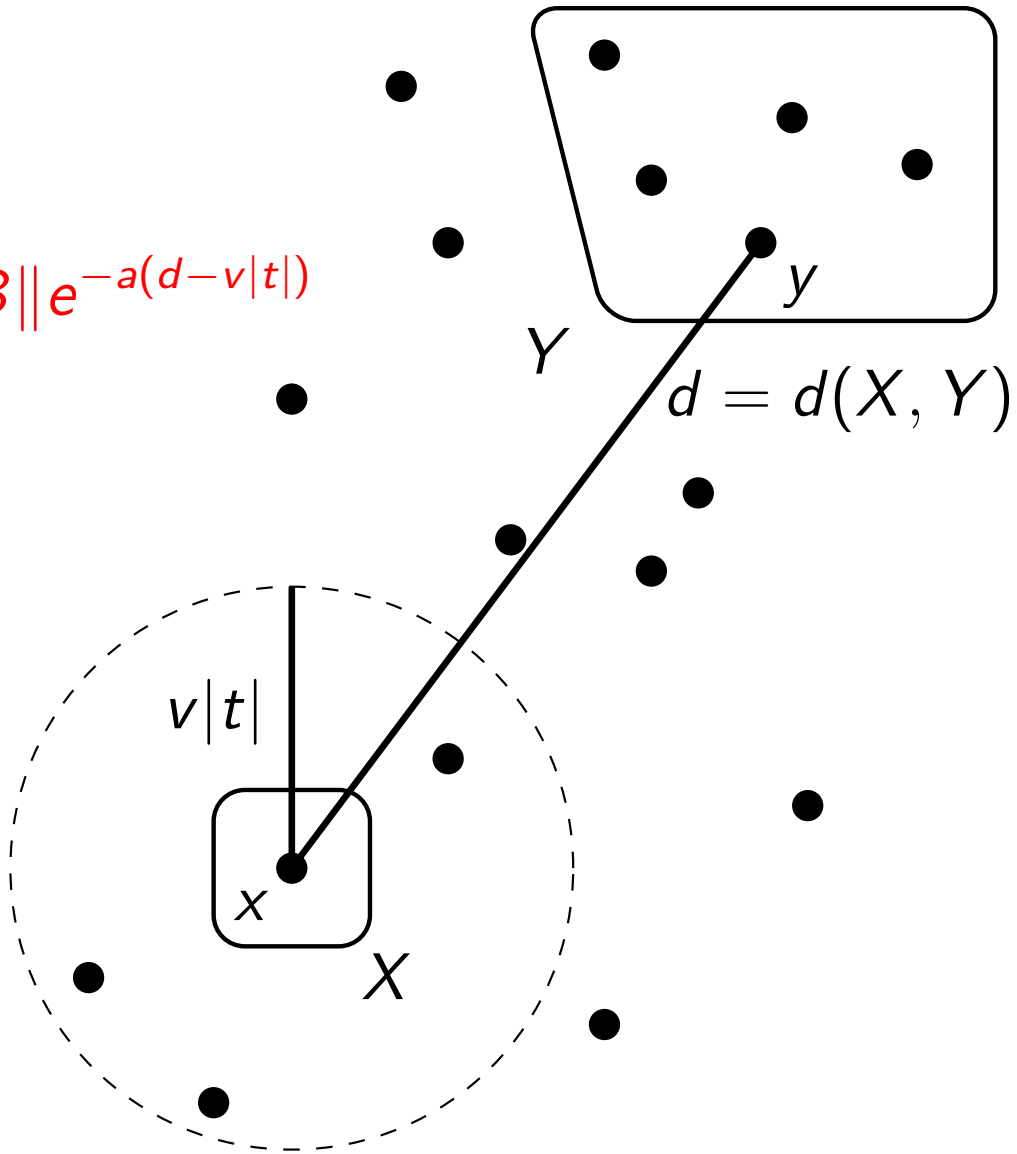
$$\operatorname{diam}(X) = \max\{d(x, y) \mid x, y \in X\}.$$

Lieb-Robinson bound :

$\exists C, v, a > 0$ s.t.

$$\| [\tau_t(A), B] \| \leq C\|A\| \, \|B\| e^{-a(d-v|t|)}$$

where $t \in \mathbb{R}$, $A \in \mathcal{A}_X$, $B \in \mathcal{A}_Y$, for finite $X, Y \subset V$, and $d = d(X, Y)$. The first such estimates were proved by Lieb & Robinson (1972).



Lieb-Robinson bounds, what do they mean?

Lieb, E.H. and Robinson, D.W.: *The Finite Group Velocity of Quantum Spin Systems*, Commun. Math. Phys. **28**, 251–257 (1972).

For a specific model, the connection with the group velocity was made mathematically explicit by Ch. Radin (1973), but this interpretation follows in general from the following observation. Up to small corrections, the diameter of the support of $\tau_t(A)$ does not grow faster than linearly in t. More precisely, by the Lemma, one has the following result:

There exist $C > 0$, such that for all $\delta > 0$, there exists A_t^δ, supported in a ball of radius $v|t| + \delta$ such that $\|A_t^\delta - \tau_t(A)\| \leq C\|A\|e^{-a\delta}$.

Lieb-Robinson bounds, why are they useful?

- "Philosophically", they show that non-relativistic theories defined by local Hamiltonians, such as the ones used in condensed matter physics, have a dynamics that does not violate locality. They provide a finite bound for the "velocity of propagation of anything" in quantum lattice systems with local interactions.

- They can be used for "practical" applications. M. Hastings (2004) was the first to realize this and since then Lieb-Robinson bounds have been used to prove several new results about the ground states of quantum lattice systems: Hastings, N-Sims, Hastings-Koma, Bravyi, Verstraete, Eisert, Osborne, and others. Quasi-locality of the dynamics + other conditions imply quasi-locality properties of ground states.

General Assumption on the Interactions:

We will assume that there is a non-increasing function $F : [0, \infty) \to (0, \infty)$, with the following properties:

(i) $\|F\| := \sup_{x \in V} \sum_{y \in V} F(d(x, y)) < \infty$,

(ii) there is a constant $C > 0$ such that for pairs $x, y \in V$,

$$\sum_{z \in V} F(d(x, z))F(d(z, y)) \leq CF(d(x, y))$$

If $V = \mathbb{Z}^\nu$, we can take $F(r) = \frac{1}{(1+r)^{\nu+\epsilon}}$, for any $\epsilon > 0$.

Suppose we have V with a function F as above, and some $a \geq 0$, such that

$$\|\Phi\|_a := \sup_{x,y \in V} \frac{e^{ad(x,y)}}{F(d(x, y))} \sum_{X \ni x,y} \|\Phi(X)\| < \infty$$

Lieb-Robinson bounds (bounded interactions)

Theorem (Lieb-Robinson 1972, Hastings 04, N-Sims 06, H-Koma 06, N-S-Ogata 06, Eisert-Osborne 06, N-S 2007)

Assume $\|\Phi\|_a < \infty$ *for some* $a > 0$. *For local observables* $A \in \mathcal{A}_X$ *and* $B \in \mathcal{A}_Y$, *one has the bound*

$$\begin{aligned} &\|[\tau_t(A), B]\| \\ &\leq \frac{2\,\|A\|\,\|B\|\,\|F\|}{C} \min(|\partial_\Phi X|, |\partial_\Phi Y|) e^{-a(d(X,Y) - 2a^{-1}\|\Phi\|_a C|t|)} \end{aligned}$$

where $\partial_\Phi X$ *is given by*

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

This means that the Lieb-Robinson velocity, v, is bounded by $a^{-1}2\|\Phi\|_a C$.

The improvements obtained by the authors listed in the theorem have mostly to do with the dependence of the prefactor on the dimensions of the local Hilbert spaces and the size of the supports.

For interactions that decay only as a power law, a similar bound with power law decay can be derived in the same way.

If one assumes $X \cap Y = \emptyset$, one can replace $e^{-a(d(X,Y)-2a^{-1}\|\Phi\|_a C|t|)}$ by $e^{-ad(X,Y)}(e^{2\|\Phi\|_a C|t|)} - 1)$, which vanishes for $t = 0$. In general, for interactions of finite range R, the commutator behaves as $|t|^k$, for small t, with $k \sim d(X,Y)/R$.

Lieb-Robinson bounds for Anharmonic Lattices

$\Lambda \subset \mathbb{Z}^\nu$, $\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} L^2(\mathbb{R})$, $p_x = -i\frac{d}{dq_x}$, and

$$H_\Lambda = \sum_{x\in\Lambda} p_x^2 + \omega^2 q_x^2 + V(q_x) \quad + \sum_{|x-y|=1} \lambda(q_x - q_y)^2 + \Phi(q_x - q_y)$$

Raz-Schlein-Sims-N (CMP 2009) prove Lieb-Robinson bounds in the following two situations:

(i) If $\lambda = 0$, it is sufficient that V is such that $p_x^2 + \omega^2 q_x^2 + V(q_x)$ is self-adjoint, and $\Phi \in L^\infty(\mathbb{R})$.

(ii) If $\lambda > 0$, $\Phi = 0$, and $V \in C^1 \cap L^1$ and such that $k\widehat{V'}(k) \in L^1(\mathbb{R})$.

More recently Raz and Sims considered the case $\lambda > 0, \Phi \neq 0$, and more general interactions. Their paper is focused on *classical* oscillator lattices.

Theorem (N-Raz-Schlein-Sims, CMP 2009)

Case (i): Assume $\lambda = 0$, V *such that* $p_x^2 + \omega^2 q_x^2 + V(q_x)$ *is self-adjoint, and* $\Phi \in L^\infty(\mathbb{R})$.

For local observables $A \in \mathcal{A}_X$ *and* $B \in \mathcal{A}_Y$, *we have bound*

$$\|[\tau_t(A), B]\| \leq 2\|A\|\|B\| \min[|\partial_\Phi X|, |\partial_\Phi Y|] e^{-(ad(X,Y) - 2^{\nu+2}\|\Phi\| e^a |t|)}. \tag{3}$$

for all $a > 0$.

Here $\partial_\Phi X$ *is given by*

$$\partial_\Phi X = \{x \in X \mid \exists y \in \Lambda \setminus X, \text{ such that } |x - y| = 1\}.$$

For $f : \Lambda \to \mathbb{C}$, define the Weyl operator $W(f)$ by

$$W(f) = e^{i \sum_{x \in \Lambda} (q_x \mathrm{Re} f_x + p_x \mathrm{Im} f_x)}.$$

Clearly, $W(f)$ is a unitary operator in $\mathcal{A}_\Lambda$.

Theorem (N-Raz-Schlein-Sims, CMP 2009)

Case (ii): Let $\lambda \geq 0$, $\Phi = 0$, and assume V is C^1, L^1, and such that $k\widehat{V'}(k) \in L^1(\mathbb{R})$. Then, for all f, g with $\operatorname{supp} f \subset X$ and $\operatorname{supp} g \subset Y$, we have

$$\left\| [\tau_t(W(f)), W(g)] \right\| \leq C \|f\|_\infty \|g\|_\infty \min(|X|, |Y|) e^{-a(d(X,Y) - v|t|)}$$

for all $a > 0$, and where

$$v = 6\sqrt{\omega^2 + 4\nu\lambda} + \frac{3C}{4a} \|k\widehat{V'}(k)\|_1 .$$

Sketch of the Proof (bounded interactions only)

Consider the function $f : \mathbb{R} \to \mathcal{A}$ defined by

$$f(t) := [\tau_t(A), B]. \tag{4}$$

Differentiate to see that f satisfies the following diff. eqn

$$f'(t) = -i\,[f(t), \tau_t\,(H_X)] - i\,[\tau_t(A), [\tau_t(H_X), B]]\,, \tag{5}$$

with the notation

$$H_Y = \sum_{\substack{Z \subset \Lambda: \\ Z \cap Y \neq \emptyset}} \Phi(Z), \tag{6}$$

for any subset $Y \subset V$. The first term in (5) above is norm-preserving, and therefore we have

$$\|\,[\tau_t(A), B]\,\| \;\leq\; \|[A, B]\| + 2\|A\| \int_0^{|t|} \|\,[\tau_s(H_X), B]\,\|\, ds \tag{7}$$

Define the quantity

$$C_B(X,t) := \sup_{A \in \mathcal{A}_X} \frac{\|[\tau_t(A), B]\|}{\|A\|}, \tag{8}$$

then (7) implies that

$$C_B(X,t) \leq C_B(X,0) + 2 \sum_{\substack{Z \subset V: \\ Z \cap X \neq \emptyset}} \|\Phi(Z)\| \int_0^{|t|} C_B(Z,s) ds. \tag{9}$$

Clearly, one has that

$$C_B(Z,0) \leq 2 \|B\| \, \delta_Y(Z), \tag{10}$$

where $\delta_Y(Z) = 0$ if $Z \cap Y = \emptyset$ and $\delta_Y(Z) = 1$ otherwise. Using this fact, iterate (9) and find that

$$C_B(X,t) \leq 2\|B\| \sum_{n=0}^{\infty} \frac{(2|t|)^n}{n!} a_n, \tag{11}$$

where the coefficients are given by

$$a_n = \sum_{\substack{Z_1\subset\Lambda:\\ Z_1\cap X\neq\emptyset}} \sum_{\substack{Z_2\subset\Lambda:\\ Z_2\cap Z_1\neq\emptyset}} \cdots \sum_{\substack{Z_n\subset\Lambda:\\ Z_n\cap Z_{n-1}\neq\emptyset}} \prod_{i=1}^{n} \|\Phi(Z_i)\|\, \delta_Y(Z_n).$$

Using the properties of the function F_a and the norm $\|\Phi\|_a$ one can estimate a_n:

$$a_1 \leq \sum_{x\in\partial_\Phi X} \sum_{y\in\partial_\Phi Y} \sum_{\substack{Z\subset\Lambda:\\ x,y\in Z}} \|\Phi(Z)\| \leq \sum_{x\in\partial_\Phi X} \sum_{y\in\partial_\Phi Y} \|\Phi\|_a F_a\left(d(x,y)\right).$$

where we defined $F_a(r) = e^{-ar}F(r)$. Note that if F satisfies (i) and (ii) then so thus $F_a(r)$, for all $a \geq 0$, with $\|F_a\| \leq \|F\|$, and $C_a \leq C$.

Next,

$$
\begin{aligned}
a_2 &\leq \sum_{x\in\partial_\Phi X}\sum_{y\in\partial_\Phi Y}\sum_{z\in\Lambda}\sum_{\substack{Z_1\subset\Lambda:\\ x,z\in Z_1}} \|\Phi(Z_1)\| \sum_{\substack{Z_2\subset\Lambda:\\ z,y\in Z_2}} \|\Phi(Z_2)\| \\
&\leq \|\Phi\|_a \sum_{x\in\partial_\Phi X}\sum_{y\in\partial_\Phi Y}\sum_{z\in\Lambda} F_a\left(d(z,y)\right) \sum_{\substack{Z_1\subset\Lambda:\\ x,z\in Z_1}} \|\Phi(Z_1)\| \\
&\leq \|\Phi\|_a^2 \sum_{x\in\partial_\Phi X}\sum_{y\in\partial_\Phi Y}\sum_{z\in\Lambda} F_a\left(d(x,z)\right) F_a\left(d(z,y)\right) \\
&\leq \|\Phi\|_a^2\, C_a \sum_{x\in\partial_\Phi X}\sum_{y\in\partial_\Phi Y} F_a\left(d(x,y)\right),
\end{aligned}
$$

Similarly

$$
a_n \leq \|\Phi\|_a^n C_a^{n-1} \sum_{x\in\partial_\Phi X}\sum_{y\in\partial_\Phi Y} F_a(d(x,y)),
$$

and this completes the proof.

Comments:

- The existence of local approximations for $\tau_t(A)$, for local A, by observables whose support has a radius $\sim v|t|$ has many applications. In addition to a few we will discuss, there are others such as speeding up and analyzing practical numerical algorithms for calculating ground states, equilibrium states, form factors, of quantum lattice models.
- Open problems: prove Lieb-Robinson bound for more general unbounded Hamiltonians, e.g., the anharmonic lattice with a quartic potential.

Existence of the dynamics in the thermodynamic limit

It is well-known that one can use the Lieb-Robinson bound to establish the existence of the dynamics for infinite lattice systems.

Let Λ_n be an increasing exhausting sequence of finite subsets of an infinite system, V, with interaction Φ. The essential observation is the following bound: for $n > m$

$$\|\tau_t^{\Lambda_n}(A) - \tau_t^{\Lambda_m}(A)\| \leq \sum_{x \in \Lambda_n \setminus \Lambda_m} \sum_{X \ni x} \int_0^{|t|} \|[\Phi(X), \tau_t^{\Lambda_m}(A)]\| \, ds.$$

Theorem

Let $a \geq 0$, and Φ such that $\|\Phi\|_a < \infty$. Then, the dynamics $\{\tau_t\}_{t\in\mathbb{R}}$ corresponding to Φ exists as a strongly continuous, one-parameter group of automorphisms on $\mathcal{A}$. In particular,

$$\lim_{n\to\infty} \|\tau_t^{\Lambda_n}(A) - \tau_t(A)\| = 0$$

for all $A \in \mathcal{A} = \overline{\bigcup_n \mathcal{A}_{\Lambda_n}}$. The convergence is uniform for t in compact sets and independent of the choice of exhausting sequence $\{\Lambda_n\}$.

The Exponential Clustering Theorem

In a relativistic quantum field theory, the speed of light plays the role of an automatic bound for the Lieb-Robinson velocity. This implies decay of correlations in the vacuum of a QFT with a gap and a unique (Ruelle, others). Fredenhagen proved an exponential bound for the decay: $\sim e^{-\gamma c^{-1}|x|}$, i.e., $\xi \leq c/\gamma$. In a QFT the gap γ is interpreted as the mass of the lightest particle.

In condensed matter physics, a gap also implies exponential decay under general conditions (Hastings 2004, N-Sims 2006, Hastings-Koma 2006).

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

Case (i): bounded interactions with $\|\Phi\|_a < \infty$ *for some* $a > 0$. *Suppose* H *has a spectral gap* $\gamma > 0$ *above a unique ground state* $\langle \cdot \rangle$. *Then, there exists* $\mu > 0$ *and a constant* $c = c(F, \gamma)$ *such that for all* $A \in \mathcal{A}_X$, $B \in \mathcal{A}_Y$,

$$|\langle AB \rangle - \langle A \rangle \langle B \rangle| \leq c\|A\| \, \|B\| \min(\partial_\Phi X, \partial_\Phi Y) e^{-\mu d(X,Y)}.$$

One can take

$$\mu = \frac{a\gamma}{\gamma + 4\|\Phi\|_a}.$$

Theorem (N-Raz-Schlein-Sims, CMP 2009)

Let H be the anharmonic lattice Hamiltonian with $\lambda \geq 0$ satisfying the conditions of Case (ii), and suppose H has a unique ground state and a spectral gap $\gamma > 0$ above it. Denote by $\langle \cdot \rangle$ the expectation in the ground state. Then, for all functions f and g with finite supports X and Y in the lattice, we have the following estimate:

$$\begin{aligned} &|\langle W(f)W(g)\rangle - \langle W(f)\rangle\langle W(g)\rangle| \\ &\leq C\|f\|_\infty \|g\|_\infty \min(|X|,|Y|)e^{-d(X,Y)/\xi} \end{aligned}$$

where $\xi = (4av + \gamma)/(a\gamma)$ and, if we assume $d(X,Y) \geq \xi$, C is a constant depending only on the dimension ν.

Idea of the proof

Suppose $H \geq 0$ with unique ground state Ω, $H\Omega = 0$, with a gap $\gamma > 0$ above 0. Let $A \in \mathcal{A}_X$ and $B \in \mathcal{A}_Y$, $d(X, Y) > 0$, $a, C, v > 0$, such that

$$\|[\tau_t(A), B]\| \leq C\|A\| \, \|B\| e^{-a(d(X,Y)-v|t|)} \, .$$

We can assume $\langle \Omega, A\Omega \rangle = \langle \Omega, B\Omega \rangle = 0$. We want to show that there is a $\xi < \infty$, independent of X, Y, A, B, s.t.

$$|\langle \Omega, AB\Omega \rangle| \leq Ce^{-d(X,Y)/\xi} \, .$$

For $z \in \mathbb{C}$, $\operatorname{Im} z \geq 0$, define

$$f(z) = \langle \Omega, A\tau_z(B)\Omega \rangle = \int_\gamma^\infty e^{izE} d\langle A^*\Omega, P_E B\Omega \rangle \,.$$

For $T > b > 0$, and Γ_T the upper semicircle of radius T centered at 0:

$$f(ib) = \frac{1}{2\pi i} \int_{\Gamma_T} \frac{f(z)}{z - ib} dz \,.$$

Then

$$|\langle \Omega, AB\Omega \rangle| \leq \limsup_{b \downarrow 0, T \uparrow \infty} \frac{1}{2\pi} \left| \int_{-T}^{T} \frac{f(t)}{t - ib} dt \right| \,.$$

Next, introduce a Gaussian cut-off and remember $f(t)$:

$$|\langle \Omega, AB\Omega \rangle| \leq \limsup_{b\downarrow 0, T\uparrow\infty} \frac{1}{2\pi} \left| \int_{-T}^{T} e^{-\alpha t^2} \frac{\langle \Omega, A\tau_t(B)\Omega \rangle}{t - ib} dt \right| + Ce^{-\gamma^2/(4\alpha)}$$

assuming $\gamma > 2\alpha b$. For $\alpha(d(X,Y)/v)^2 \gg 1$, the Lieb-Robinson bounds lets us commute $\tau_t(B)$ with A in this estimate. Using the spectral representation of τ_t, we get

$$|\langle \Omega, AB\Omega \rangle| \leq \limsup_{b\downarrow 0, T\uparrow\infty} \frac{1}{2\pi} \left| \int_{\gamma}^{\infty} \int_{-T}^{T} dt \frac{e^{-iEt} e^{-\alpha t^2}}{t - ib} d\langle B^*\Omega, P_E A\Omega \rangle \right| + \text{err.}$$

The $t-$integral can be uniformly bounded by $e^{-\gamma^2/(4\alpha)}$. Optimizing α gives the result.

Non-separability, Entanglement, and Entropy

Two-component system: $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ (Alice & Bob).

Density matrix ρ on $\mathcal{H}$.

ρ is separable if there exists convex combination coefficients t_α and density matrices $\rho_A^{(\alpha)}$ and $\rho_B^{(\alpha)}$, such that there is a decomposition of the form

$$\rho = \sum_\alpha t_\alpha \rho_A^{(\alpha)} \otimes \rho_B^{(\alpha)}$$

Otherwise ρ is called non-separable.

In the case of a pure state $\psi \in \mathcal{H}$, ψ ($|\psi\rangle\langle\psi|$) is separable iff it is a product state:

$$\psi = \psi_A \otimes \psi_B$$

Non-separablity is a quantum property in the sense that every classical probability measure on a product space is separable:

$$\mu = \sum_{xy} \mu(x, y) \delta_x \otimes \delta_y$$

Another word for non-separable is entangled. E.g., for two qubits

$$\psi = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle)$$

is maximally entangled (w.r.t. any conventional measure of entanglement).

Entanglement Entropy

$$S_E(\rho) = \min_{\rho=\sum_\alpha t_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|} t_\alpha S(\rho_A^{(\alpha)})$$

where

$$\rho_A^{(\alpha)} = \mathrm{Tr}_{\mathcal{H}_B} |\psi_\alpha\rangle \langle\psi_\alpha|$$

and, for any density matrix σ, $S(\sigma)$ is the von Neumann entropy:

$$S(\rho) = -\mathrm{Tr}\rho \log \rho$$

ρ is separable iff $S_E(\rho) = 0$.

S_E of a pure state

For a pure state $\psi \in \mathcal{H}_A \otimes \mathcal{H}_B$, S_E is simply the entropy of its restriction $\rho_A = \mathrm{Tr}_{\mathcal{H}_B} |\psi\rangle \langle\psi|$. One way to calculate this efficiently is by using the Schmidt decomposition:

$$\psi = \sum_\alpha c_\alpha \phi_A^{(\alpha)} \otimes \phi_B^{(\alpha)}$$

where $\{\phi_A^{(\alpha)}\}$ and $\{\phi_B^{(\alpha)}\}$ are o.n. sets and $\sum_\alpha |c_\alpha|^2 = \|\psi\|^2$. Then

$$\rho_A = \sum_\alpha |c_\alpha|^2 \left|\phi_A^{(\alpha)}\right\rangle \left\langle\phi_A^{(\alpha)}\right|$$

Therefore

$$S_E = -\sum_\alpha |c_\alpha|^2 \log |c_\alpha|^2$$

Structure of gaped ground states

The Exponential Clustering Theorem says that a non-vanishing gap γ implies a finite correlation length ξ. Can one say more? E.g., with the goal of devising better algorithms to compute ground states? Or to do quantum computation?

The AKLT model (the model that changed the world, named after Affleck, Kennedy, Lieb, & Tasaki, CMP 1988) and the structure of Valence Bond Solid states give us a hint.

$$H^{AKLT}_{[a,b]} = \sum_{x=a}^{b-1} [\frac{1}{3} + \frac{1}{2}\mathbf{S}_x \cdot \mathbf{S}_{x+1} + \frac{1}{6}(\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2] = \sum_{a=1}^{b-1} P^{(2)}_{x,x+1}$$

acting on $(\mathbb{C}^3)^{\otimes(b-a+1)}$. $P^{(2)}_{x,x+1}$ is the $\perp$ projection onto the spin 2 subspaces of two spin 1's at x and $x+1$. $E_0 = 0$.

Essential properties of the AKLT chain

- Unique ground state for the infinite chain: pick $\psi_L \in \ker H_{[-L,L]}$, $\|\psi_L\| = 1$, $A \in \mathcal{A}_X$, then

$$\omega(A) = \lim_{L\to\infty} \langle \psi_L, A\psi_L \rangle$$

  exists and is independent of the chose sequence (hence ω is translation and SU(2) invariant).

- Finite correlation length: there exists $\xi > 0$, $C > 0$, s.t., for all $A \in \mathcal{A}_X, B \in \mathcal{A}_Y$

$$|\omega(AB) - \omega(A)\omega(B)| \leq C\|A\|\|B\|e^{-d(X,Y)/\xi}.$$

  In fact, this holds with $e^{-1/\xi} = 1/3$.

- Spectral gap: there exists $\gamma > 0$, s.t. for all $b > a$, the gap of $H_{[a,b]}$ satisfies $E_1 \geq \gamma$. For the infinite chain this is expressed by

$$\omega(A^* H_X A) \geq \gamma \omega(A^* A).$$

for all X and all $A \in \mathcal{A}_X$, with

$$H_X = \sum_{\substack{\{x,x+1\} \\ \{x,x+1\} \cap X \neq \emptyset}} P^{(2)}_{x,x+1}$$

One can compute γ numerically: $\gamma \sim .4097....$

The AKLT chain was the first proven example of the existence of the Haldane phase.

This is important, but the impact of the explicit construction of the exact ground state of the AKLT Hamiltonian has been even greater. It led to analytic and numerical techniques to compute and approximate the complex entangled states that occur in many condensed matter systems.

The AKLT state

Recall the Clebsch-Gordan series for the decomposition of the tensor product of two irreducible representations of SU(2):

$$D^{(s_1)} \otimes D^{(s_2)} \cong D^{(|s_1-s_2|)} \oplus D^{(|s_1-s_2|+1)} \oplus \cdots \oplus D^{(s_1+s_2)}$$

Let $\phi \in \mathbb{C}^2 \otimes \mathbb{C}^2$ be the singlet state: $\phi = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, and $W : \mathbb{C}^3 \to \mathbb{C}^2 \otimes \mathbb{C}^2$ be the isometry implementing the embedding $D^{(1)} \subset D^{(1/2)} \otimes D^{(1/2)}$. For any spin-1 observable $A \in M_3$, $WAW^* \in M_2 \otimes M_2$. Then, for every $n \geq 1$, and$|\alpha\rangle, |\beta\rangle \in \mathbb{C}^2$,

$$\psi^{(n)}_{\alpha\beta} = (W^* \otimes \cdots \otimes W^*)(|\alpha\rangle \otimes \phi \otimes \cdots \otimes \phi \otimes |\beta\rangle)$$

is a ground state of $H_{[1,n]}$.

- Why is $\psi^{(n)}_{\alpha\beta}$ a ground state?
  $H^{AKLT}_{[1,n]}\psi^{(n)}_{\alpha,\beta} = 0$, because each term vanishes:

$$P^{(2)}_{x,x+1}(W^* \otimes W^*)(|\alpha\rangle \otimes \phi \otimes |\beta\rangle) = 0$$

  since there is no spin-2 component in $|\alpha\rangle \otimes \phi \otimes |\beta\rangle$
- Why unique thermodynamic limit? Why is $\xi < \infty$?
  Rewrite

$$\frac{\langle \psi^{(n)}_{\alpha\beta}, A_1 \otimes \cdots \otimes A_n \psi^{(n)}_{\alpha\beta}\rangle}{\langle \psi^{(n)}_{\alpha\beta}, \psi^{(n)}_{\alpha\beta}\rangle}$$

  as

$$\mathrm{Tr} P_\alpha \mathbb{E}_{A_1} \circ \mathbb{E}_{A_2} \circ \cdots E_{A_n}(P_\beta)$$

  where, for $A \in M_3$ and $B \in M_2$, $\mathbb{E}_A(B) \in M_2$ is defined as

$$\mathbb{E}_A(B) = V^* A \otimes BV$$

  with V ...

with $V : \mathbb{C}^2 \to \mathbb{C}^3 \otimes \mathbb{C}^2$ is the isometry corresponding to $D^{(1/2)} \subset D^{(1)} \otimes D^{(1/2)}$. For a suitable constant c,

$$V\,|\alpha\rangle = c(W^* \otimes \mathbb{1}_2)(|\alpha\rangle \otimes \phi)$$

and the thermodynamic limit is given by

$$\frac{1}{2}\mathrm{Tr}\,\mathbb{E}_{A_1} \circ \mathbb{E}_{A_2} \circ \cdots E_{A_n}(\mathbb{1}_2)$$

One can check that

$$\mathbb{E}_{\mathbb{1}}(B) = \frac{1}{2}(\mathrm{Tr}\,B)\mathbb{1}_2 - \frac{1}{3}(B - \frac{1}{2}\mathrm{Tr}\,B)$$

In particular $\mathbb{E}_{\mathbb{1}}(\mathbb{1}_2) = V^*V = \mathbb{1}_2$ and $\mathrm{Tr}\,\mathbb{E}_{\mathbb{1}}(B) = \mathrm{Tr}\,B$. Everything follows.

- Why $\gamma > 0$?

  The ground state ω of the infinite chain has the following structure: Let $\rho_{[a,b]}$ be the density matrix describing its restriction to $\mathcal{A}_{[a,b]}$. Then, the rank of $\rho_{[a,b]}$ is 4. Let $G_{[a,b]}$ be the orthogonal projection onto its range.
  Then, for $\ell \geq 0, a \geq \ell + 1$, one can show that

$$\| G_{[a-\ell,a+\ell+1]} \left[G_{[1,a]} \otimes G_{[a+1,L]} \right] - G_{[1,L]} \right] \| \leq Ce^{-\ell/\xi}$$

This property allows one to prove a uniform lower bound for the gap (Fannes-N-Werner 1992, Spitzer-Starr 2002). In brief:

$$\gamma \geq \frac{1}{2}(1 - ce^{-\ell/\xi}) \times (\text{gap of } H_{[-\ell,\ell]}).$$

The Area Law for the entanglement entropy

The AKLT state ω satisfy an "area bound" on the entropy of its local restrictions. In general, this means that for $X \subset \Lambda$ and $\rho_X \in \mathcal{A}_X$ is the density matrix describing the restriction of the state to $\mathcal{A}_X$, then

$$S(\rho_X) = -\mathrm{Tr}\rho_x \log \rho_X \leq C|\partial X|$$

If X is an interval, for the AKLT state we have $S(\rho_X) = \log 4$. Conjecture: area law holds for gapped ground states in general of arbitrary quantum spin systems with bounded spins and bounded finite-range interactions.

The existence of a large class of models (VBS models) with AKLT-like ground states supports this conjecture. In one dimension there is even a density result (Fannes, N, Werner 1992).

VBS models also exist in higher dimensions and their ground state are sometimes called PEPS (Products of Entangled Pairs, Verstraete).

Therefore, the AKLT model may be somewhat special but the general properties of its ground state are not.

In particular, gapped ground states have an approximate product structure.

An approximation theorem for gapped ground states

We will consider a system of the following type: Let Λ be a finite subset of $\mathbb{Z}^d$. At each $x \in \Lambda$, we have a finite-dimensional Hilbert space of dimension n_x. Let

$$H_V = \sum_{\{x,y\} \subset \Lambda, |x-y|=1} \Phi(x,y),$$

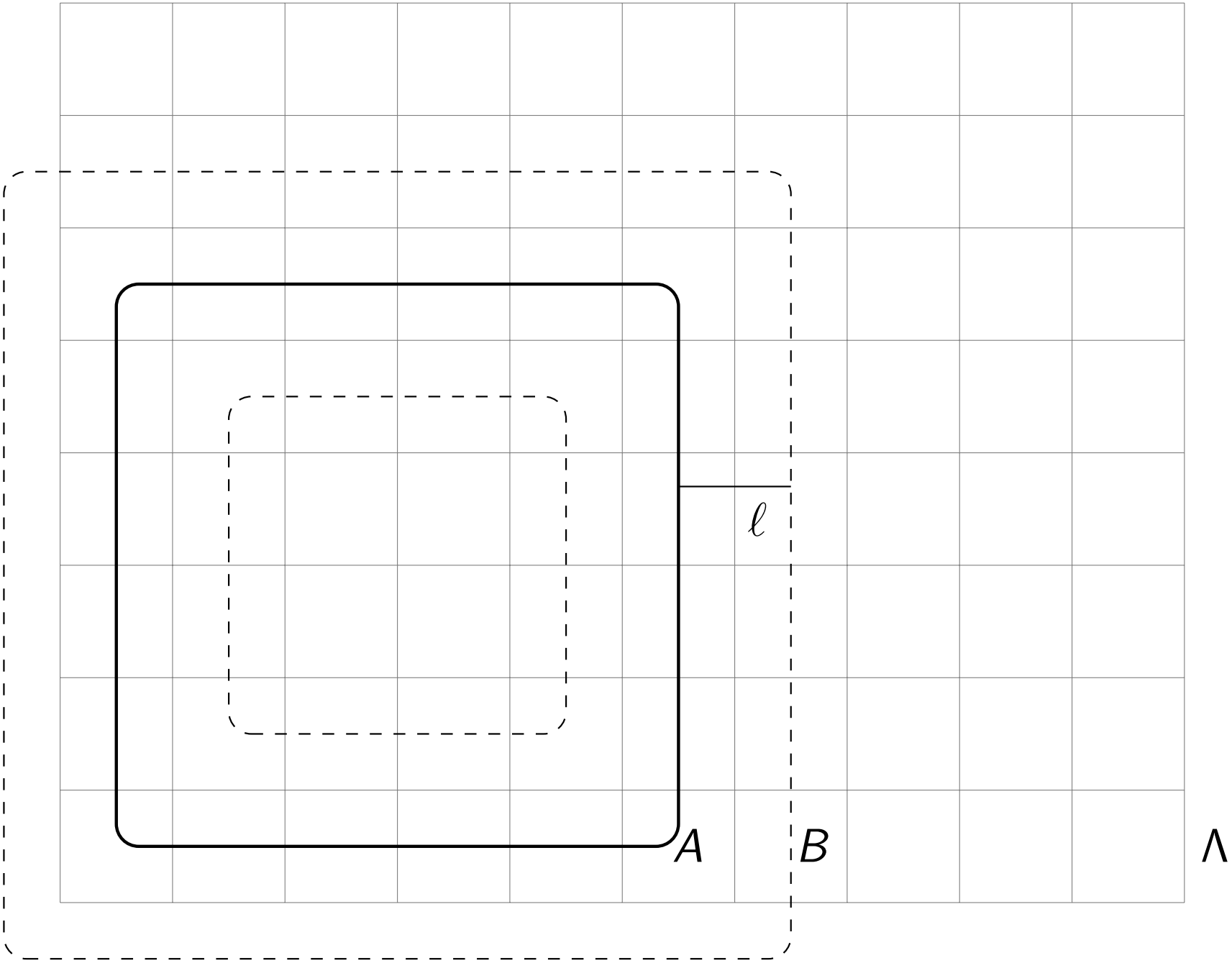
with $\|\Phi(x,y)\| \leq J$. Suppose H_V has a unique ground state and denote by P_0 the corresponding projection, and let $\gamma > 0$ be the gap above the ground state energy.

For a set $A \subset \Lambda$, the boundary of A, denoted by ∂A, is

$$\partial A = \{x \in A \mid \text{there exists } y \in \Lambda \setminus A, \text{with } |x-y| = 1\}.$$

and for $\ell \geq 1$ define

$$B(\ell) = \{x \in \Lambda \mid d(x, \partial A) < \ell\}.$$


ℓ
A
B
Λ

The following generalizes a result by Hastings (2007):

Theorem (Hamza-Michalakis-N-Sims, in prep.)

There exists $\xi > 0$ (given explicitly in terms of d, J, and γ), such that for any sufficiently large $m > 0$, and any $A \subset \Lambda$, there exist two orthogonal projections $P_A \in \mathcal{A}_A$, and $P_{\Lambda\setminus A} \in \mathcal{A}_{\Lambda\setminus A}$, and an operator $P_B \in \mathcal{A}_{B(m)}$ with $\|P_B\| \leq 1$, such that

$$\|P_B(P_A \otimes P_{\Lambda\setminus A}) - P_0\| \leq C(\xi)|\partial A|^2 e^{-m/\xi}$$

where $C(\xi)$ is an explicit polynomial in ξ.

Sketch of the proof

(several ideas by Hastings & many estimates by Hamza and Sims)

(1) The first step is the bring the Hamiltonian in a form similar to the Hamiltonian of the AKLT model. Assume $E_0 = 0$. We aim at a decomposition, for each sufficiently large ℓ,

$$H_\Lambda = K_A + K_{B(\ell)} + K_{\Lambda \setminus A}\,,$$

with the following properties:

- $\operatorname{supp} K_X \subset X$, for $X = A, B(\ell), \Lambda \setminus A$.
- $\|K_X \psi_0\| \leq e^{-c\ell}$, for each X and for some $c > 0$ (we only assumed $H_\Lambda \psi_0 = 0$).

We start from

$$H_\Lambda = H_I + H_B + H_E \,, \tag{12}$$

where

$$\begin{aligned} I &= I(\ell) = \{x \in A \mid \text{for all } y \in \partial A, d(x,y) \geq \ell\} \\ E &= E(\ell) = \{x \in V \setminus A \mid \text{for all } y \in \partial A, d(x,y) \geq \ell\} \,. \end{aligned}$$

The sets $I(\ell)$ and $E(\ell)$ are the interior and exterior of A. $B(\ell)$ is boundary of thickness 2ℓ:

$$B(\ell) = \{x \in \Lambda \mid d(x, \partial A) < \ell\} \,.$$

Note that Λ is the disjoint union of I, B, and E. Now define

$$H_I = \sum_{\substack{X \subset \Lambda: \\ X \cap I \neq \emptyset}} \Phi(X), \quad H_B = \sum_{\substack{X \subset \Lambda: \\ X \subset B}} \Phi(X), \quad H_E = \sum_{\substack{X \subset \Lambda: \\ X \cap E \neq \emptyset}} \Phi(X).$$

For $\ell > 1$, there are no repeated terms and (12) holds.

$\|H_X\psi_0\|$ is not necessarily small but we can arrange it so that each term has 0 expectation in ψ_0. The next step: for $X \in \{I, B, E\}$ define

$$(H_X)_\alpha = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} \tau_t(H_X)\, e^{-\alpha t^2}\, dt\,,$$

for $\alpha > 0$. We still have

$$H_\Lambda = (H_I)_\alpha + (H_B)_\alpha + (H_E)_\alpha\,,$$

We can show $\|H_X\psi_0\|$ is small for α small, but the support is no longer X. The easiest way to correct this is by redefining them with a suitably restricted dynamics:

e.g.,

$$K_A^{(\alpha)} = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{itH_A} H_I e^{-itH_A} \, e^{-\alpha t^2} \, dt \, ,$$

and similarly define $K_{\Lambda\setminus A}^{(\alpha)}$ using $H_{\Lambda\setminus A}$, and $K_B^{(\alpha)}$ using $H_{B(2\ell)}$. A good choice for α is $av^2/(2\ell)$, where a and v are the constants appearing in the Lieb-Robinson bound. With this choice all errors are bounded by

$$\epsilon(\ell) \equiv C(d, a, v) J^2 |\partial A| \ell^{d-1/2} e^{-\ell/\xi}$$

with

$$\xi = 2 \max(a^{-1}, av^2/\gamma^2)$$

To summarize:

$$\|H_\Lambda - (K_A^{(\alpha)} + K_B^{(\alpha)} + K_{\Lambda\setminus A}^{(\alpha)})\| \leq \epsilon(\ell)$$

and for $X = A, B, \Lambda \setminus A$,

$$\|K_X^{(\alpha)}\psi_0\| \leq \epsilon(\ell)$$

(2) Now define the projections P_A and $P_{\Lambda\setminus A}$ as the spectral projections of $K_A^{(\alpha)}$ and $K_{\Lambda\setminus A}^{(\alpha)}$ corresponding to the eigenvalues $\leq \sqrt{\epsilon(\ell)}$.
This gives

$$\|(\mathbb{1} - P_A)\psi_0\| \leq \frac{1}{\sqrt{\epsilon(\ell)}}\|K_A^{(\alpha)}\psi_0\| \leq \sqrt{\epsilon(\ell)}$$

and similary for $P_{\Lambda\setminus A}$. Since the projections commute we have the identity
$2(\mathbb{1} - P_A P_{\Lambda\setminus A}) = (\mathbb{1} - P_A)(\mathbb{1} + P_{\Lambda\setminus A}) + (\mathbb{1} - P_{\Lambda\setminus A})(\mathbb{1} + P_A)$,
and we get

$$\|P_0 - P_0 P_A P_{\Lambda\setminus A})\| = \|P_0(\mathbb{1} - P_A P_{\Lambda\setminus A})\| \leq 2\sqrt{\epsilon(\ell)}\,.$$

(3) As the final step, we need to replace the P_0 multiplying $P_A P_{\Lambda\setminus A}$ by something supported in $B(m)$ for a suitable m. We start from the observation that for a s.a. operator with a gap, such as H_Λ, the ground state projection P_0 can be approximated by P_α defined by

$$P_\alpha = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{itH_V} e^{-\alpha t^2} dt \,.$$

If the gap is γ, and with our choice of α, we have

$$\|P_\alpha - P_0\| \leq e^{-\gamma^2/(4\alpha)} \leq e^{-\ell/\xi}$$

We will modify this formula for P_α in two ways: replace e^{itH_Λ} by $e^{it(K_A^{(\alpha)}+K_B^{(\alpha)}+K_{\Lambda\setminus A}^{(\alpha)})}e^{-it(K_A^{(\alpha)}+K_{\Lambda\setminus A}^{(\alpha)})}$, then approximate the result with an operator supported in $B(3\ell)$:

$$\begin{aligned}\tilde{P}_B &= \sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{\infty} e^{it(K_A^{(\alpha)}+K_B^{(\alpha)}+K_{\Lambda\setminus A}^{(\alpha)})}e^{-it(K_A^{(\alpha)}+K_{\Lambda\setminus A}^{(\alpha)})}e^{-\alpha t^2}dt \\ P_B &= \mathrm{Tr}_{\mathcal{H}_{\Lambda\setminus B(3\ell)}}\tilde{P}_B\end{aligned}$$

Then, $\|P_0P_AP_{\Lambda\setminus A}-\tilde{P}_BP_AP_{\Lambda\setminus A}\|$ and $\|\tilde{P}_B-P_B\|$ can both be estimated to be small.

Area Law for Gapped 1-Dim'l Systems

Suppose $d = 1$, $V = [1, L] \subset \mathbb{Z}$ and $n_x \leq n$, for all $x \in [1, L]$. For $1 \leq a \leq b \leq L$, let $\rho_{[a,b]}$ denote the density matrix of P_0 restricted to $\mathcal{A}_{[a,b]}$.

Theorem (Hastings 07)

There exist constants C and $\xi < \infty$ depending only on J and γ, such that

$$S(\rho_{[a,b]}) \leq C\xi \log(\xi) \log(n) 2^{\xi \log(n)}$$

One can take $\xi = 12v/\gamma$.

The approximation theorem is not sufficient to prove the area law by itself, but it is an essential step. Here is how. Consider the (essentially unique) Schmidt decomposition of the pure state $\psi_0 \in \mathcal{H}_A \otimes \mathcal{H}_{\Lambda\setminus A}$:

$$\psi_0 = \sum_{\alpha=1}^{r} \sigma_\alpha \psi_A^\alpha \otimes \psi_{\Lambda\setminus A}^\alpha \,,$$

with o.n. vectors $\psi_X^\alpha \in \mathcal{H}_X$ and $\sigma_\alpha > 0$. r is called the Schmidt rank of ψ_0. For any density matrix ρ, we have

$$S(\rho) \leq \log(\mathrm{rank}\rho)$$

If ρ_A is the restriction of ψ_0, the rank of ρ_A is given by the Schmidt rank of ψ_0 with respect to this decompostion. Therefore, we would like to show that the Schmidt rank is bounded by $C^{|\partial A|}$.

The rank of ρ_A when P_0 is of the form $P_B(P_A \otimes P_{\Lambda\setminus A})$ can be bounded in a similar way.

First, suppose P_A and $P_{\Lambda\setminus A}$ are of rank 1, and

$$P_B = \sum_{j=1}^{R} E_A^j \otimes E_{\Lambda\setminus A}^j$$

for operators $E_X^j \in \mathcal{A}_X$. Then P_0 is of rank one, projecting on a vector of Schmidt rank $\leq R$. Note that $\operatorname{supp} P_B \subset B$ implies $R \leq (\dim \mathcal{H}_{B\cap A})^2$.

By using the spectral decomposition for general P_A and $P_{\Lambda\setminus A}$, we see that

$$\text{rank}\rho_A \leq R \leq (\dim \mathcal{H}_{B\cap A})^2 \times \text{rank}P_A \times \text{rank}P_{\Lambda\setminus A}.$$

For general models, one has to struggle with the fact that it is not clear how to bound $\mathrm{rank} P_A$ and $\mathrm{rank} P_{\Lambda \setminus A}$. In one dimension, Hastings succeeded in bypassing this difficulty in a clever but circuitous way.

For VBS models, in any dimension, $\mathrm{rank} P_A$ and $\mathrm{rank} P_{\Lambda \setminus A}$ are easily seen to be bounded by $c^{|\partial A|}$. So all VBS models satisfy an area law (even without a gap, as long as they satisfy a non-degeneracy condition).

Open Problem: prove an Area Law in higher dimensions.

Lieb-Schultz-Mattis Theorem

The Lieb-Schultz-Mattis (LSM) theorem is a classic result (Annals of Physics, 1961) about the spin-1/2 Heisenberg antiferromagnetic chain. It was generalized to other 1D models by Affleck and Lieb (Lett. Math. Phys., 1985).

A standard example where the LSM theorem applies is the half-integer spin antiferromagnetic Heisenberg chain: $V = [1, L]$:

$$H_L = \sum_{x=1}^{L-1} \mathbf{S}_x \cdot \mathbf{S}_{x+1}$$

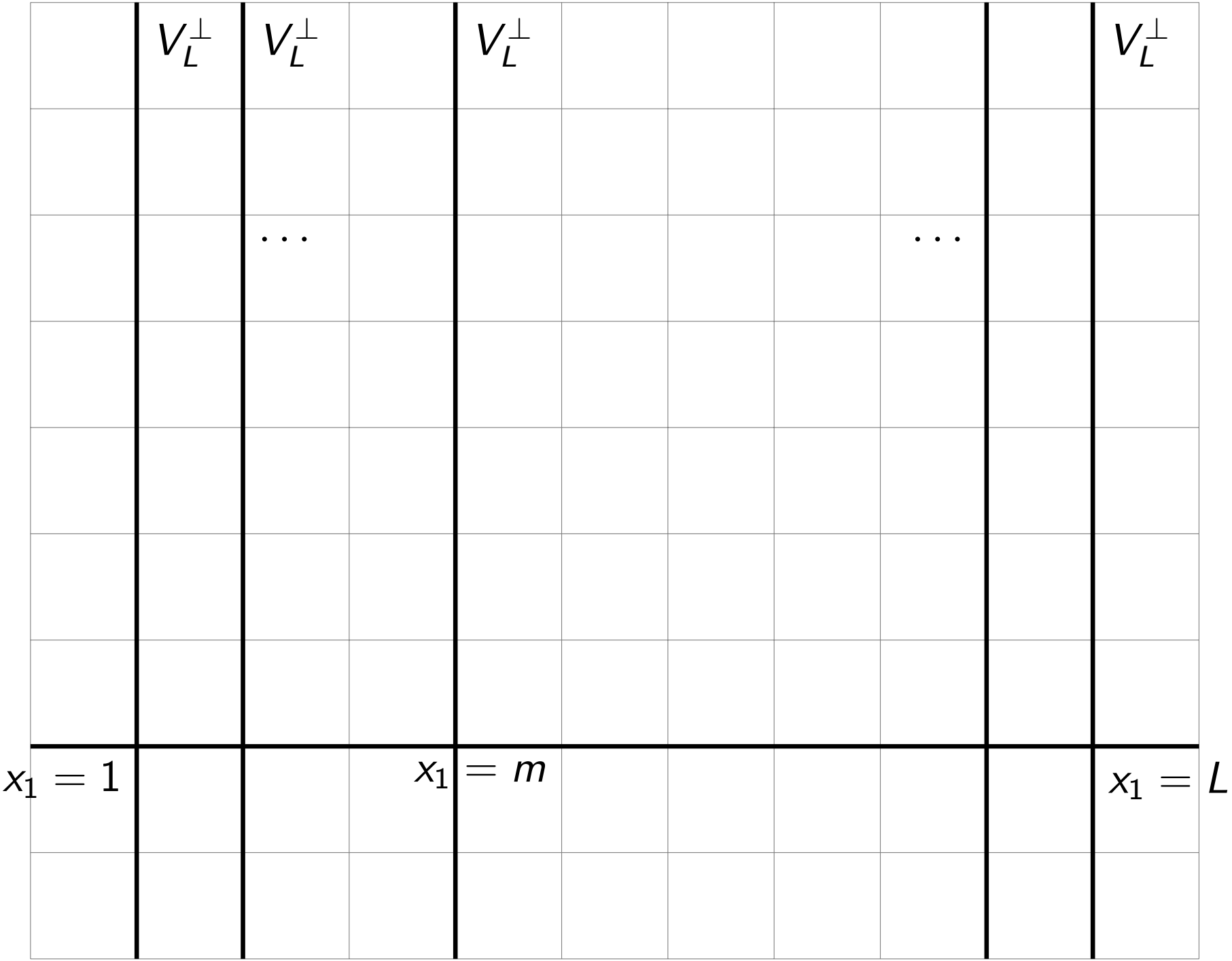
It also applies to the XXZ chain in the disordered regime.

The LSM Theorem states that if the ground state of H_L is unique, then the gap to the first exited state is bounded by C/L. A result of Lieb and Mattis (1966), shows that for the particular model H_L with L even, this is indeed the case. The generalization by Affleck and Lieb in 1985 includes chains with spins of arbitrary half-integer magnitude.

We now discuss the proof of a higher-dimensional version of this result as given by N-Sims (CMP 2007), which is a rigorous version of a result by Hastings (PRB 2004). It relies in an essential way on Lieb-Robinson bounds and the Exponential Clustering Theorem.

Setup

- For simplicity, we will only consider systems defined on subsets $V \subset \mathbb{Z}^d$, $d \geq 1$ of the following form: $V = [1, L] \times V_L^\perp \subset \mathbb{Z}^d$, with $V_L^\perp \subset \mathbb{Z}^{d-1}$, such that $|V_L^\perp| \leq CL^{d-1}$.
- We will assume periodic boundary conditions in the first coordinate. The spin systems on each copy of $V_L^\perp$ are the same.
- $V_L^\perp$ can have a mixture of spins of different magnitudes, s_x, but we have to assume that the total spin in each copy of $V^\perp$ is a half-integer: $\sum_{x \in V_L^\perp} s_x = k + 1/2$, for some nonnegative integer k.


$V_L^\perp$
$V_L^\perp$
$V_L^\perp$
$V_L^\perp$
$\cdots$
$\cdots$
$x_1 = 1$
$x_1 = m$
$x_1 = L$

The new LSM Theorem

The result holds for a large class of models H_V. For this talk it suffices to focus on the simplest examples. E.g., the theorem applies is the half-integer spin antiferromagnetic Heisenberg Hamiltonian on V, with *odd* $|V_L^\perp|$, and translation invariance in the first coordinate.

Theorem (Hastings PRB 2004, N-Sims CMP 2007)

If the ground state of H_V is non-degenerate, then the gap above it, γ_L, satisfies

$$\gamma_L \leq C \frac{\log L}{L}$$

for some constant C and all L.

- The interactions should be finite-range and real, but are not limited to pair interactions.
- Only rotation invariance about one axis is used, but the ground state has to be non-degenerate.
- The spins can have a mixture of magnitudes as long as they are uniformly bounded and the total spin in each copy of $V_L^{\perp}$ is half-integral.
- The lattice structure of V_L is not used except for the translation invariance in the horizontal direction.

Structure of the proof

If ψ_0 is the normalized unique ground states, the variational principle gives, for any normalized ψ_1 such that $|\langle\psi_0, \psi_1\rangle| \neq 1$, the bound

$$0 < \gamma \leq \frac{\langle\psi_1, (H - E_0)\psi_1\rangle}{1 - |\langle\psi_0, \psi_1\rangle|^2}$$

So, there are three steps to obtain such a bound:

(1) construction of the trial state ψ_1

(2) estimate of its energy

(3) estimate of its inner product with the ground state.

The upper bounds provided by these estimates contain γ_L in such a way the assumption that $\gamma_L > C(\log L)/L$, with sufficiently large C, leads to a contradiction.

The proof is complicated by the fact that the ground state is unknown, but interesting because it required new (mathematical) understanding of the general properties of quantum spin dynamics and ground state correlations.
Conceptually, the variational state is the ground state of a modified Hamiltonian, H_θ, in which the interactions in one hyperplane have been twisted by an angle θ.
The idea of Hastings (2004) was to describe this state as the solution of a differential equation in the variable θ with the original ground state as initial condition.
Lieb-Robinson bounds and the Exponential Clustering Theorem play a crucial role in estimating the energy of the variational state and proving its orthogonality to the ground state.

1: Construction of the trial state

Twisted interactions: let (x, y) be a horizontal bond in V: $x = (m, v), y = (m+1, v)$, for some $m \in [1, L]$, and $v \in V_L^\perp$. Then, for $\theta \in \mathbb{R}$ we define the twisted Heisenberg interaction at (x, y) by

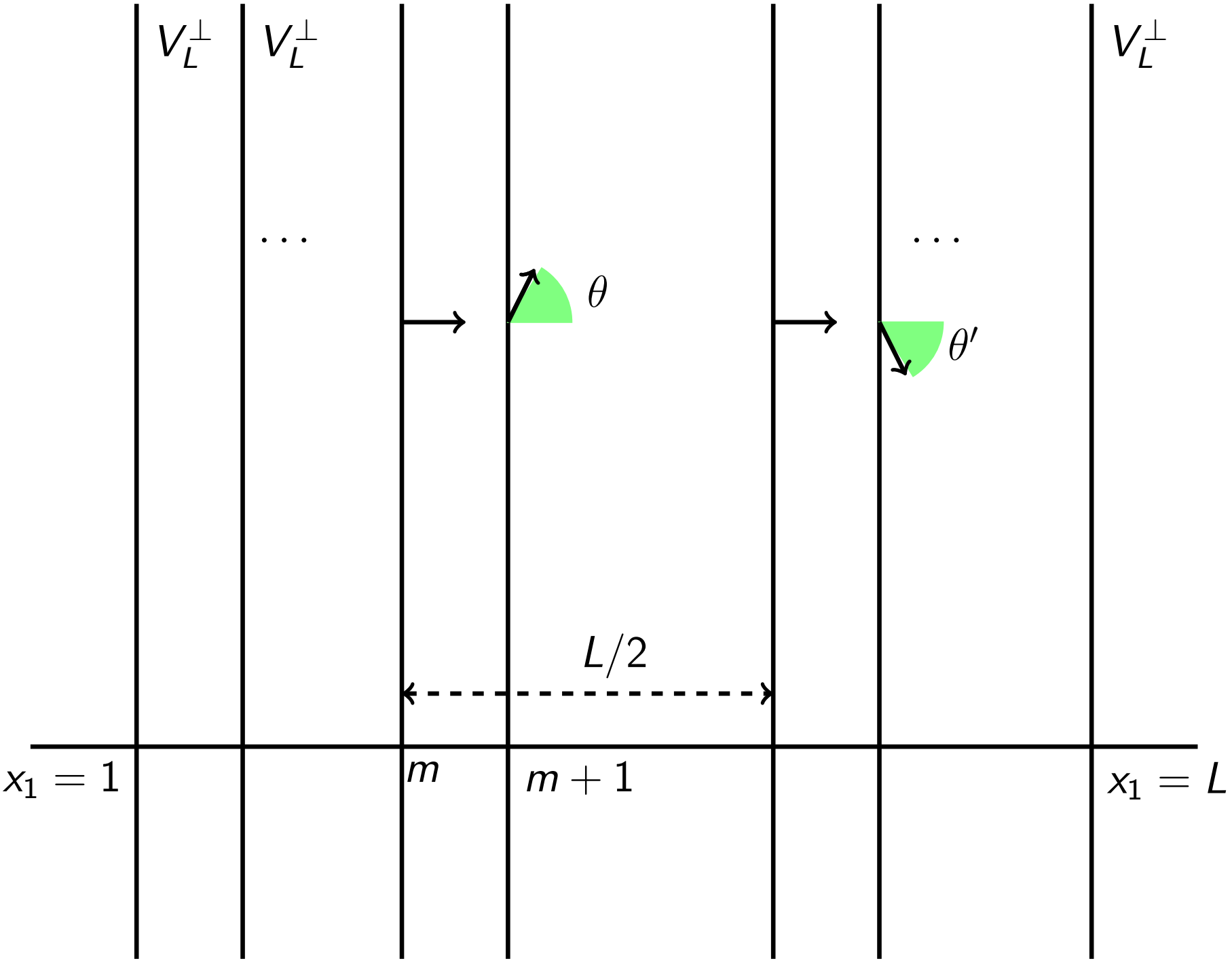
$$h_{xy}(\theta) = \mathbf{S}_x \cdot e^{-i\theta S_y^3} \mathbf{S}_y e^{i\theta S_y^3}$$

Twisted Heisenberg Hamiltonian on $V_L = [1, L] \times V_L^\perp$:

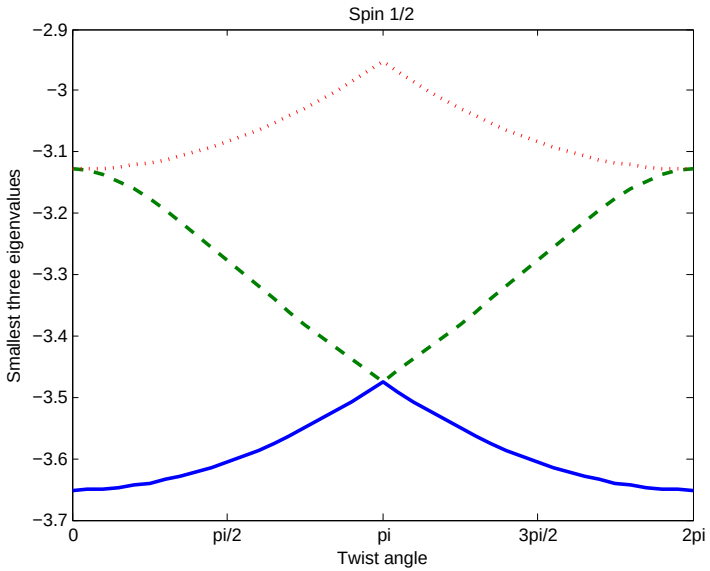
$$H_{\theta,\theta'} = \sum_{|x-y|=1} h_{xy}(\theta_{xy})$$

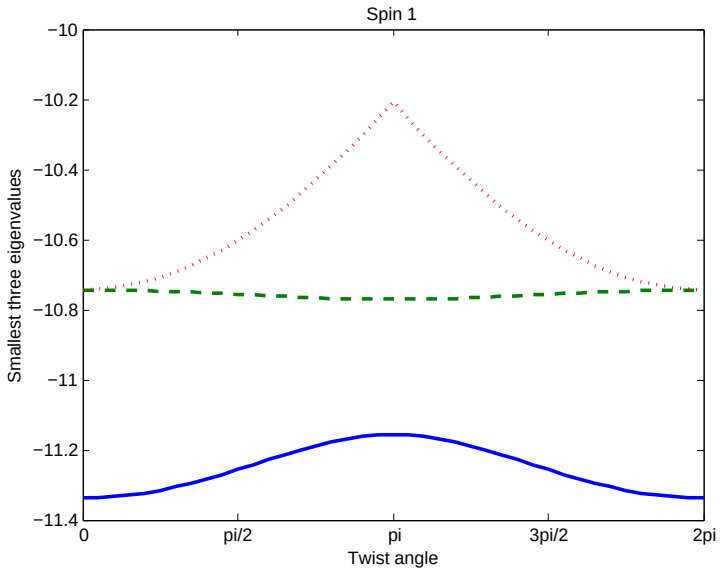
where

$$\theta_{xy} = \begin{cases} \theta & \text{if } x = (m, v), y = (m+1, v) \text{ for some } v \in V_L^\perp \\ \theta' & \text{if } x = (m + L/2, v), y = (m + 1 + L/2, v) \text{ for } v \in V_L^\perp \\ 0 & \text{else} \end{cases}$$


$V_L^\perp$
$V_L^\perp$
$V_L^\perp$
$\cdots$
$\cdots$
θ
θ'
$L/2$
$x_1 = 1$
m
$m+1$
$x_1 = L$

The three lowest energies of $H(\theta, 0)$, as a function of θ, behave differently depending on whether the spins are half-integer (left), or integer (right):





Hastings' idea (PRB 2004): in the half-integer spin case we can obtain the first excited state by applying a "quasi-adiabatic evolution" to the ground state, where θ is the evolution parameter.

It is easy to see that $H_{\theta,-\theta}$ is unitarily equivalent to $H = H_{0,0}$. In particular, for the ground state energy $E_0(\theta, \theta')$ we have

$$\partial_\theta E_0(\theta, -\theta) = 0.$$

By using this in the derivative of the eigenvalue equation $H_{\theta,-\theta}\psi_0(\theta, -\theta) = E_0\psi_0(\theta, -\theta)$, one obtains

$$\partial\psi_0(\theta) = -\frac{1}{H_{\theta,-\theta} - E_0}[\partial_\theta H_{\theta,-\theta}]\psi_0(\theta).$$

This can formally be written using the Heisenberg dynamics $\tau_t(A) = e^{itH} A e^{-itH}$, for any observable A, as follows:

$$\partial\psi_0(\theta) = -\int_0^\infty \tau_{it}(\partial_\theta H_{\theta,-\theta})\psi_0(\theta)\, dt$$

To make things well-defined we introduce parameters $a, T > 0$ and define

$$B_{a,T}(A, H) = -\int_0^T dt[A_a(it, H) - A_a(it, H)^*]$$

where

$$A_a(it, H) = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} ds \frac{e^{-as^2}}{s - it}\tau_s(A)$$

Note that $\partial_\theta H_{\theta,-\theta}$ contains terms localized at bonds (x, y) of the form $x = (m, v), y = (m + 1, v)$ and $x = (m + L/2, v), y = (m + 1 + L/2, v)$, for some $v \in V_L^\perp$. We denote these two types of terms grouped together by $\partial_1 H$ and $\partial_2 H$. Then,

$$B_{a,T}(\partial_\theta H_{\theta,-\theta}, H) = B_{a,T}(\partial_1 H, H) - B_{a,T}(\partial_2 H, H)$$

Hastings' insight: we can use this equation for $\psi_0(\theta, -\theta)$ with $B_{a,T}(\partial_\theta H_{\theta,-\theta}, H)$ replaced by $B_{a,T}(\partial_1 H, H)$, and suitably chosen parameters a and T, to obtain an equation for an approximation of $\psi_0(\theta, 0)$.

Hastings' Equation for the variational state is then:

$$\partial_\theta \psi_{a,T}(\theta) = B_{a,T}(\theta)\psi_{a,T}(\theta),$$

with $B_{a,T}(\theta) = B_{a,T}(\partial_1 H, H_{\theta,-\theta})$ and initial condition

$$\psi_{a,T}(0) = \psi_0(0,0)$$

Then, $\psi_1 = \psi_{a,T}(2\pi)$, with $a = \gamma_L/L$, and $T = L/2$, is the variational state we will use.

Remarks: 1) this is equation is norm preserving. 2) It is easy to derive on $O(1)$ a priori upper bound for γ_L.

Locality property of the trial state

Let $\Lambda_{m,L} \subset V_L$ be the subvolume of the form $[m+2-L/4, m-2+L/4] \times V_L^{\perp}$. This is slightly less than half of the system.

Let $\rho_{a,T}(\theta)$ and $\rho_0(\theta, -\theta)$ be the density matrices corresponding to the states $\psi_{a,T}(\theta)$ and $\psi_0(\theta, -\theta)$.

Theorem

Suppose there exists a constant $c > 0$ such that $L\gamma_L \geq c$ and choose $a = \gamma_L/L$ and $T = L/2$. Then, there exists constants $C > 0$ and $k > 0$ such that

$$\sup_{\theta \in [0,2\pi]} \| Tr_{V_L \setminus \Lambda_{m,L}} [\rho_{a,T}(\theta) - \rho_0(\theta, -\theta)] \|_1 \leq C L^{2d} e^{-kL\gamma_L}.$$

This theorem states that dropping one of the terms in the $B-$operator in Hastings Equation does not change much the effect of the other term in its own half of the system.

The proof of this theorem combines to important facts:

(i) $\psi_{a,T}(\theta) \sim X(\theta)\psi_0(0,0)$, for some $X(\theta) \in \mathcal{A}_{\Lambda_{m,L}}$, i.e., an operator localized in $\Lambda_{m,L}$.

(ii) The spatial correlations in $\psi_0(0,0)$ decay exponentially fast with a rate $\sim \gamma_L$.

These two facts are provided by the Lieb-Robinson bound and the Exponential Clustering Theorem, respectively.

2: Energy Estimate

The main idea here is to use the locality property of the trial state and the unitary equivalence of the Hamiltonians $H_{\theta,-\theta}$ to obtain a uniform estimate of the derivative of the function

$$E(\theta) = \langle \psi_{a,T}(\theta), H_{\theta,0}\psi_{a,T}(\theta)\rangle.$$

Since $E(0) = E_0$ and $E(2\pi)$ is the energy of the trial state $\psi_1 = \psi_{a,T}(2\pi)$, this provides a bound for the difference. Explicitly, we can prove the following result.

Theorem

Suppose there exists a constant $c > 0$ such that $L\gamma_L \geq c$ and choose $a = \gamma_L/L$ and $T = L/2$. Then, there exists constants $C > 0$ and $k > 0$ such that

$$|\langle \psi_1, H_L\psi_1\rangle - E_0| \leq CL^{3d-1}e^{-kL\gamma_L}.$$

3: Orthogonality Estimate

By construction, the "quasi-adiabatic" dynamics is norm preserving. So, $\|\psi_1\| = \|\psi_0\| = 1$. To prove that ψ_1 is sufficiently orthogonal to ψ_0 we need to use that the total spin in each transversal system $V_L^\perp$ is half-integral.

Theorem

Suppose there exists a constant $c > 0$ such that $L\gamma_L \geq c$ and choose $a = \gamma_L/L$ and $T = L/2$. Then, there exists constants $C > 0$ and $k > 0$ such that

$$|\langle \psi_{a,T}(2\pi), \psi_0 \rangle| \leq CL^{2d} e^{-kL\gamma_L}.$$

This result is proved by using the invariance of $\psi_0(\theta, -\theta)$ under twisted translations.

Let T be a unitary implementing the translation symmetry in the horizontal direction (in which we have periodic boundary conditions), chosen such that $T\psi_0 = \psi_0$. This is possible since ψ_0 is the unique ground state and $T^* H T = 0$.

Define

$$T_{\theta,\theta'} = T U_m(\theta) U_{m+L/2}(\theta')$$

where $U_n(\theta)$ applies the rotation $e^{i\theta S_x^3}$ to all sites for the form $x = (n, v)$, for some $v \in V_L^\perp$.

Then, it is easy to see that

$$H_{\theta,-\theta} = W^* H(0,0) W,$$

with

$$W = \bigotimes_{m<n\leq m+L/2} U_n(\theta)$$

and that $W^* T W = T_{\theta,-\theta}$ commutes with $H_{\theta,-\theta}$.
Therefore

$$T_{\theta,-\theta}\psi_0(\theta,-\theta) = \psi_0(\theta,-\theta).$$

The idea is again to use the locality properties to study the solution of Hastings' Equation. We can show

$$T_{\theta,0}\psi_{a,T}(\theta) \cong \psi_{a,T}(\theta).$$

Note that, due to the half-integral total spin in each $V_L^{\perp}$, $U_m(2\pi) = -\mathbb{1}$. Therefore

$$T_{2\pi,0} = -T$$

and therefore $T\psi_1 \cong -\psi_1$. Since $T\psi_0 = \psi_0$, this implies that ψ_1 is (nearly) orthogonal to ψ_0.

Concluding remarks

- Studying specific models is important but thinking about general mechanisms is useful too.
- The fun is not over yet!

There are enough open problems for everyone:

- area law in $d > 1$
- Haldane's conjecture
- general stability of gapped ground states
- lower bounds for small gaps; nature of the excitations
- long-time dynamics?
- topological phases, what do they really look like?
- provable convergence of numerical algorithms

Some References

1. O. Bratteli and D.W. Robinson D.W., *Operator Algebras and Quantum Statistical Mechanics. Volume 2.*, Second Edition. Springer-Verlag, 1997.
2. E. Lieb, T. Schultz, and D. Mattis, *Two soluble models of an antiferromagnetic chain*, Ann. Phys. (N.Y.) **16**, 407–466 (1961)
3. E.H. Lieb and D.W. Robinson, *The finite group velocity of quantum spin systems*, Comm. Math. Phys. **28**, 251–257 (1972)
4. M.B. Hastings, *Lieb-Schultz-Mattis in higher dimensions*, Phys. Rev. B **69**, 104431–14 (2004)
5. B. Nachtergaele and R. Sims: Lieb-Robinson Bounds and the Exponential Clustering Theorem. *Comm. Math. Phys.* **265**, 119–130 (2006)
6. M.B. Hastings and T. Koma, *Spectral gap and exponential decay of correlations*, Commun. Math. Phys. **265**, 781–804 (2006)
7. B. Nachtergaele, Y. Ogata, and R. Sims: Propagation of Correlations in Quantum Lattice Systems. *J. Stat. Phys.* **124**, no. 1, 1–13 (2006)
8. B. Nachtergaele and R. Sims: A multi-dimensional Lieb-Schultz-Mattis theorem. *Comm. Math. Phys.* **276**, 437–472 (2007),
9. B. Nachtergaele, H. Raz, B. Schlein, and R. Sims, *Lieb-Robinson Bounds for Harmonic and Anharmonic Lattice Systems*, Commun. Math. Phys., to appear, arXiv.org:0712.3820.
10. B. Nachtergaele, and R. Sims: Locality Estimates for Quantum Spin Systems, in V. Sidovaricius (Ed), Proceedings of ICMP XV, Rio de Janeiro 2006, to appear, arXiv:0712.3318.
11. E. Hamza, S. Michalakis, B. Nachtergaele, and R. Sims, in preparation.