PHASE TRANSITIONS IN CLASSICAL AND QUANTUM HEISENBERG MODELS

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CONTENTS

REFERENCES

"Reflection positivity, infrared bounds, continuous symmetry breaking", Balint Tóth, Prague lectures '96,
http://www.math.bme.hu/~balint/oktatas/statiszikus_fizika/jegyzet/

"Reflection positivity & phase transitions in lattice spin models", Marek Biskup, Prague lectures '06, Lect. Notes Math. 1970, 1-86 (2009)

"Phase transitions & continuous symmetry breaking", Jürg Fröhlich, Vienna lectures '11
http://www.mathphy.uni-tuebingen.de/~chha/speakers.html

"Quantum Heisenberg models & their probabilistic representations", C. Goldschmidt, D.U., P. Windridge, Contemp. Math. 552, 177-224 (2011)

1. CLASSICAL HEISENBERG MODEL

1.1. SETTING

Finite lattice $\Lambda = \{-\frac{L_1}{2}+1, \dots, \frac{L_1}{2}\} \times \dots \times \{-\frac{L_d}{2}+1, \dots, \frac{L_d}{2}\}$

$\mathcal{E}$ = set of edges of Λ, i.e. nearest-neighbors with per. b.c.

At each site x there is a "classical spin" $\sigma_x \in S^2 \subset \mathbb{R}^3$
(N.b. dimension of space is $d = 1, 2, 3, \dots$, but dimension of spin is always 3.)

State space $\Omega_\Lambda = \bigtimes_{x \in \Lambda} S^2 = (S^2)^\Lambda$

Hamiltonian: $H(\underline{\sigma}) = -2 \sum_{\{x,y\} \in \mathcal{E}} \sigma_x \cdot \sigma_y - \vec{h} \cdot \sum_{x \in \Lambda} \sigma_x$

with $\vec{h} \in \mathbb{R}^3$: external magnetic field

Partition function: $Z(\beta, \Lambda, \vec{h}) = \int_{\Omega_\Lambda} d\underline{\sigma} \; e^{-\beta H(\underline{\sigma})}$

Haar measure on S^2, $\int d\sigma = 1$

Order parameter for spontaneous magnetization:

$$\left\langle \left(\frac{1}{|\Lambda|} \sum_{x \in \Lambda} \sigma_x \right)^2 \right\rangle = \frac{1}{|\Lambda|^2} \sum_{x,y \in \Lambda} \sum_{i=1}^{3} \langle \sigma_x^i \sigma_y^i \rangle$$

where $\langle \cdot \rangle = \frac{1}{Z(\beta, \Lambda, \vec{h})} \int_{\Omega_\Lambda} d\underline{\sigma} \cdot e^{-\beta H(\underline{\sigma})}$

Main question: occurrence of ferromagnetism? That is, is the above expression positive, uniformly in Λ, when $\vec{h} = 0$?

- β small: no, as can be proved by high temperature expansions (+ cluster expansion method)
- $d = 1, 2$, all β: no (Mermin–Wagner theorem)
- β large, $d \geq 3$: yes. Amazing result of Fröhlich, Simon, Spencer (1976), reflection positivity & infrared bounds, to be explained below.

1.2 OCCURRENCE OF SPONTANEOUS MAGNETIZATION

We look at correlation functions $\langle \sigma_x^i \sigma_y^i \rangle$. They do not depend on $i = 1, 2, 3$ (rotation invariance of spins). They only depend on $x - y$ (translation invariance).

Notation: $\chi(x) = \langle \sigma_0^3 \sigma_x^3 \rangle = \langle \sigma_y^3 \sigma_{y+x}^3 \rangle$.

Let us introduce the dual lattice for Fourier theory, Λ^*, and the lattice dispersion relation $\varepsilon(k)$, $k \in \Lambda^*$:

$$\Lambda^* = \frac{2\pi}{L_1} \left\{ -\frac{L_1}{2} + 1, \dots, \frac{L_1}{2} \right\} \times \dots \times \frac{2\pi}{L_d} \left\{ -\frac{L_d}{2} + 1, \dots, \frac{L_d}{2} \right\}$$

$$\varepsilon(k) = 2 \sum_{i=1}^{d} (1 - \cos k_i)$$

Theorem (Long-range order, Fröhlich–Simon–Spencer '76)

Assume $\vec{h} = 0$, and $L_1, \dots, L_d$ are even. Then we have the lower bound

$$\frac{1}{|\Lambda|} \sum_{x \in \Lambda} \chi(x) \geq \frac{1}{3} - \frac{1}{\beta |\Lambda|} \sum_{k \in \Lambda^* \setminus \{0\}} \frac{1}{\varepsilon(k)}$$

Consequences: In thermodynamic limit $L_1, \dots, L_d \to \infty$,

$$\liminf_{L_1, \dots, L_d \to \infty} \left\langle \left(\frac{1}{|\Lambda|} \sum_{x \in \Lambda} \sigma_x \right)^2 \right\rangle \geq 1 - \underbrace{\frac{3}{(2\pi)^d \beta}}_{\text{small when } \beta \text{ large}} \underbrace{\int_{[-\pi, \pi]^d} \frac{dk}{\varepsilon(k)}}_{< \infty \text{ if } d \geq 3}$$

In words, the classical Heisenberg model exhibits spontaneous magnetization at sufficiently low temperatures!

<u>Structure of proof</u>:

LRO (theorem above)

$\Uparrow$ Fourier

IRB $\quad \hat{\chi}(k) \leq \frac{1}{\beta \varepsilon(k)}$

$\Uparrow$ $v_x = \eta \cos(kx)$

GD $\quad Z(\underline{v}) \leq Z(0)$

$\Uparrow$ really nice!

RP $\quad Z(v_1, v_2)^2 \leq Z(v_1, Rv_1)\, Z(Rv_2, v_2)$

These steps are explained in Sections 1.3 – 1.6 below.

1.3. INFRARED BOUND (IRB) IMPLIES LRO

Definition of <u>Fourier transform</u>: If $f \in \ell^2(\Lambda)$,

$$\hat{f}(k) = \sum_{x \in \Lambda} e^{-ikx} f(x), \quad k \in \Lambda^*$$

$$f(x) = \frac{1}{|\Lambda|} \sum_{k \in \Lambda^*} e^{ikx} \hat{f}(k), \quad x \in \Lambda$$

<u>Lemma</u> (IRB $\Rightarrow$ LRO)

Assume that $\hat{\chi}(k) \leq \frac{1}{\beta \varepsilon(k)}$. Then we get the lower bound in the theorem above.

<u>Proof</u>:

$$\frac{1}{3} = \chi(0) \overset{\text{inv. Fourier}}{=} \frac{1}{|\Lambda|} \hat{\chi}(0) + \frac{1}{|\Lambda|} \underbrace{\sum_{k \in \Lambda^* \setminus \{0\}} \hat{\chi}(k)}_{\in \mathbb{R}}$$

$$= \int_{S^2} d\sigma\, (\sigma_0^3)^2 = \frac{1}{3} \int_{S^2} d\sigma\, \|\sigma_0\|^2$$

Then $\frac{1}{|\Lambda|} \sum_{x \in \Lambda} \chi(x) = \frac{1}{|\Lambda|} \hat{\chi}(0) \geq \frac{1}{3} - \frac{1}{2\beta|\Lambda|} \sum_{k \in \Lambda^* \setminus \{0\}} \frac{1}{\varepsilon(k)}$

$\square$

1.4. GAUSSIAN DOMINATION (GD) IMPLIES IRB

We introduce a partition function $Z(\underline{v})$ that depends on an external real field $\underline{v} = (v_x)_{x\in\Lambda}$. At this stage, we need the discrete Laplacian Δ:

$$(\Delta v)_x = \sum_{y:\{x,y\}\in\mathcal{E}} (v_y - v_x)$$

As a matrix in $\ell^2(\Lambda)$: $\quad \Delta_{xy} = \begin{cases} -2d & \text{if } x=y \\ 1 & \text{if } \{x,y\}\in\mathcal{E} \\ 0 & \text{oth.} \end{cases}$

Exercise: check the useful identity

$$(f, -\Delta g) = \sum_{\{x,y\}\in\mathcal{E}} (f_x - f_y)(g_x - g_y)$$

inner product in $\ell^2(\Lambda)$

This identity is the discrete analogue of $-\int f \frac{d^2}{dx^2} g = \int \frac{df}{dx}\frac{dg}{dx}$.

The Heisenberg Hamiltonian is ($\vec{h}=0$)

$$H(\underline{\sigma}) = -2\sum_{\{x,y\}\in\mathcal{E}} \sigma_x\sigma_y = \sum_{\{x,y\}\in\mathcal{E}} (\sigma_x - \sigma_y)^2 - 2d|\Lambda|$$

Definition: $\quad Z(\underline{v}) = \int_{\Omega_\Lambda} d\underline{\sigma}\, \exp\Big\{-\beta \sum_{\{x,y\}\in\mathcal{E}} (\sigma_x + \underbrace{v_x}_{\equiv v_x \vec{e}_3} - \sigma_y - v_y)^2\Big\}$

We have $Z(0) = Z(\beta,\Lambda,0)\, e^{2d\beta|\Lambda|}$

Lemma (GD $\Rightarrow$ IRB)

Assume that $Z(\underline{v}) \le Z(0)$ $\forall\, \underline{v}$. Then $\hat{\chi}(k) \le \frac{1}{2\beta\varepsilon(k)}$.

Proof: $\quad Z(\underline{v}) = \int_{\Omega_\Lambda} d\underline{\sigma}\, \exp\Big\{-\beta\sum (\sigma_x-\sigma_y)^2 - 2\beta \underbrace{\sum (\sigma_x^3-\sigma_y^3)(v_x-v_y)}_{-(\underline{\sigma},\Delta\underline{v})} - \beta \underbrace{\sum (v_x-v_y)^2}_{(\underline{v},\Delta\underline{v})}\Big\}$

Let $\underline{h} = -\Delta\underline{v}$. Then

$$Z(\underline{v}) \le Z(0) \iff \langle e^{-2\beta(\underline{\sigma},\underline{h})}\rangle \le e^{-\beta(\underline{v},\Delta\underline{v})}$$

We use the inequality with $v_x = \cos(kx)$, $k\in\Lambda^*$.

$$(-\Delta v)_x = -\mathrm{Re}\,(\Delta e^{ikx}) = -\mathrm{Re}\Big(\sum_{j=1}^d e^{ikx+ik_j} + e^{ikx-ik_j} - 2\Big)e^{ikx}$$

$$= -2\,\mathrm{Re}\, e^{ikx}\Big(\sum_{j=1}^d \cos k_j - 1\Big) = \varepsilon(k)\, v_x$$

We see that $\underline{h} = \varepsilon(k)\,\underline{v}$. Consider the field $\eta\underline{v}$, η small.

$$\langle e^{-2\beta\eta\varepsilon(k)(\underline{\sigma},\underline{v})}\rangle \le e^{\beta\eta^2\varepsilon(k)\|\underline{v}\|^2}$$

$$\| $$

$$1 - 2\beta\eta\varepsilon(k)\underbrace{\langle(\underline{\sigma},\underline{v})\rangle}_{=0} + 2\beta^2\eta^2\varepsilon(k)^2 \underbrace{\sum_{x,y}\cos(kx)\cos(ky)\langle\sigma_x^3\sigma_y^3\rangle}_{=\sum_{x,z}\cos(kx)\cos(k(x-z))\,\chi(z)} + O(\eta^4)$$

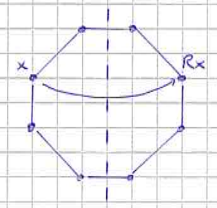
$$\sum_z \cos(k(x-z))\,\chi(z) = \mathrm{Re}\sum_z e^{ikx}e^{-ikz}\chi(z) = \mathrm{Re}\, e^{ikx}\underbrace{\hat{\chi}(k)}_{\in\mathbb{R}\text{ by symmetry}} = \cos(kx)\,\hat{\chi}(k)$$

We get $1 + 2\beta^2\eta^2\varepsilon(k)^2\hat{\chi}(k)\|\underline{v}\|^2 + O(\eta^4) \le 1 + \beta\eta^2\varepsilon(k)\|\underline{v}\|^2 + O(\eta^4)$,

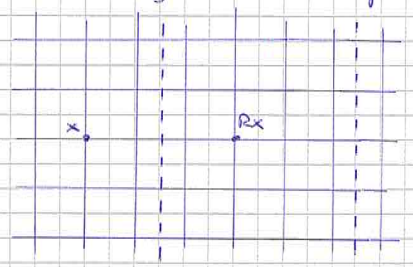
so that $2\beta\,\varepsilon(k)\,\hat{\chi}(k) \le 1$. $\square$

1.5. REFLECTION POSITIVITY (RP) IMPLIES GD

Let $R : \Lambda \to \Lambda$ denote the following reflection map:



$d = 1$



$d = 2$

Let $\Lambda = \Lambda_1 \cup \Lambda_2$ with $\Lambda_1 \cap \Lambda_2 = \emptyset$, $\Lambda_2 = R\Lambda_1$.
Denote $\underline{v} = (v_1, v_2)$, where v_1 is a field on Λ_1 and v_2 is a field on Λ_2.

<u>Lemma</u> (RP $\Rightarrow$ GD)

Assume that $Z(v_1, v_2)^2 \leq Z(v_1, Rv_1)\, Z(Rv_2, v_2)$ for any reflection R across edges, in all lattice directions. Then $Z(\underline{v}) \leq Z(0)$ $\forall$ real field $\underline{v}$.

<u>Proof</u>: Observe that $Z(\text{const}) = Z(0)$, so we need to show that there exists a constant maximizer.
The existence of maximizers follows from $\lim_{v_x \to \pm\infty} Z(\underline{v}) = 0$ for any x, and any fixed $(v_y)_{y \neq x}$.

Let $\underline{v}^*$ be a maximizer. Then (v_1^*, Rv_1^*) is also a maximizer, $\forall$ reflection R. It is then possible to construct a sequence of maximizers and reflections so that maximizers are eventually constant:

$\square$

1.6. PROOF OF REFLECTION POSITIVITY

The concept of reflection positivity is due to Osterwalder and Schrader in the context of field theory. It can be formulated in a general way for lattice systems, see Fröhlich, Israël, Lieb, Simon ('80s). In these notes, we just consider the case of the classical Heisenberg model, following FSS (just below), and we shall see the extension to the quantum Heisenberg model later, following DLS.

<u>Lemma</u>

For every reflection R, we have $Z(v_1, v_2)^2 \leq Z(v_1, Rv_1)\, Z(Rv_2, v_2)$.

Proof: The partition function $Z(v_1, v_2)$ has the form

$$Z(v_1,v_2) = \int_{\Omega_{\Lambda_1}} d\underline{\sigma}_1 \int_{\Omega_{\Lambda_2}} d\underline{\sigma}_2 \; e^{-F(\underline{\sigma}_1,v_1) - F(\underline{\sigma}_2,v_2)} \exp\Big\{-\beta \sum_{\substack{x\in\Lambda_1\\ y\in\Lambda_2\\ \{x,y\}\in\mathcal{E}}} \sum_{i=1}^{3} (\sigma^i_{x,1} + v^i_{x,1} - \sigma^i_{y,2} - v^i_{y,2})^2\Big\}$$

The two half domains, Λ_1 and Λ_2, are coupled by the last exponential. The key insight is to introduce fields to decouple them. Recall that

$$e^{-\frac{1}{2}a^2} = \int_{-\infty}^{\infty} \frac{d\xi}{\sqrt{2\pi}} \, e^{-\frac{1}{2}\xi^2} e^{i\xi a}$$

Introducing a field for each term in the exponential, we get

$$Z(v_1,v_2) = \Big(\prod_{\substack{x\in\Lambda_1\\ y\in\Lambda_2\\ \{x,y\}\in\mathcal{E}}} \prod_{i=1}^{3} \int_{-\infty}^{\infty} \frac{d\xi^i_{xy}}{\sqrt{2\pi}} \, e^{-\frac{1}{2}\xi^{i\,2}_{xy}} \Big)$$

$$\cdot \int_{\Omega_{\Lambda_1}} d\underline{\sigma}_1 \; e^{-F(\underline{\sigma}_1,v_1)} \exp\Big\{ i\sqrt{2\beta} \sum_{\substack{x\in\Lambda_1\\ y\in\Lambda_2\\ \{x,y\}\in\mathcal{E}}} \sum_{i=1}^{3} \xi^i_{xy} \, (\sigma^i_{x,1} + v^i_{x,1})$$

$$\cdot \int_{\Omega_{\Lambda_2}} \cdots$$

Cauchy-Schwarz inequality:

$$Z(v_1,v_2)^2 \le \Big(\prod \prod \int \frac{d\xi^i_{xy}}{\sqrt{2\pi}} \, e^{-\frac{1}{2}\xi^{i\,2}_{xy}} \Big) \int_{\Omega_{\Lambda_1}} d\underline{\sigma}_1 \; e^{-F(\underline{\sigma}_1,v_1)} \, e^{i\sqrt{2\beta}\sum\sum \xi^i_{xy}(\sigma^i_{x1} + v^i_{x1})}$$

$$\cdot \int_{\Omega_{\Lambda_1}} d\underline{\sigma}_1' \; e^{-F(\underline{\sigma}_1',v_1)} \, e^{-i\sqrt{2\beta}\sum\sum \xi^i_{xy}(\sigma'^i_{x1} + v^i_{x1})} \quad \cdot \text{ same in } \Lambda_2$$

$$= Z(v_1, Rv_1) \, Z(Rv_2, v_2) . \qquad \square$$

2. GENERAL SETTING OF QUANTUM SPIN SYSTEMS

References: D. Ruelle, "Statistical Mechanics", 1969
R.B. Israel, "Convexity in the Theory of Lattice Gases", 1979
B. Simon, "The Statistical Mechanics of Lattice Gases", 1993
J. Fröhlich's Vienna lectures

Statistical mechanics is about macroscopic behavior of systems that satisfy known microscopic laws. A standard approach is to start with finite systems and let the system size tend to infinity. Another approch is to introduce the notion of infinite-volume state, and formulate a property in order to characterize equilibrium states (this is the KMS condition).

We choose a fixed infinite lattice, $\mathbb{Z}^d$ for concreteness. Let $\mathcal{H}_0$ the local Hilbert space. We suppose $\dim \mathcal{H}_0 < \infty$ here. (The relevant space for spin $\frac{1}{2}$ is $\mathbb{C}^2$.) For each $x \in \mathbb{Z}^d$, let $\mathcal{H}_x$ be a copy of $\mathcal{H}_0$.

Let $\mathcal{A}_0$ the algebra of operators on $\mathcal{H}_0$ ($\mathcal{A}_0$ is C^*-algebra) and $\mathcal{A}_x$ the copy of $\mathcal{A}_0$.

For each finite subset $\Lambda \subset \mathbb{Z}^d$, let

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

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

(To be precise, $\mathcal{A}_\Lambda$ is the algebra of all linear combinations of operators of the form $A_{x_1} \otimes A_{x_2} \otimes \dots \otimes A_{x_n}$, if $\Lambda = \{x_1, \dots, x_n\}$.)

There is a natural inclusion relation between these algebras: if $\Lambda' \subset \Lambda$ and $a \in \mathcal{A}_{\Lambda'}$, we can construct the operator $a \otimes Id_{\Lambda \setminus \Lambda'}$ in $\mathcal{A}_\Lambda$. Notice that $\underbrace{\|a\|}_{\text{op. norm in } \mathcal{H}_{\Lambda'}} = \underbrace{\|a \otimes Id_{\Lambda \setminus \Lambda'}\|}_{\text{op. norm in } \mathcal{H}_\Lambda}$.

With this construction in mind, we have $\mathcal{A}_{\Lambda'} \subset \mathcal{A}_\Lambda$ if $\Lambda' \subset \Lambda$.

In order to describe infinite-volume systems, it may be tempting to consider the Hilbert space $\bigotimes_{x \in \mathbb{Z}^d} \mathcal{H}_x$. But this is not appropriate — this would be a non-separable Hilbert space, to be avoided at all costs!

Instead, we consider the C^*-algebra of all local operators, i.e. $\bigcup_{\Lambda \text{ finite}} \mathcal{A}_\Lambda$. This is a normed space. Its completion is the <u>algebra of quasi-local observables</u>, denoted $\mathcal{A}$.

An (infinite-volume) <u>state</u> is a positive normalized linear functional ρ on $\mathcal{A}$. That is, it satisfies

$$\rho(Id) = 1 \qquad \text{(normalized)}$$
$$\rho(A^*A) \geq 0 \qquad \text{(positive)}$$

A (translation-invariant) <u>interaction</u> is a family $\{\Phi_X\}_{X \subset \mathbb{Z}^d}$ of operators defined for each finite, ~~connected~~ subset X of $\mathbb{Z}^d$, that satisfies

$$\Phi_X \in \mathcal{A}_X$$
$$\Phi_{X+a} = \tau_a \Phi_X \quad \forall a \in \mathbb{Z}^d \qquad (\tau_a \text{ is transl. op. } \mathcal{A}_X \to \mathcal{A}_{X+a})$$
$$\Phi_X^* = \Phi_X$$

We introduce the following norm on interactions:

$$\|\Phi\|_r = \sum_{X \ni 0} \|\Phi_X\| e^{r|X|}, \qquad r \geq 0$$

This yields Banach spaces of interactions.

A given interaction give rise to a family of <u>Hamiltonians</u> indexed by domains. For Λ a finite subset of $\mathbb{Z}^d$, let

$$H_\Lambda^\Phi = \sum_{X \subset \Lambda} \Phi_X$$

(Remark: the case of domains with periodic boundary conditions does not quite fit this framework; it needs a separate treatment.)

Now that we have Hamiltonians, we can define <u>finite-volume Gibbs states</u>. Let

$$Z_\Lambda^{\beta,\phi} = \underbrace{\mathrm{Tr}}_{\text{trace in } \mathcal{H}_\Lambda} e^{-\beta H_\Lambda^\phi}$$

and for $a \in \mathcal{A}_\Lambda$, let

$$\rho_\Lambda^{\beta,\phi}(a) = \frac{1}{Z_\Lambda^{\beta,\phi}} \mathrm{Tr}\, a\, e^{-\beta H_\Lambda^\phi}$$

We get <u>infinite-volume equilibrium states</u> by considering cluster points of $(\rho_\Lambda^{\beta,\phi})_{\Lambda \subset \mathbb{Z}^d}$, with $\Lambda \nearrow \mathbb{Z}^d$ (we do not want cluster points where Λ tend to $\mathbb{N}^d$, or to a line ...)

[A better way to describe the infinite-volume limit is to observe that the set of finite subsets of $\mathbb{Z}^d$ is a "directed set" where the partial order is the inclusion. Then $(\rho_\Lambda^{\beta,\phi})$ is a net, and there exist converging subnets by a compactness argument. The limits of converging subnets, with $\Lambda_\alpha \nearrow \mathbb{Z}^d$, are infinite-volume states.]

In practice, it is enough to consider the sequence $(\rho_{\Lambda_n}^{\beta,\phi})$ where Λ_n is the box of size n centered at the origin (or at $(\frac{1}{2}, \dots, \frac{1}{2})$) and to consider the cluster points of this sequence.

Let us now look at the KMS condition that characterize infinite-volume equilibrium states. We need to introduce the operator that describes the <u>time evolution</u> of observables:

$$\hat{\alpha}_{t,\phi}(a) = e^{itH_\Lambda^\phi} a\, e^{-itH_\Lambda^\phi}, \quad a \in \mathcal{A}_\Lambda$$

Using cyclicity of the trace, and using the definition above with $t \in \mathbb{C}$, we get the following identity: if $a, b \in \mathcal{A}_\Lambda$,

$$\rho_\Lambda^{\beta,\phi}(a\, \hat{\alpha}_{t,\phi}(b)) = \frac{1}{Z_\Lambda^{\beta,\phi}} \mathrm{Tr}\, a\, e^{itH_\Lambda^\phi} b\, e^{-itH_\Lambda^\phi} e^{-\beta H_\Lambda^\phi}$$

$$= \frac{1}{Z_\Lambda^{\beta,\phi}} \mathrm{Tr}\, e^{itH_\Lambda^\phi + \beta H_\Lambda^\phi} b\, e^{-itH_\Lambda^\phi - \beta H_\Lambda^\phi} a\, e^{-\beta H_\Lambda^\phi}$$

$$= \rho_\Lambda^{\beta,\phi}(\hat{\alpha}_{t-i\beta,\phi}(b)\, a).$$

The idea behind KMS is to use the infinite-volume version of this identity as the definition of equilibrium. We first need to extend $\hat{\alpha}_{t,\phi}$ to the whole of $\mathcal{A}$.

<u>Lemma</u> Let $\mathrm{ad}_A(B) = [A, B]$. Then

$$e^A B\, e^{-A} = \sum_{n \geq 0} \frac{1}{n!} \mathrm{ad}_A^n(B).$$

<u>Proof</u>: The left side is equal to

$$\sum_{k,m \geq 0} \frac{(-1)^m}{k!\, m!} A^k B A^m = \sum_{n \geq 0} \sum_{k=0}^{n} \frac{(-1)^{n-k}}{k!\,(n-k)!} A^k B A^{n-k}$$

We prove by induction that

$$\frac{1}{n!}\,\mathrm{ad}_A^n(B) = \sum_{k=0}^{n} \frac{(-1)^{n-k}}{k!\,(n-k)!}\, A^k B A^{n-k}$$

This is clear for $n=0$. For $n \geq 1$,

$$\frac{1}{n!}\,\mathrm{ad}_A^n(B) = \frac{1}{n!}\left[A\,\mathrm{ad}_A^{n-1}(B) - \mathrm{ad}_A^{n-1}(B)\,A\right]$$

$$= \frac{1}{n!}A^n B + \frac{(-1)^n}{n!} B A^n + \frac{1}{n}\sum_{k=1}^{n-1} A^k B A^{n-k} (-1)^{n-k}\left(\frac{1}{(k-1)!\,(n-k)!} + \frac{1}{k!\,(n-1-k)!}\right)$$

$$= \sum_{k=0}^{n} \frac{(-1)^{n-k}}{k!\,(n-k)!}\, A^k B A^{n-k} \qquad \square$$

We now construct the infinite-volume "time" evolution operator, for all $t \in \mathbb{C}$.

<u>Theorem</u> Assume $t \in \mathbb{C}$ and $\|\Phi\|_r < \infty$ for some $r > 0$.

There exists a unique bounded operator $\alpha_{t,\Phi} : \mathcal{A} \to \mathcal{A}$ such that

$$\lim_{\Lambda \nearrow \mathbb{Z}^d} \|\alpha^{\Lambda}_{t,\Phi}(a) - \alpha_{t,\Phi}(a)\| = 0$$

norm in $\mathcal{A}$

$$\alpha_{s+t}(a) = \alpha_s(\alpha_t(a)) \quad \forall s,t \in \mathbb{C}.$$

The proof is done as follows:

(1) If $|t| < \varepsilon$ and ε is small enough, $(\alpha^{\Lambda}_{t,\Phi}(a))_{\Lambda \subset \mathbb{Z}^d}$ is a Cauchy net for each fixed $a \in \mathcal{A}_\Lambda$ for some finite Λ.

(2) By the uniform boundedness theorem, there exists $\alpha_{t,\Phi}$ with the properties above, at least for $|t| < \varepsilon$.

(3) We use the group property to extend it to all $t \in \mathbb{C}$.

<u>Proof</u>: We show that for any $\eta > 0$, there exists Λ such that $\|\alpha^{\Lambda'}_{t,\Phi}(a) - \alpha^{\Lambda}_{t,\Phi}(a)\| < \eta$ for all $\Lambda' \supset \Lambda$.

By the lemma above,

$$\alpha^{\Lambda}_{t,\Phi}(a) = \sum_{n \geq 0} \frac{(it)^n}{n!}\,\mathrm{ad}^n_{H^{\Phi}_{\Lambda}}(a)$$

$$= \sum_{n \geq 0} \frac{(it)^n}{n!} \sum_{X_1,\dots,X_n \subset \Lambda} [\Phi_{X_1}, [\Phi_{X_2}, \dots [\Phi_{X_n}, a] \dots]]$$

In order for the terms to differ from 0, it is necessary that $X_1 \cap \mathrm{supp}\, a \neq \emptyset$, $X_2 \cap (X_1 \cup \mathrm{supp}\, a) \neq \emptyset$, etc..., where $\mathrm{supp}\, a$ is the support of a, i.e., the smallest set Y such that $a \in \mathcal{A}_Y$. If $\Lambda' \supset \Lambda$, we have

$$\alpha^{\Lambda'}_{t,\Phi}(a) - \alpha^{\Lambda}_{t,\Phi}(a) = \sum_{n \geq 0} \frac{(it)^n}{n!} \sum_{X_1 \cap \mathrm{supp}\, a \neq \emptyset} \sum_{X_2 \cap (X_1 \cup \mathrm{supp}\, a) \neq \emptyset} \cdots$$

$$\cdots \sum_{X_n \cap (X_1 \cup \dots \cup X_{n-1} \cup \mathrm{supp}\, a) \neq \emptyset} \mathbb{1}_{\cup X_i \not\subset \Lambda}\, [\Phi_{X_n}, [X_{n-1}, \dots [\Phi_{X_1}, a] \dots]]$$

Let us introduce

$$K_N = \sum_{n=0}^{N} \frac{(2|t|)^n}{n!} \sum_{X_1 \ni 0} \sum_{X_2 \cap X_1 \neq \emptyset} \cdots \sum_{X_n \cap (X_1 \cup \dots \cup X_{n-1}) \neq \emptyset} e^{r|X_1| + \dots + r|X_n|}\, \|\Phi_{X_1}\| \cdots \|\Phi_{X_n}\|$$

We have $\|\alpha^{\Lambda'}_{t,\Phi}(a) - \alpha^{\Lambda}_{t,\Phi}\| \leq |\mathrm{supp}\, a|\, \|a\| \lim_{N \to \infty} K_N$. We prove that K_N is bounded by some K uniformly in N. Then $\|\alpha^{\Lambda'} - \alpha^{\Lambda}\|$ is bounded by a convergent series, which must go to 0 when $\Lambda \nearrow \mathbb{Z}^d$.

It is not too hard to check that $K_N \leq 1 + \sum_{X \ni 0} 2|H| \|\Phi_X\| \, K_{N-1}^{|X|}$.

It is then easy to prove by induction that $K_N \leq \varkappa$ for some $\varkappa$ slightly larger than 1, provided $\|\Phi\|_r < \infty$ for some $r > 0$, and provided that $|t| < \varepsilon$. Then $(\alpha^{\Lambda}_{t,\Phi})_\Lambda$ is indeed a Cauchy net for small $|t|$, and the limit $\alpha_{t,\Phi}$ is a bounded operator $\mathcal{A} \to \mathcal{A}$ by the uniform boundedness theorem.

If s and t are both less than ε (but not necessarily $s+t$), we have

$$\Phi^{\Lambda}_{s+t,\Phi}(a) = \underbrace{\Phi^{\Lambda}_{s,\Phi}(\Phi_{t,\Phi}(a))}_{\to \Phi_{s,\Phi}(\Phi_{t,\Phi}(a))} + \underbrace{\Phi^{\Lambda}_{s,\Phi}\big(\underbrace{\Phi^{\Lambda}_{t,\Phi}(a) - \Phi_{t,\Phi}(a)}_{\to 0}\big)}_{\to 0}$$

This proves that $\Phi^{\Lambda}_{t,\Phi}(a)$ converges for all $t \in \mathbb{C}$, and the limit satisfies the group property. $\square$

We can now formulate the KMS condition. A state ρ on $\mathcal{A}$ <u>satisfies the KMS condition for the interaction Φ</u> (i.e., it is an infinite-volume equilibrium state) if for all $a, b \in \mathcal{A}$, we have

$$\rho(a\, \alpha_{t,\Phi}(b)) = \rho(\alpha_{t-i\beta,\Phi}(b)\, a).$$

(Compare with finite-volume expression above!) It is not hard to see that the limits $\Lambda \nearrow \mathbb{Z}^d$ of finite-volume Gibbs states are KMS. Also, while it may seem very abstract and general, the set of KMS states does not contain undesirable pathologies.

<u>Thermodynamic functions & Gibbs variational principle</u>

We introduce the <u>entropy</u> s_Λ, which is a function of states, and the <u>free energy</u> f_Λ, which is a function of interactions.

If ρ is a state on $\mathcal{A}$, then for any finite $\Lambda \subset \mathbb{Z}^d$ there exists a unique functional ρ_Λ on $\mathcal{A}_\Lambda$ such that

$$\rho(a) = \mathrm{Tr}\, \rho_\Lambda a \quad , \quad \forall a \in \mathcal{A}_\Lambda.$$

We define

$$s_\Lambda(\rho) = -\frac{1}{|\Lambda|} \mathrm{Tr}_{\mathcal{H}_\Lambda}(\rho_\Lambda \log \rho_\Lambda)$$

$$f_\Lambda(\beta, \Phi) = -\frac{1}{\beta|\Lambda|} \log \mathrm{Tr}\, e^{-\beta H^{\Phi}_\Lambda}$$

$$u_\Lambda(\rho, \Phi) = \frac{1}{|\Lambda|} \rho(H^{\Phi}_\Lambda) \qquad \text{(average energy)}$$

<u>Theorem</u> (Ruelle)

Assume Φ, ρ are translation-invariant, $\|\Phi\|_r < \infty$ for suitable r. Then the limits of $s_\Lambda, f_\Lambda, u_\Lambda$ as $\Lambda \nearrow \mathbb{Z}^d$ (in the sense of Fisher) exist, and the limiting functions enjoy convexity/concavity properties.

(See a good reference for precise statements!)

<u>Theorem</u> (Gibbs variational principle)

$$s(\rho) \leq \beta u(\rho, \phi) - \beta f(\beta, \phi),$$

with equality iff ρ satisfies the KMS condition.

This is a much more attractive characterization of infinite-volume equilibrium states! It works only for translation-invariant states and interactions, though, unlike the KMS condition.

or periodic

Finally, let us remark that translation-invariant states can also be defined as functionals that are tangent to the free energy: if the domain Λ is finite, the Gibbs state can be written as

$$\rho_\Lambda^\phi(a) = -\frac{d}{dh} \frac{1}{\beta|\Lambda|} \log \operatorname{Tr} e^{-\beta H_\Lambda^\phi - \beta h \sum_{x \in \Lambda} \tau_x a} \Big|_{h=0}$$

$$= \frac{d}{dh} f_\Lambda(\beta, \phi + h\phi_a) \Big|_{h=0}$$

where ϕ_a is the interaction from a:

$$\phi_{a,X} = \begin{cases} \tau_x a & \text{if } X = \operatorname{supp} a + x \\ 0 & \text{otherwise} \end{cases}$$

In infinite-volume limit, one can look at the linear functionals that are tangent to $f(\beta, \phi)$.

Finally, it is not hard to check that the set of equilibrium states has the structure of a simplex. It is actually a Choquet simplex, i.e. every state can be written as an average (with suitable measure) over extremal states.

One can define phase transitions as the change of the number of extremal states. There are typically just one equilibrium state at high temperatures, but there may be many at low temperatures. See Fröhlich's notes for more details.

3. QUANTUM HEISENBERG MODEL

3.1. DEFINITION OF THE MODEL

Let $S \in \frac{1}{2}\mathbb{N}$. The spin-$S$ model involves local Hilbert spaces $\mathbb{C}^{2S+1} = \mathcal{H}_0$.

On $\mathbb{C}^{2S+1}$, Let S^1, S^2, S^3 be operators that satisfy the relations

$$(S^1)^2 + (S^2)^2 + (S^3)^2 = S(S+1)\,\mathrm{Id}$$
$$[S^1, S^2] = iS^3, \quad [S^2, S^3] = iS^1, \quad [S^3, S^1] = iS^2$$

Let $\vec{S} = (S^1, S^2, S^3)$ and, with $\vec{a} \in \mathbb{R}^3$, $S^{\vec{a}} = \vec{a} \cdot \vec{S}$.

<u>Lemma</u>

(a) $[S^{\vec{a}}, S^{\vec{b}}] = i S^{\vec{a} \times \vec{b}}$

(b) $e^{-iS^{\vec{a}}} S^{\vec{b}} e^{iS^{\vec{a}}} = S^{R_{\vec{a}}\vec{b}}$

vector $\vec{b}$ rotated around $\vec{a}$ by angle $\|\vec{a}\|$

<u>Proof</u>: (a) follows from linearity & commutation relations. For (b), replace $\vec{a}$ by $s\vec{a}$, and check that both sides satisfy the same differential equation.

$$\frac{d}{ds} e^{-iS^{s\vec{a}}} S^{\vec{b}} e^{iS^{s\vec{a}}} = -i\left[S^{\vec{a}}, e^{-iS^{s\vec{a}}} S^{\vec{b}} e^{iS^{s\vec{a}}}\right]$$

$$\frac{d}{ds} S^{R_{s\vec{a}}\vec{b}} = \left(\frac{d}{ds} R_{s\vec{a}}\vec{b}\right)\cdot\vec{S} = (\vec{a} \times R_{s\vec{a}}\vec{b})\cdot\vec{S} = -i\left[S^{\vec{a}}, S^{R_{s\vec{a}}\vec{b}}\right]$$

$\square$

<u>Case $S = \frac{1}{2}$</u>: Pauli matrices

$$S^1 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S^2 = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S^3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

<u>Case $S = 1$</u>:

$$S^1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad S^2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad S^3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

The most natural Hamiltonians are

$$H^{\text{ferro}}_{\Lambda,h} = -\sum_{\{x,y\}\in\mathcal{E}} \vec{S}_x \cdot \vec{S}_y - h \sum_{x\in\Lambda} S^3_x$$

$$H^{\text{anti}}_{\Lambda,h} = +\sum_{\{x,y\}\in\mathcal{E}} \vec{S}_x \cdot \vec{S}_y - h \sum_{x\in\Lambda} S^3_x$$

Here, the notation $\vec{S}_x \cdot \vec{S}_y$ means the operator in $\mathcal{H}_x \otimes \mathcal{H}_y$ given by $S^1_x S^1_y + S^2_x S^2_y + S^3_x S^3_y$. It is Hermitian. When $S = \frac{1}{2}$, one can check that its eigenvalues are $-\frac{3}{4}$ (multiplicity 1) and $\frac{1}{4}$ (multiplicity 3).

Motivation for the Heisenberg Hamiltonian with spin $S=\frac{1}{2}$:
In $\mathcal{H}_x \otimes \mathcal{H}_y$, consider the symmetry group of rotations, represented by unitary operators $U^{\vec{a}} = e^{i S^{\vec{a}} \otimes \vec{S}^{\vec{a}}}$, $\vec{a} \in \mathbb{R}^3$.
One can check that the group yields irreducible decomposition $\mathcal{H}_x \otimes \mathcal{H}_y$ = singlet $\oplus$ triplet, where singlet is the subspace spanned by $\frac{1}{\sqrt{2}}\left(|\frac{1}{2},-\frac{1}{2}\rangle - |-\frac{1}{2},\frac{1}{2}\rangle\right)$, and triplet is the subspace spanned by $|\frac{1}{2},\frac{1}{2}\rangle$, $|-\frac{1}{2},-\frac{1}{2}\rangle$, and $\frac{1}{\sqrt{2}}\left(|\frac{1}{2},-\frac{1}{2}\rangle + |-\frac{1}{2},\frac{1}{2}\rangle\right)$.

The interaction operator should be rotation invariant, so it must be of the form $c_1 P_{\text{singlet}} + c_2 P_{\text{triplet}}$. Up to constants and a shift by the identity operator, we get $\pm \vec{S}_x \cdot \vec{S}_y$. This suggests $\pm \sum_{\{x,y\}\in\mathcal{E}} \vec{S}_x \cdot \vec{S}_y$.

In these notes, we consider the following Hamiltonian:

$$H^{(u)}_{\Lambda,h} = -2 \sum_{\{x,y\}\in\mathcal{E}} \left(S^1_x S^1_y + u S^2_x S^2_y + S^3_x S^3_y \right) - h \sum_{x\in\Lambda} S^3_x$$

Most interesting cases are
- $u = +1$: Heisenberg ferromagnet
- $u = 0$: XY model
- $u = -1$: $(h=0)$ If Λ is bipartite, $\Lambda = \Lambda_A \overset{\cup}{\cdot} \Lambda_B$, then
  $U^{-1} H^{(u)}_\Lambda U = 2 \sum \left(S^1_x S^1_y - u S^2_x S^2_y + S^3_x S^3_y \right) = H^{\text{anti}}_\Lambda$,
  with $U = \prod_{x\in\Lambda_B} e^{i\pi S^2_x}$.

3.2. OCCURRENCE OF SPONTANEOUS MAGNETIZATION

The order parameter for spontaneous magnetization in the quantum Heisenberg model is

$$\left\langle \left(\frac{1}{|\Lambda|} \sum_{x\in\Lambda} \vec{S}_x \right)^2 \right\rangle = \frac{1}{|\Lambda|^2} \sum_{x,y\in\Lambda} \sum_{i=1}^{3} \langle S^i_x S^i_y \rangle$$

As in the classical case, we show that correlations do not decay. It is enough to prove it for $i=3$. The beautiful result of Dyson, Lieb, Simon (1978) can be formulated as follows:

<u>Theorem</u> (Long-range order, Dyson-Lieb-Simon)
Assume that $\vec{h}=0$, $L_1, \dots, L_d$ even, <u>and $u \in [-1,0]$</u>.
Then we have the lower bound

$$\frac{1}{|\Lambda|} \sum_{x\in\Lambda} \langle S^3_0 S^3_x \rangle \geq \frac{1}{3} S(S+1) - \frac{1}{\sqrt{2}\,|\Lambda|} \sum_{k\neq 0} \sqrt{\frac{\varepsilon_u(k)}{\varepsilon(k)}} - \underbrace{\frac{1}{2\beta|\Lambda|} \sum_{k\neq 0} \frac{1}{\varepsilon(k)}}_{\text{small for } \beta \text{ large, if } 1/\varepsilon(k) \text{ is integrable}}$$

Here, $\varepsilon_u(k) = \sum_{i=1}^{d} \left((1-u\cos k_i) \langle S^1_0 S^1_{e_i} \rangle + (u - \cos k_i) \langle S^2_0 S^2_{e_i} \rangle \right)$.

It is easy to check that $\varepsilon_u(k) \leq S(S+1)$, so the right side is positive for $d \geq 3$ and S large enough, uniformly in Λ. Results can be pushed to $d \geq 3$ and all $S \in \frac{1}{2}\mathbb{N}$ (Kennedy, Lieb, Shastry, ideas of Neves, Perez).
Also, $\beta = \infty$, $d=2$, and $S \geq 1$.

The proof mirrors the one of FSS for classical systems, but several extra difficulties had to be solved. One difficulty is that the IRB does not hold for the usual correlation function. The reason is that

$$\underbrace{\langle \vec{S}_0 \cdot \vec{S}_0 \rangle}_{=3/4} - \underbrace{\langle \vec{S}_0 \cdot \vec{S}_x \rangle}_{\leq \frac{1}{4} \ \forall \text{state}} \geq \frac{1}{2}$$

On the other hand, assuming IRB,

$$|\langle \vec{S}_0 \cdot \vec{S}_0 \rangle - \langle \vec{S}_0 \cdot \vec{S}_x \rangle| = \left| \sum_{k \in \Lambda^*} (1 - e^{ikx}) \widehat{\langle \vec{S}_0 \cdot \vec{S}_x \rangle}(k) \right|$$

$$\leq \frac{1}{|\Lambda|} \frac{\text{const}}{\beta} \sum_{k \in \Lambda^* \setminus \{0\}} \frac{|1 - e^{ikx}|}{\varepsilon(k)}$$

This tends to 0 when $\beta \to \infty$, contradiction.

<u>Structure of the proof</u>

LRO $\Leftarrow$ IRB for corr. fct

$\Uparrow$

IRB for Duhamel fct

$\Uparrow$

GD

$\Uparrow$

RP (requires $u \leq 0$)

This time, we follow the logical order, starting with RP.
Proof will be complete in page 33.

3.3 REFLECTION POSITIVITY FOR QUANTUM SYSTEMS

It is enough for our purpose to consider the claim of Dyson, Lieb, Simon. A more general approach can be found in Fröhlich, Israel, Lieb, Simon.

<u>Lemma</u> (Reflection positivity)

$\mathcal{H} = h \otimes h$, $\dim h < \infty$. Matrices A, B, C_i, D_i, $i = 1, \dots, k$, in the small space h. Then

$$\left| \mathrm{Tr}_{\mathcal{H}} e^{A \otimes \mathrm{Id} + \mathrm{Id} \otimes B - \sum_{i=1}^{k} (C_i \otimes \mathrm{Id} - \mathrm{Id} \otimes D_i)^2} \right|^2$$

$$\leq \mathrm{Tr}_{\mathcal{H}} e^{A \otimes \mathrm{Id} + \mathrm{Id} \otimes \bar{A} - \sum^{k} (C_i \otimes \mathrm{Id} - \mathrm{Id} \otimes \bar{C}_i)^2} \cdot \mathrm{Tr}_{\mathcal{H}} e^{\bar{B} \otimes \mathrm{Id} + \mathrm{Id} \otimes B - \sum^{k} (\bar{D}_i \otimes \mathrm{Id} - \mathrm{Id} \otimes D_i)^2}$$

where $\bar{A}$ denotes the complex conjugate of A (not the adjoint) with respect to a fixed basis (the inequality holds $\forall$ basis).

<u>Proof</u>: Recall Trotter's formula $e^{A+B} = \lim_{n \to \infty} (e^{\frac{1}{n}A} e^{\frac{1}{n}B})^n$

As before, we introduce fields to decouple the two Hilbert spaces. Here, proof for $k=1$ (otherwise, use more fields).

$$\left| \mathrm{Tr}\, e^{A\otimes \mathrm{Id} + \mathrm{Id}\otimes B - (C\otimes \mathrm{Id} - \mathrm{Id}\otimes D)^2} \right|^2 =$$

$$= \lim_{n\to\infty} \left| \mathrm{Tr} \left(e^{\frac{1}{n} A\otimes \mathrm{Id}}\, e^{\frac{1}{n}\mathrm{Id}\otimes B}\, e^{-\frac{1}{n}(C\otimes \mathrm{Id} - \mathrm{Id}\otimes D)^2} \right)^n \right|^2$$

$$= \lim_{n\to\infty} \left| \int d\nu(s_1)\dots d\nu(s_n)\, \mathrm{Tr} \prod_{j=1}^{n} e^{\frac{1}{n}A\otimes \mathrm{Id}}\, e^{\frac{1}{n}\mathrm{Id}\otimes B} \cdot e^{\frac{i s_j}{\sqrt{n}}(C\otimes \mathrm{Id} - \mathrm{Id}\otimes D)} \right|^2$$

$$\boxed{e^{-M^2} = \int_{-\infty}^{\infty} \underbrace{\frac{ds}{2\sqrt{\pi}}\, e^{-\frac{s^4}{4}}}_{d\nu(s)}\, e^{isM}}$$

$$= \lim_{n\to\infty} \left| \int d\nu(s_1)\dots d\nu(s_n)\, \mathrm{Tr}_{\mathcal{H}} \prod_{j=1}^{n} e^{\frac{1}{n}A}\, e^{\frac{i s_j}{\sqrt{n}}C}\, \mathrm{Tr}_{\mathcal{H}} \prod_{j=1}^{n} e^{\frac{1}{n}B}\, e^{-\frac{i s_j}{\sqrt{n}}D} \right|^2$$

$$\boxed{\mathrm{Tr}\, M\otimes N = \mathrm{Tr}\, M\, \mathrm{Tr}\, N}$$

Cauchy-Schwarz

$$\leq \lim_{n\to\infty} \left(\int d\nu(s_1)\dots d\nu(s_n)\, \mathrm{Tr}_{\mathcal{H}} \prod_{j=1}^{n} e^{\frac{1}{n}A}\, e^{\frac{i s_j}{\sqrt{n}}C}\, \mathrm{Tr}_{\mathcal{H}} \prod_{j=1}^{n} e^{\frac{1}{n}\overline{A}}\, e^{-i\frac{s_j}{\sqrt{n}}\overline{C}} \right)$$

$$\left(\dots\, e^{\frac{1}{n}\overline{B}}\, e^{\frac{i s_j}{\sqrt{n}}\overline{D}} \quad e^{\frac{1}{n}B}\, e^{-i\frac{s_j}{\sqrt{n}}D} \right)$$

We used $\overline{MN} = \overline{M}\,\overline{N}$. Retracing the steps backwards, we get the lemma. $\square$

3.4. PARTITION FCT WITH FIELDS & GD

Given a field $\underline{v} = (v_x)_{x\in\Lambda}$ with $v_x \in \mathbb{R}$, let

$$H(\underline{v}) = H^{(u)}_{\Lambda,0} - \sum_{x\in\Lambda} h_x S_x^3$$

where $\underline{h} = \Delta \underline{v}$. The partition function with field is

$$Z(\underline{v}) = \mathrm{Tr}_{\mathcal{H}_\Lambda}\, e^{-\beta H(\underline{v})}$$

Let us also define

$$Z'(\underline{v}) = Z(\underline{v})\, e^{+\frac{1}{4}\beta(\underline{v},\Delta\underline{v})}\, e^{\beta C_\Lambda}$$

The property of "Gaussian domination" is

$$Z(\underline{v}) \leq Z(0)\, e^{-\frac{1}{4}\beta(\underline{v},\Delta\underline{v})} \iff Z'(\underline{v}) \leq Z'(0)$$

As in the classical case, it is a consequence of the following lemma:

<u>Lemma</u> (RP of quantum Heisenberg model)

If $u \leq 0$, then for any reflection R across edges,

$$Z'(v_1, v_2)^2 \leq Z'(v_1, Rv_1)\, Z'(Rv_2, v_2).$$

⚠ The "constant" C_Λ contains the term $-2\sum_{x\in\Lambda}\left((S_x^1)^2+u(S_x^2)^2+(S_x^3)^2\right)$.
It is constant only for $S=\frac{1}{2}$.

<u>Proof</u>: We have

$$H(\underline{v}) = \sum_{\{x,y\}\in\mathcal{E}}\left((S_x^1-S_y^1)^2+(\sqrt{u}\,S_x^2-\sqrt{u}\,S_y^2)^2+(S_x^3+\tfrac{v_x}{2}-S_y^3-\tfrac{v_y}{2})^2\right) + C_\Lambda - \frac{1}{4}\sum_{\{x,y\}\in\mathcal{E}}(v_x-v_y)^2$$

$$H'(\underline{v}) = H(\underline{v}) + \frac{1}{4}\sum_{\{x,y\}\in\mathcal{E}}(v_x-v_y)^2 - C_\Lambda$$

Then $Z'(\underline{v}) = \mathrm{Tr}\, e^{-\beta H'(\underline{v})}$ can be cast in a reflection positive form, by defining

$$A = -\beta\sum_{\substack{\{x,y\}\in\mathcal{E}_1\\ \text{edges in } \Lambda_1}}\left((S_x^1-S_y^1)^2+(\sqrt{u}\,S_x^2-\sqrt{u}\,S_y^2)^2+(S_x^3+\tfrac{1}{2}v_x-S_y^3-\tfrac{1}{2}v_y)^2\right)$$

B = same in Λ_2

$$C_i^1 = \sqrt{\beta}\,S_{x_i}^1,\quad D_i^1 = \sqrt{\beta}\,S_{y_i}^1,\quad C_i^2 = \sqrt{\beta}\,S_{x_i}^2,\quad D_i^2 = \sqrt{\beta}\,S_{y_i}^2,$$

$$C_i^3 = \sqrt{\beta}\,(S_{x_i}^3+\tfrac{1}{2}v_{x_i}),\quad D_i^3 = \sqrt{\beta}\,(S_{y_i}^3+\tfrac{1}{2}v_{y_i})$$

where $\{x_i,y_i\}$ are edges crossing the reflection plane, with $x_i\in\Lambda_1$, $y_i\in\Lambda_2$.

We have $\overline{S_x^1} = S_x^1$, $\overline{S_x^3} = S_x^3$ in the usual basis.
Also, $\overline{\sqrt{u}\,S_x^2} = \sqrt{u}\,S_x^2$ <u>if $u\le 0$</u>.

The present lemma then follows from the previous lemma. □

3.5. GD IMPLIES IRB FOR DUHAMEL FUNCTION

Definition: <u>Duhamel correlation function</u>:

$$(S_0^3, S_x^3) = \frac{1}{Z_{\Lambda,0}^{(u)}(\beta)}\,\frac{1}{\beta}\int_0^\beta ds\,\mathrm{Tr}\,S_0^3\,e^{-sH_{\Lambda,0}^{(u)}}\,S_x^3\,e^{-(\beta-s)H_{\Lambda,0}^{(u)}}$$

<u>Lemma</u> (GD $\Rightarrow$ IRB)

$$\widehat{(S_0^3, S_x^3)}(k) \le \frac{1}{2\beta\,\varepsilon(k)}.$$

<u>Proof</u>: Choose $v_x = \eta\cos(kx)$ in GD inequality. We have

$$Z(\underline{v}) = Z(0) + \frac{1}{2}\left(\underline{h},\ \frac{\partial^2 Z(\underline{v})}{\partial h_x\,\partial h_y}\Big|_{\underline{h}=0}\underline{h}\right) + O(\eta^4)$$

(Recall that $\underline{h} = \Delta\underline{v} = -\varepsilon(k)\,\underline{v}$.)
Also, $Z(\underline{v}) = Z^{(u)}(\beta,\Lambda,\underline{h}) = \mathrm{Tr}\,e^{-\beta H_{\Lambda,\underline{h}}^{(u)}}$.
We can check (using Duhamel's formula) that

$$\frac{1}{Z^{(u)}(\beta,\Lambda,\underline{h})}\,\frac{\partial^2}{\partial h_x\,\partial h_y}\,Z^{(u)}(\beta,\Lambda,\underline{h})\Big|_{\underline{h}=0} = \beta^2\,(S_x^3, S_y^3)$$

Then

$$Z(\underline{v}) = Z(0) + Z(0)\,\frac{1}{2}\eta^2\,\varepsilon(k)^2\sum_{x,y\in\Lambda}\beta^2\cos(kx)\cos(ky)\,(S_x^3,S_y^3) + O(\eta^4)$$

$$= Z(0) + Z(0)\,\frac{\beta^2}{2}\eta^2\,\varepsilon(k)^2\,\widehat{(S_0^3,S_x^3)}(k)\sum_x\cos^2(kx) + O(\eta^4).$$

Also, $e^{-\frac{1}{4}\beta(\underline{v},\Delta\underline{v})} = e^{\frac{1}{4}\beta\,\varepsilon(k)\,\eta^2\sum_x\cos^2(kx)}$.

Looking at order η^2, we get the lemma. □

3.6 DUHAMEL FUNCTION AND FALK-BRUCH INEQUALITY

We need to transfer the IRB for the Duhamel correlation function to the usual corr. function. This can be done using Falk-Bruch's inequality.

Let us consider a more general setting, which has the advantage to alleviate the notation.

Let $\mathcal{H}$ a finite-dimensional Hilbert space, and H a Hermitian operator. The set of linear maps $\mathcal{H} \to \mathcal{H}$ is also a Hilbert space. On this space, we consider the Duhamel inner product

$$(A, B) = \frac{1}{Z} \int_0^1 ds \, \mathrm{Tr}_{\mathcal{H}} \, e^{-(1-s)H} A^* e^{-sH} B$$

where $Z = \mathrm{Tr}\, e^{-H}$. Exercise: check that it is inner product.

Useful identity:

$$\frac{d}{ds} \mathrm{Tr}\, e^{-(1-s)H} A^* e^{-sH} B = \mathrm{Tr}\, e^{-(1-s)H} [H, A^*] e^{-sH} B$$
$$= \mathrm{Tr}\, e^{-(1-s)H} A^* e^{-sH} [B, H]$$

Then $\quad ([A,H], B) = (A, [B,H])$

and $\quad (A, [B,H]) = \frac{1}{Z} \int_0^1 ds \, \frac{d}{ds} \mathrm{Tr}\, e^{-(1-s)H} A^* e^{-sH} B = \langle [B, A^*] \rangle$

Here, $\langle \cdot \rangle = \frac{1}{Z} \mathrm{Tr} \cdot e^{-H}$.

Let $F(s) = \mathrm{Tr}\, e^{-(1-s)H} A^* e^{-sH} A$.

$$\frac{d^2}{ds^2} F(s) = \mathrm{Tr}\, e^{-(1-s)H} [A,H]^* e^{-sH} [A,H] \geq 0,$$

so F is convex (it is actually log-convex, i.e., $F''F - (F')^2 \geq 0$).

$$\frac{1}{2} \langle A^*A + AA^* \rangle = \frac{1}{2Z} \left(F(0) + F(1) \right) \geq \frac{1}{Z} \int_0^1 F(s)\, ds = (A,A)$$

(identity iff $[A,H] = 0$).

We will not use it, but let us notice that we get BOTOAYGOB inequality from Cauchy-Schwarz:

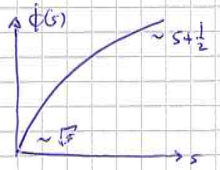
$$\underbrace{|(A, [B,H])|^2}_{\geq |\langle [B, A^*] \rangle|^2} \leq \underbrace{(A,A)}_{\leq \frac{1}{2}\langle A^*A + AA^* \rangle} \underbrace{([B,H], [B,H])}_{= (B, [[B,H], H]) = \langle [[B,H], B^*] \rangle}$$

One of the inequalities above gives an upper bound for the Duhamel function, namely $(A,A) \leq \frac{1}{2} \langle A^*A + AA^* \rangle$. But we need a lower bound in order to extend the IRB bound to the usual correlation function. This is provided by Falk-Bruch inequality (see also DLS).

Let $\phi(s) = \sqrt{s} \coth \frac{1}{\sqrt{s}}$.

Exercise: check that

$\sqrt{s} \leq \phi(s) \leq \sqrt{s} + s$.



Since ϕ is monotone increasing, the following is a lower bound for (A,A).

<u>Lemma</u> (Falk-Bruch inequality)

$$\frac{2\langle A^*A + AA^*\rangle}{\langle [A^*,[H,A]]\rangle} \leq \phi\left(\frac{4\,(A,A)}{\langle [A^*,[H,A]]\rangle}\right)$$

<u>Proof</u>: Recall the function $F(s)$. The inequality can be written as

$$2\,\frac{F(0)+F(1)}{F'(1)-F'(0)} \leq \phi\left(\frac{4\int_0^1 F(s)\,ds}{F'(1)-F'(0)}\right)$$

If $\{\varphi_j\}$ is an orthonormal set of eigenvectors of H with eigenvalues λ_j, we can write

$$F(s) = \sum_{i,j} |(\varphi_i, A\varphi_j)|^2 e^{-\beta\lambda_i} e^{(\lambda_i-\lambda_j)s}$$
$$= \int_{-\infty}^{\infty} e^{st}\,d\mu(t),$$

where μ is a positive measure. We have

$$\int_0^1 F(s)\,ds = \int \frac{e^t-1}{t}\,d\mu(t)$$

$$F(0)+F(1) = \int (e^t+1)\,d\mu(t)$$

$$F'(1)-F'(0) = \int t(e^t-1)\,d\mu(t)$$

Define the probability measure $d\nu(t) = \left(\int t(e^t-1)\,d\mu(t)\right)^{-1} \underbrace{t(e^t-1)}_{\geq 0}\,d\mu(t)$.

We have

$$\frac{\int F(s)\,ds}{F'(1)-F'(0)} = \int \frac{1}{t^2}\,d\nu(t)$$

$$\frac{F(0)+F(1)}{F'(1)-F'(0)} = \int \frac{1}{t}\coth\frac{t}{2}\,d\nu(t)$$

The last step is to use Jensen's inequality (recall that ϕ is concave):

$$\phi\left(\frac{4\int_0^1 F(s)\,ds}{F'(1)-F'(0)}\right) = \phi\left(\int \frac{4}{t^2}\,d\nu(t)\right) \geq \int \phi\left(\frac{4}{t^2}\right)d\nu(t)$$
$$= \int \frac{2}{t}\coth\frac{t}{2}\,d\nu(t) = 2\,\frac{F(0)+F(1)}{F'(1)-F'(0)}. \qquad \square$$

In order to see that the Fourier transform of (S_0^3, S_x^3) can be written in the form (A,A), let us define the Fourier transform of operators: Let

$$\hat{S}_k^3 = \sum_{x\in\Lambda} e^{-ikx} S_x^3, \quad k\in\Lambda^*$$
$$S_x^3 = \frac{1}{|\Lambda|}\sum_{k\in\Lambda^*} e^{ikx}\hat{S}_k^3, \quad x\in\Lambda.$$

We can then check that

$$\widehat{\langle S_0^3 S_x^3\rangle}(k) = \sum_{x\in\Lambda} e^{-ikx}\langle S_0^3 S_x^3\rangle = \frac{1}{|\Lambda|}\sum_{x,y\in\Lambda} e^{-ik(x-y)}\langle S_x^3 S_y^3\rangle = \frac{1}{|\Lambda|}\langle \hat{S}_{-k}^3 \hat{S}_k^3\rangle.$$

The same relation applies to other correlation functions, including Duhamel. Notice that $(S_k^3)^* = S_{-k}^3$, and that $\widehat{(S_0^3, S_x^3)}(k) = (\hat{S}_k^3, \hat{S}_k^3)\frac{1}{|\Lambda|}$ (there is no $-k$ because of the definition of the Duhamel inner product).

We can now apply the Falk-Bruch inequality, and using $\phi(s) \leq \sqrt{s}+s$, we get

Lemma (IRB for usual correlation function)

$$\widehat{\langle S_0^3 S_x^3\rangle}(k) \leq \sqrt{\frac{\mathcal{E}_u(k)}{2\,\mathcal{E}(k)}} + \frac{1}{2\beta\,\mathcal{E}(k)}$$

where $\mathcal{E}_u(k) = \sum_{i=1}^{d} \left((1-u\cos k_i)\langle S_0^1 S_{e_i}^1\rangle + (u-\cos k_i)\langle S_0^2 S_{e_i}^2\rangle \right)$.

As will be apparent in the proof of this lemma, $\mathcal{E}_u(k)$ can be written as $\langle \hat{S}^3_{-k}, [H^{(u)}_{\Lambda,0}, \hat{S}^3_k]\rangle = \left([H^{(u)}_{\Lambda,0}, \hat{S}^3_k], [H^{(u)}_{\Lambda,0}, \hat{S}^3_k] \right)$, up to positive factors, so $\mathcal{E}_u(k) \geq 0$ for all $k \in \Lambda^*$.
When $L_1 = L_2 = \dots = L_d$, we can check that $\mathcal{E}_1(k) = \langle S_0^1 S_{e_1}^1\rangle\, \mathcal{E}(k)$ and $\mathcal{E}_{-1}(k) = -\langle S_0^1 S_{e_1}^1\rangle\, \mathcal{E}(k+\pi)$ (in order to see this, use $H^{(-1)}_{\Lambda,0} \simeq H^{\text{antiferro}}_{\Lambda}$, and spin rotation invariance).

Proof: Let $A = \hat{S}^3_k$ and $H = \beta H^{(u)}_{\Lambda,0}$. Let us calculate the double commutator in Falk-Bruch inequality.

$$[H,A] = \sum_{x\in\Lambda} e^{-ikx}\,[H, S_x^3]$$

$$= -2\beta \sum_{x,y:\,\{x,y\}\in\mathcal{E}} e^{-ikx}\left[S_x^1 S_y^1 + u S_x^2 S_y^2 + S_x^3 S_y^3,\ S_x^3 \right]$$

$$= -2\beta \sum_{x,y:\,\{x,y\}\in\mathcal{E}} e^{-ikx}\left(-i S_x^2 S_y^1 + u i S_x^1 S_y^2 \right)$$

$$[A^*,[H,A]] = 2\beta i \sum_{x,y:\,\{x,y\}\in\mathcal{E}} e^{-ikx}\left[e^{ikx} S_x^3 + e^{iky} S_y^3,\ S_x^2 S_y^1 - u S_x^1 S_y^2 \right]$$

$$= 2\beta \cdot \sum_{x,y:\,\{x,y\}\in\mathcal{E}} \left(S_x^1 S_y^1 - e^{-ik(x-y)} S_x^2 S_y^2 + u S_x^2 S_y^2 - u e^{-ik(x-y)} S_x^1 S_y^1 \right)$$

$$= 4\beta \sum_{\{x,y\}\in\mathcal{E}} \left((1-u\cos k(x-y))\, S_x^1 S_y^1 + (u-\cos k(x-y))\, S_x^2 S_y^2 \right).$$

We have found $\langle [A^*,[H,A]]\rangle = 4\beta|\Lambda|\,\mathcal{E}_u(k)$. The lemma now follows from

$$\frac{4\langle \hat{S}^3_{-k}\hat{S}^3_k\rangle}{4\beta|\Lambda|\,\mathcal{E}_u(k)} \leq \phi\left(\frac{4\,(\hat{S}^3_k, \hat{S}^3_k)}{4\beta|\Lambda|\,\mathcal{E}_u(k)} \right) \Longleftrightarrow \frac{\widehat{\langle S_0^3 S_x^3\rangle}(k)}{\beta\,\mathcal{E}_u(k)} \leq \phi\left(\frac{\widehat{(S_0^3, S_x^3)}(k)}{\beta\,\mathcal{E}_u(k)} \right),$$

and from $\phi(s) \leq \sqrt{s} + s$. $\square$

We finally obtain the lower bound of the theorem of p. 26.

$$\frac{1}{3}S(S+1) = \langle S_0^3 S_0^3\rangle = \frac{1}{|\Lambda|}\sum_{k\in\Lambda^*} \widehat{\langle S_0^3 S_x^3\rangle}(k)$$

Then $\frac{1}{|\Lambda|}\sum_{x\in\Lambda}\langle S_0^3 S_x^3\rangle = \frac{1}{|\Lambda|}\,\widehat{\langle S_0^3 S_x^3\rangle}(0) = \frac{1}{3}S(S+1) - \frac{1}{|\Lambda|}\sum_{k\neq 0}\widehat{\langle S_0^3 S_x^3\rangle}(k)$

Using the IRB of the previous lemma, the theorem follows.