Reflection Positivity and Phase Transitions

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Lattice spin systems

Condensed matter: Atoms form a regular lattice and electrons move in this periodic potential.

Each electron carries a “spin”, i.e. an intrinsic magnetic moment.

**Heisenberg model**: There is exactly one localised electron on each atom, that is characterised by its spin.

Interactions are nearest-neighbour only, and they are invariant under spin rotations.

Important model for magnetism, and more generally for condensed matter physics and quantum information.

Further simplification: classical spin models.
Classical spin models

Lattice $\Lambda = \{-\frac{L}{2} + 1, \ldots, \frac{L}{2}\}^d$ with periodic boundary conditions

State space: $(\mathbb{S}^{N-1})^\Lambda$

Hamiltonian: $H_\Lambda(\sigma) = \sum_{xy \in \Lambda} (\sigma_x - \sigma_y)^2$

Special cases: $N = 0$: self-avoiding random walk; $N = 1$: Ising; $N = 2$: XY model; $N = 3$: classical Heisenberg

Ising model: Phase transitions in dimension 2 and higher; exactly two extremal Gibbs states at low temperatures

For $N \geq 2$: model has continuous symmetry, that prevents ordering in 2D (Mermin-Wagner); spontaneous magnetisation is expected in $d \geq 3$

$N = 2$: [Fröhlich, Pfister ’83] prove that, whenever the free energy is differentiable in $\beta$, there is either a unique extremal Gibbs state, or all extremal states are labelled by the elements of the symmetry group $SO(2)$
Results from RP & IRB

Spectacular results come from the method of **reflection positivity** and **infrared bounds**: the model has spontaneous magnetisation at low enough temperatures!

Finite volume Gibbs state: \[ \langle \cdot \rangle = \frac{1}{Z(\Lambda)} \int_{(S^{N-1})^\Lambda} e^{-\beta H_\Lambda(\sigma)} \, d\sigma \]

**Theorem** [Fröhlich, Simon, Spencer ’76]

\[
\frac{1}{|\Lambda|^2} \sum_{x,y \in \Lambda} \langle \sigma_x \sigma_y \rangle \geq 1 - \frac{3}{\beta |\Lambda|} \sum_{k \in \Lambda^* \setminus \{0\}} \frac{1}{\varepsilon(k)}
\]

Here, \( \Lambda^* = \frac{2\pi}{L} \{-\frac{L}{2} + 1, \ldots, \frac{L}{2}\}^d \) and \( \varepsilon(k) = 2 \sum_{i=1}^d (1 - \cos k_i) \)

As a consequence,

\[
\liminf_{L \to \infty} \left\langle \left( \frac{1}{|\Lambda|} \sum_{x \in \Lambda} \sigma_x \right)^2 \right\rangle \geq 1 - \frac{3}{(2\pi)^d \beta} \int_{[-\pi,\pi]^d} \frac{dk}{\varepsilon(k)}
\]

Hence **there cannot be a single extremal state!** \((d \geq 3, \beta \text{ large})\)
Overview of the method of proof

Let $\kappa(x) = \langle \sigma_0^3 \sigma_x^3 \rangle$ the two-point fct and $\hat{\kappa}(k)$ its Fourier transform:

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

Notice that

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

The goal is to show that

$$\frac{1}{|\Lambda|} \hat{\kappa}(0) > c > 0$$

For $v \in \mathbb{R}^\Lambda$, let

$$Z(v) = \int_{(S^{N-1})^\Lambda} \exp \left\{ -\beta \sum_{xy \in \Lambda} (\sigma_x + v_x - \sigma_y - v_y)^2 \right\} \, d\sigma$$

Notice that $Z(v = 0) = Z(\Lambda)$
Overview of the method of proof

One proves a series of 4 lemmas:

**Lemma 1: Reflection positivity**

\[ Z(v_1, v_2)^2 \leq Z(v_1, Rv_1) Z(Rv_2, v_2) \]

**L2: RP \Rightarrow gaussian domination**

\[ Z(v) \leq Z(0) \]

**L3: GD \Rightarrow infrared bound**

\[ \hat{\kappa}(k) \leq \frac{1}{\beta \varepsilon(k)} \]

**Lemma 4: IRB \Rightarrow theorem**

\[
\frac{1}{|\Lambda|} \hat{\kappa}(0) \geq \frac{1}{3} - \frac{1}{\beta |\Lambda|} \sum_{k \in \Lambda^* \setminus \{0\}} \frac{1}{\varepsilon(k)}
\]
Lemma 1: Reflection positivity

\[ Z(v_1, v_2)^2 \leq Z(v_1, Rv_1) \, Z(Rv_2, v_2) \]

\[
Z(v_1, v_2) = \int_{\Lambda_1} d\sigma_1 \int_{\Lambda_2} d\sigma_2 \, e^{-F(\sigma_1, v_1) - F(\sigma_2, v_2)} \\
\exp\left\{ -\beta \sum_{xy \in P} \sum_{i=1}^{d} (\sigma_{1x}^i + v_{1x}^i - \sigma_{2y}^i - v_{2y}^i)^2 \right\} \\
= \left( \prod_{xy \in P} \prod_{i=1}^{d} \int_{-\infty}^{\infty} d\xi_{xy}^i \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(\xi_{xy}^i)^2} \right) \\
\cdot \int_{\Lambda_1} d\sigma_1 \, e^{-F(\sigma_1, v_1)} \, \exp\left\{ i\sqrt{2\beta} \sum_{xy \in P} \sum_{i=1}^{d} \xi_{xy}^i (\sigma_{1x}^i - v_{1x}^i) \right\} \int_{\Lambda_2} d\sigma_2 \ldots
\]

Lemma follows from Cauchy-Schwarz
From reflection positivity to gaussian domination

**L2: RP \Rightarrow gaussian domination**

\[ Z(v) \leq Z(0) \]

Suppose \((v_1, v_2)\) is maximiser. Then \((v_1, Rv_1)\) is also maximiser by RP

(Periodic boundary conditions are not shown here)
From reflection positivity to gaussian domination

**L2: RP \implies gaussian domination**

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\[ \text{\includegraphics[width=0.5\textwidth]{diagram.png}} \]
From reflection positivity to gaussian domination

\[ L2: \text{RP} \Rightarrow \text{gaussian domination} \]

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Suppose $(v_1, v_2)$ is maximiser. Then $(v_1, Rv_1)$ is also maximiser by RP

There is a space-invariant maximiser!
From gaussian domination to the infrared bound

L3: GD $\Rightarrow$ infrared bound

$$\hat{\kappa}(k) \leq \frac{1}{\beta \varepsilon(k)}$$

$$Z(v) = \int_{(S^{N-1})^\Lambda} d\sigma \exp\left\{ -\beta \sum (\sigma_x - \sigma_y)^2 - 2\beta (\sigma, \Delta v) - \beta \sum (v_x - v_y)^2 \right\}$$

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

Take $v_x = \cos kx$, for fixed $k \in \Lambda^*$. Then $-\Delta v = \varepsilon(k)v$

For small field $\eta v$, the inequality becomes

$$1 + \eta^2 \beta^2 \varepsilon(k)^2 \hat{\kappa}(k) \|v\|^2 + O(\eta^4) \leq 1 + \eta^2 \beta \varepsilon(k) \|v\|^2 + O(\eta^4)$$

This implies the IRB
Lemma 4: IRB ⇒ theorem

$$\frac{1}{|\Lambda|} \hat{\kappa}(0) \geq \frac{1}{3} - \frac{1}{\beta|\Lambda|} \sum_{\kappa \in \Lambda^* \backslash \{0\}} \frac{1}{\varepsilon(k)}$$

We have $$\langle (\sigma_0^3)^2 \rangle = \frac{1}{3}$$; by the inverse Fourier transform,

$$\frac{1}{3} = \kappa(0) = \frac{1}{|\Lambda|} \hat{\kappa}(0) + \frac{1}{|\Lambda|} \sum_{k \in \Lambda^* \backslash \{0\}} \hat{\kappa}(k)$$

The lemma follows immediately.
Quantum Heisenberg models

Lattice $\Lambda = \{-\frac{L}{2} + 1, \ldots, \frac{L}{2}\}^d$ with periodic b.c. as before

Hilbert space $\mathcal{H}_\Lambda = \bigotimes_{x \in \Lambda} \mathbb{C}^{2S+1}$, $S \in \frac{1}{2} \mathbb{N}$

Spin operators $S^1, S^2, S^3$ on $\mathbb{C}^2$ such that $[S^1, S^2] = iS^3$, etc...

$S^i_x = S^i \otimes \text{Id}_\Lambda \setminus \{x\}$

Hamiltonian:

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

- $u = 1$: Heisenberg ferromagnet
- $u = -1$: unitarily equivalent to Heisenberg antiferromagnet
- $u = 0$: quantum XY model

Gibbs state $\langle a \rangle = \text{Tr} \ a \ e^{-\beta H^{(u)}_\Lambda} / \text{Tr} \ e^{-\beta H^{(u)}_\Lambda}$
Difficulties in the quantum case

Let $\kappa(x) = \langle S_0^3 S_x^3 \rangle$. The infrared bound cannot hold!

Indeed, in the case $S = \frac{1}{2}$,

$$\langle \vec{S}_0 \cdot \vec{S}_0 \rangle - \langle \vec{S}_0 \cdot \vec{S}_x \rangle \geq \frac{1}{2}$$

$$= \frac{3}{4} \quad \leq \frac{1}{4}$$

However, assuming the infrared bound to hold,

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

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

which goes to 0 as $\beta \to \infty$, contradiction
Theorem [Dyson, Lieb, Simon ’78] Assume that \( u \in [-1, 0] \). Then

\[
\frac{1}{|\Lambda|^2} \sum_{x, y \in \Lambda} \langle S_x^3 S_y^3 \rangle \geq \frac{1}{3} S(S + 1) - \frac{1}{\sqrt{2}|\Lambda|} \sum_{k \in \Lambda^* \backslash \{0\}} \sqrt{\frac{\varepsilon_u(k)}{\varepsilon(k)}} \\
- \frac{1}{2\beta|\Lambda|} \sum_{k \in \Lambda^* \backslash \{0\}} \frac{1}{\varepsilon(k)}
\]

where \( \varepsilon_u(k) = \sum_{i=1}^{d} ((1 - u \cos k_i)\langle S^1_0 S^1_{e_i} \rangle + (u - \cos k_i)\langle S^2_0 S^2_{e_i} \rangle) \)

Since \( \varepsilon_u(k) \leq S(S + 1) \), the lower bound is positive for \( S \) large enough.

A better lower bound was proposed in [Kennedy, Lieb, Shastry ’88]
Changes in the quantum case

The proof follows [Fröhlich, Simon, Spencer ’76] but with some changes.

First, the infrared bound holds for the Duhamel two-point function:

\[
(S_0^3, S_x^3) = \frac{1}{Z(\Lambda)} \int_0^\beta \text{Tr} \, S_0^3 \, e^{-sH_\Lambda(u)} \, S_x^3 \, e^{-(\beta-s)H_\Lambda(u)}
\]

Unlike \( \langle S_0^3 S_0^3 \rangle \), we do not have \( (S_0^3, S_0^3) = \text{const} \)

Solution: Falk-Bruch inequality [Falk, Bruch ’69]. With \( \Phi(s) = \sqrt{s} \coth \frac{1}{\sqrt{s}} \),

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

This allows to transfer the infrared bound for the Duhamel function, to a lower bound for the usual two-point function.
Reflection positivity for quantum systems

**Lemma**

Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, finite-dimensional, with $\mathcal{H}_1 \cong \mathcal{H}_2$. Matrices $A, B, C_i, D_i$ in small space $\mathcal{H}_1$. Then

$$\left| \text{Tr} \mathcal{H} e^{A \otimes 1 \otimes 1 \otimes B - \sum^k (C_i \otimes 1 - 1 \otimes D_i)^2} \right|^2 \leq \text{Tr} \mathcal{H} e^{A \otimes 1 \otimes 1 \otimes \bar{A} - \sum^k (C_i \otimes 1 - 1 \otimes \bar{C}_i)^2} \cdot \text{Tr} \mathcal{H} e^{\bar{B} \otimes 1 \otimes 1 \otimes B - \sum^k (\bar{D}_i \otimes 1 - 1 \otimes D_i)^2}$$

Here, $\bar{A}$ is the complex conjugate of $A$.

This gives the restriction $u \in [-1, 0]$, which excludes the quantum Heisenberg ferromagnet!

More general approach in [Fröhlich, Israel, Lieb, Simon ’78–80]
Conclusion

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- Does not apply to irregular lattices, nor to quantum Heisenberg ferromagnet.

Further developments in statistical physics: chessboard estimates; matrix models (spin nematics); random loop models.

Our knowledge of statistical physics would be much poorer without the methods of reflection positivity!
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THANK YOU!