Reflection Positivity and Phase Transitions

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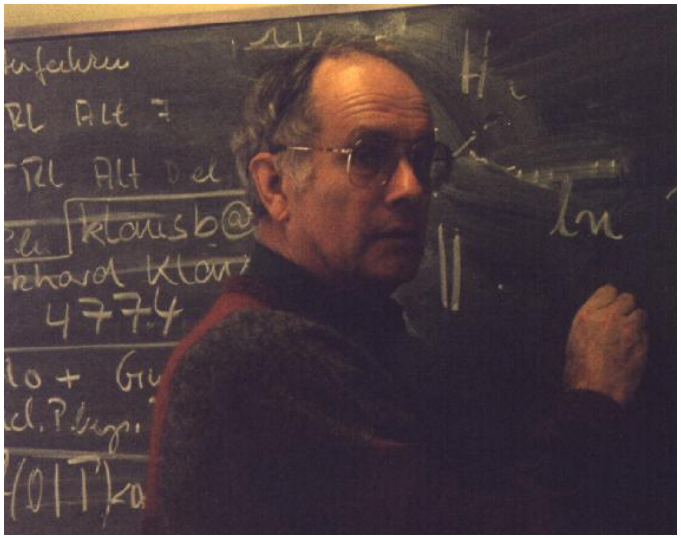
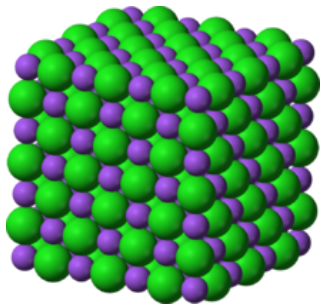
"Positive Reflections", in memory of Robert Schrader
ETH Zürich, 23 May 2016



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



Crystalline structure of sodium chloride (table salt)

Source: Wikipedia

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

$N = 2$: **[Fröhlich, Pfister '83]** prove that, whenever the free energy is differentiable in β, 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: $\langle\cdot\rangle = \frac{1}{Z(\Lambda)}\int_{(\mathbb{S}^{N-1})^\Lambda} \cdot\, \mathrm{e}^{-\beta H_\Lambda(\sigma)}\,\mathrm{d}\sigma$

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

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

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,

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

Hence **there cannot be a single extremal state!** ($d \geqslant 3, \beta$ large)

Overview of the method of proof

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

$$\widehat{\kappa}(k) = \sum_{x \in \Lambda} \mathrm{e}^{-\mathrm{i}kx}\, \kappa(x), \quad k \in \Lambda^*$$

Notice that

$$\kappa(x) = \frac{1}{|\Lambda|} \sum_{k \in \Lambda^*} \mathrm{e}^{\mathrm{i}kx}\, \widehat{\kappa}(k)$$

The goal is to show that $\boxed{\frac{1}{|\Lambda|}\widehat{\kappa}(0) > c > 0}$

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

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

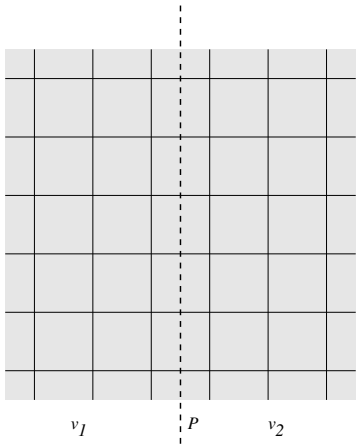
Notice that $Z(v = 0) = Z(\Lambda)$

Overview of the method of proof

One proves a series of 4 lemmas:

Lemma 1: Reflection positivity

$$Z(v_1, v_2)^2 \leqslant Z(v_1, Rv_1)\, Z(Rv_2, v_2)$$



L2: RP $\Rightarrow$ gaussian domination

$$Z(v) \leqslant Z(0)$$

L3: GD $\Rightarrow$ infrared bound

$$\widehat{\kappa}(k) \leqslant \frac{1}{\beta\varepsilon(k)}$$

Lemma 4: IRB $\Rightarrow$ theorem

$$\frac{1}{|\Lambda|}\widehat{\kappa}(0) \geqslant \frac{1}{3} - \frac{1}{\beta|\Lambda|} \sum_{k\in\Lambda^*\setminus\{0\}} \frac{1}{\varepsilon(k)}$$

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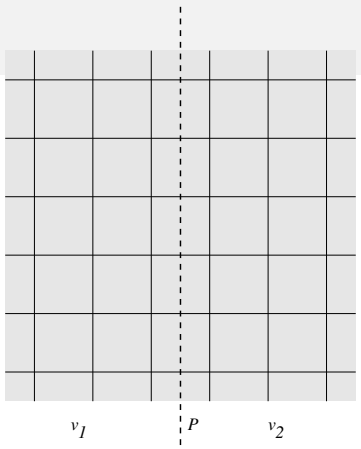


$$Z(v_1,v_2) = \int_{\Lambda_1} \mathrm{d}\sigma_1 \int_{\Lambda_2} \mathrm{d}\sigma_2\, \mathrm{e}^{-F(\sigma_1,v_1)-F(\sigma_2,v_2)}$$

$$\exp\Big\{-\beta \sum_{xy\in P} \sum_{i=1}^{d} (\sigma^i_{1x} + v^i_{1x} - \sigma^i_{2y} - v^i_{2y})^2\Big\}$$

$$= \Big(\prod_{xy\in P} \prod_{i=1}^{d} \int_{-\infty}^{\infty} \frac{\mathrm{d}\xi^i_{xy}}{\sqrt{2\pi}}\, \mathrm{e}^{-\frac{1}{2}(\xi^i_{xy})^2} \Big)$$

$$\cdot \int_{\Lambda_1} \mathrm{d}\sigma_1\, \mathrm{e}^{-F(\sigma_1,v_1)}\, \exp\Big\{\mathrm{i}\sqrt{2\beta} \sum_{xy\in P} \sum_{i=1}^{d} \xi^i_{xy}(\sigma^i_{1x} - v^i_{1x})\Big\} \int_{\Lambda_2} \mathrm{d}\sigma_2 \ldots$$

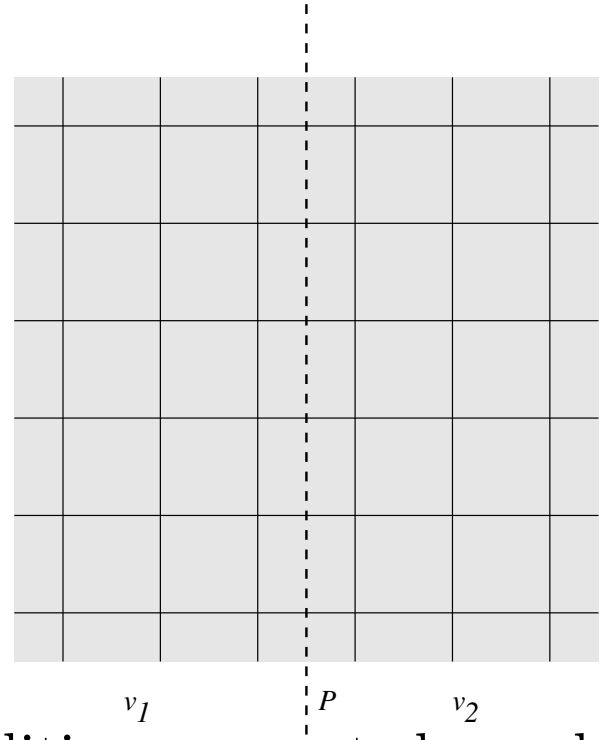
Lemma follows from Cauchy-Schwarz

From reflection positivity to gaussian domination

L2: RP $\Rightarrow$ gaussian domination

$$Z(v) \leqslant Z(0)$$

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



(Periodic boundary conditions are not shown here)

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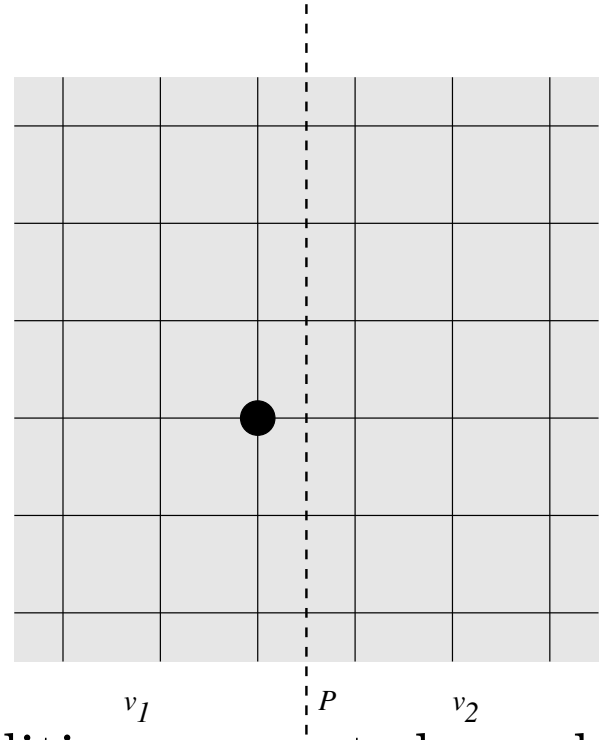

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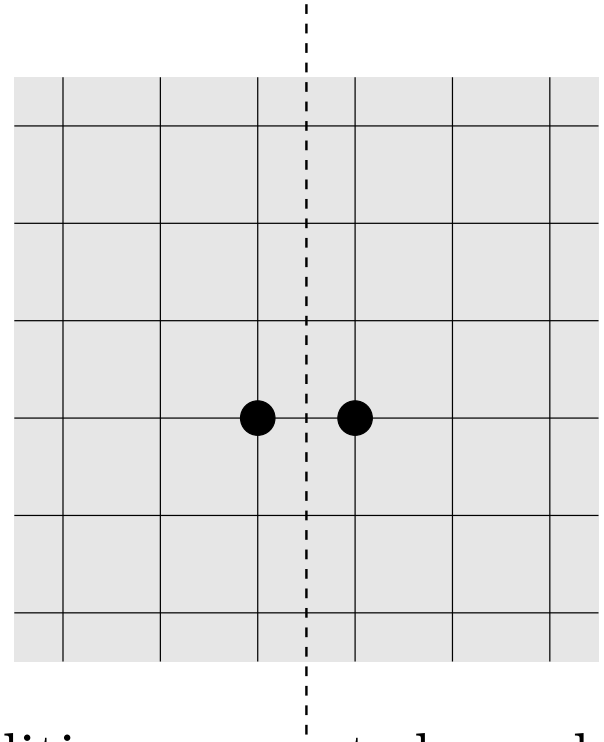

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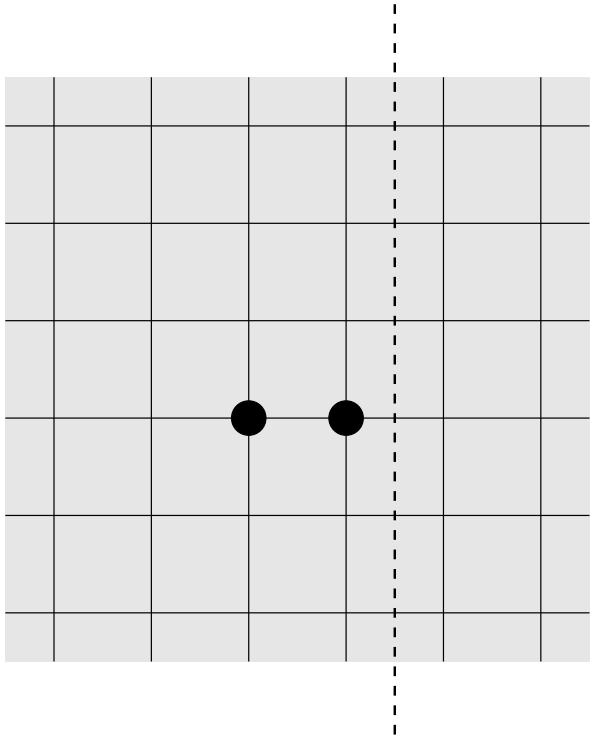

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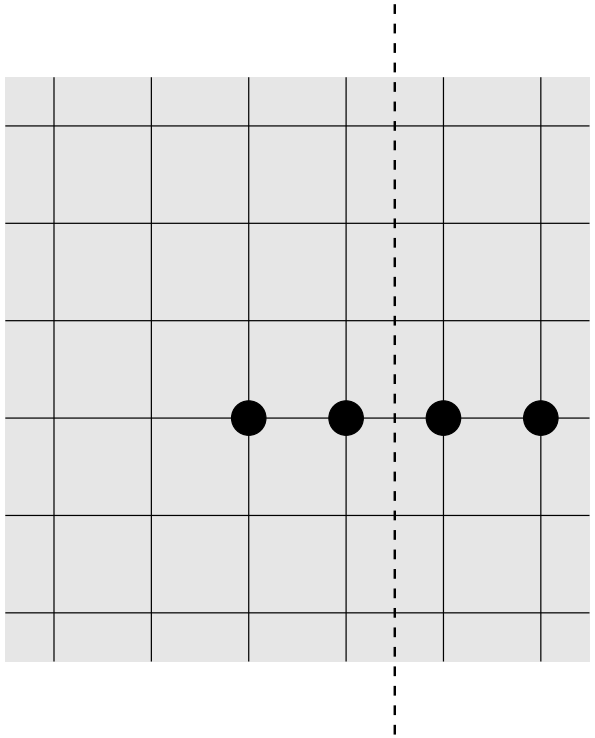

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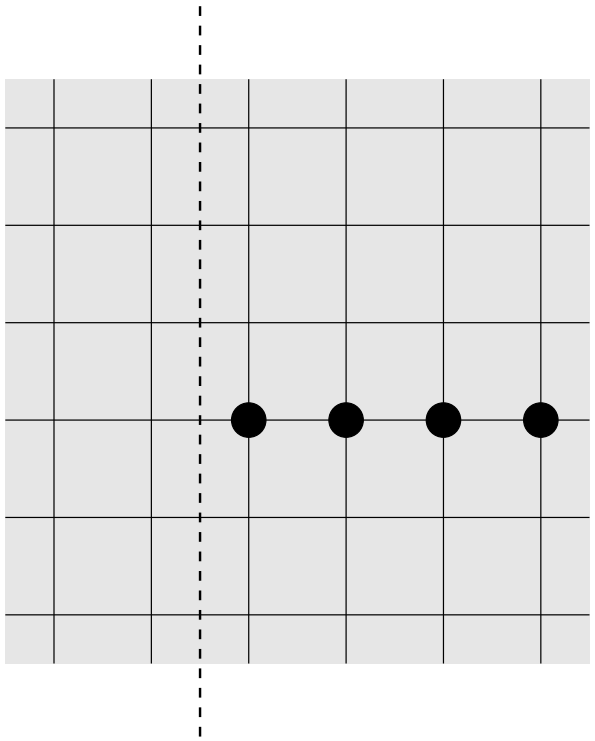

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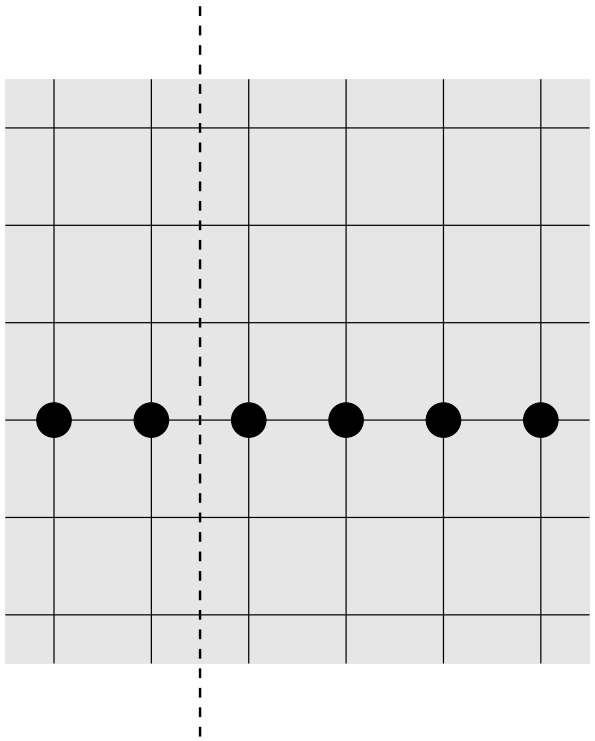

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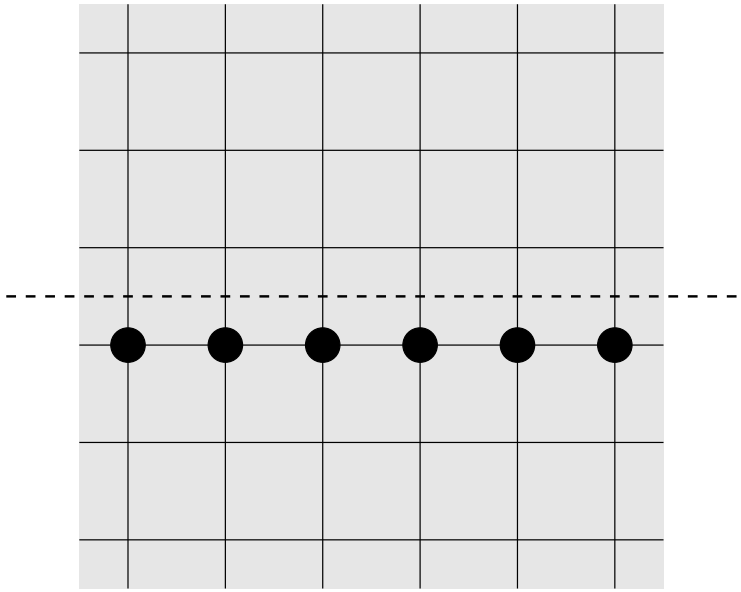

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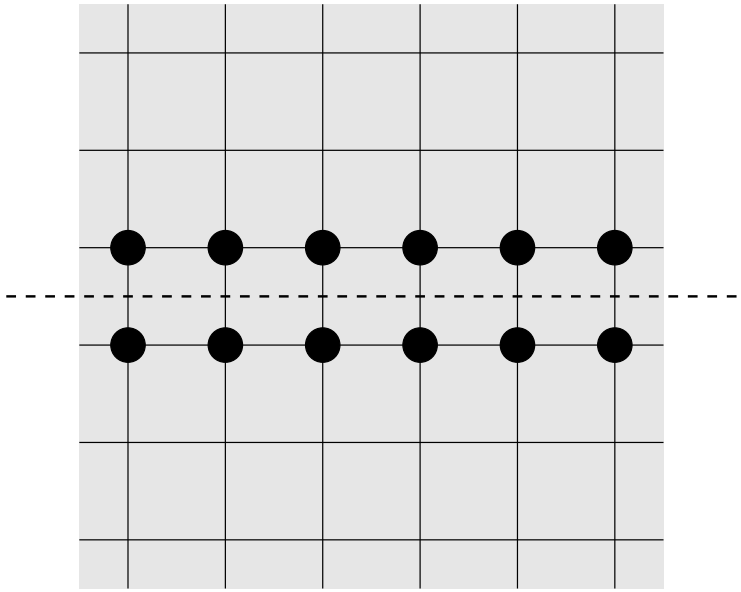

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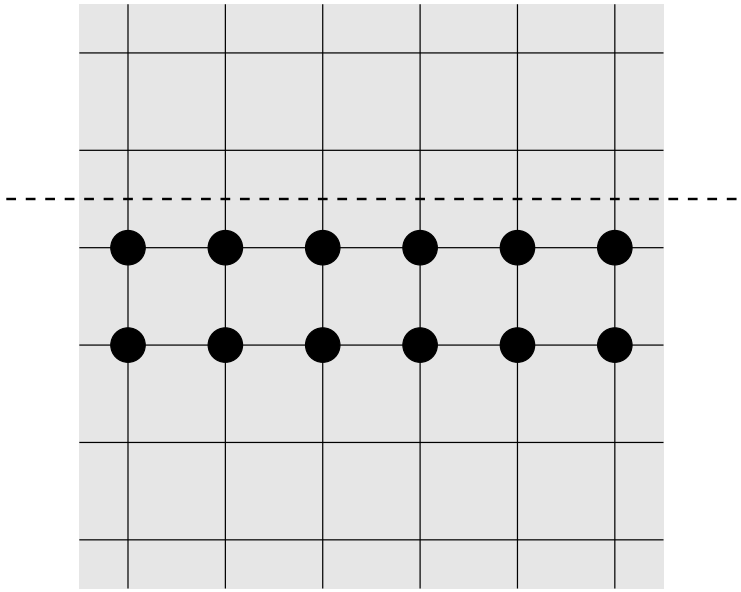

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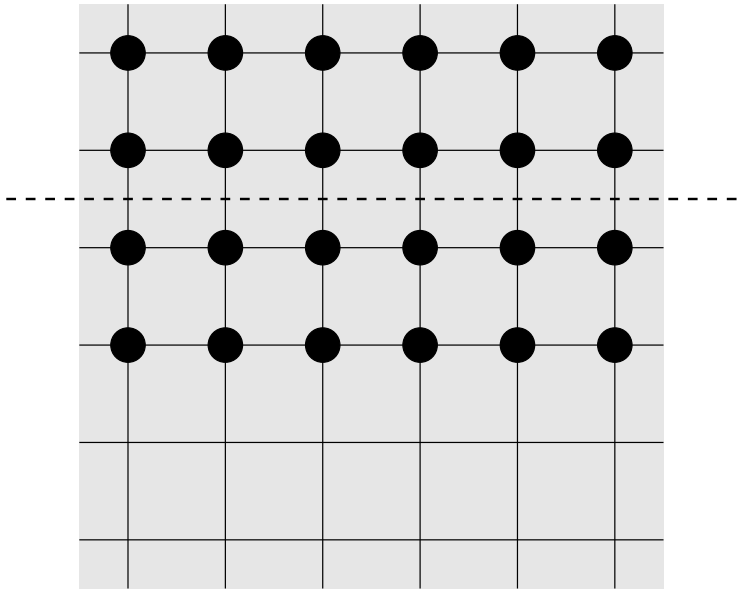

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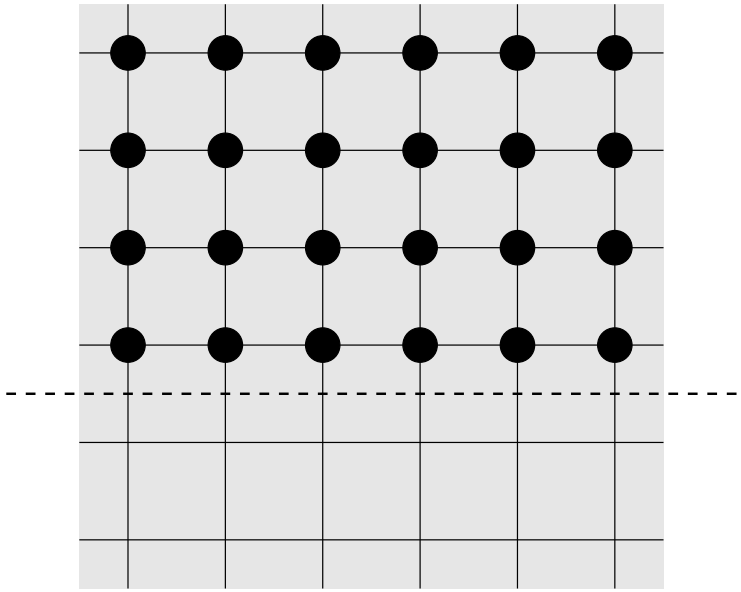

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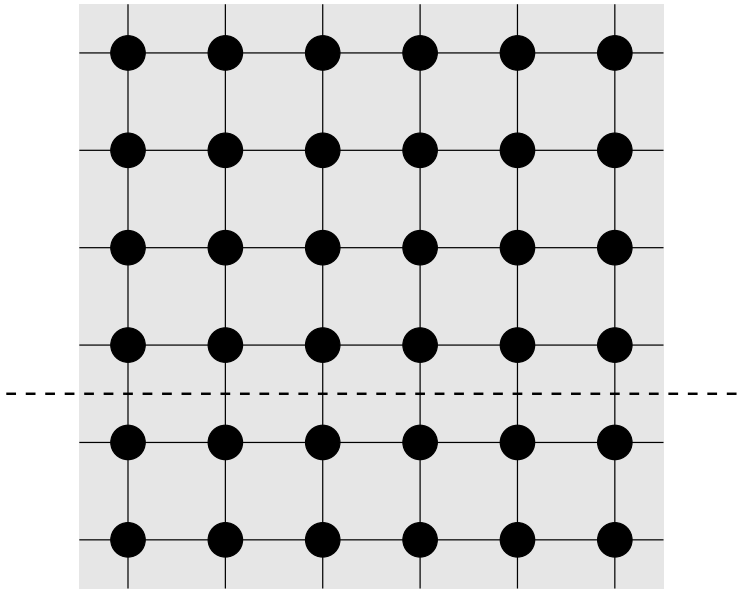

There is a space-invariant maximiser!

From gaussian domination to the infrared bound

L3: GD $\Rightarrow$ infrared bound

$$\widehat{\kappa}(k) \leqslant \frac{1}{\beta\varepsilon(k)}$$

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

$$Z(v) \leqslant Z(0) \quad \Leftrightarrow \quad \big\langle \mathrm{e}^{2\beta(\sigma,\Delta v)} \big\rangle \leqslant \mathrm{e}^{-\beta(v,\Delta v)}$$

Take $v_x = \cos kx$, for fixed $k \in \Lambda^*$. Then $-\Delta v = \varepsilon(k) v$
For small field ηv, the inequality becomes

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

This implies the IRB

From the infrared bound to spontaneous magnetisation

Lemma 4: IRB $\Rightarrow$ theorem

$$\frac{1}{|\Lambda|}\widehat{\kappa}(0) \geqslant \frac{1}{3} - \frac{1}{\beta|\Lambda|}\sum_{k\in\Lambda^*\setminus\{0\}}\frac{1}{\varepsilon(k)}$$

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

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

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 $[S^1, S^2] = \mathrm{i}S^3$, etc...
$S^i_x = S^i \otimes \mathrm{Id}_{\Lambda\setminus\{x\}}$
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 $\langle a \rangle = \mathrm{Tr}\, a\, \mathrm{e}^{-\beta H^{(u)}_\Lambda} \big/ \mathrm{Tr}\ \mathrm{e}^{-\beta H^{(u)}_\Lambda}$

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 $S = \frac{1}{2}$,

$$\underbrace{\langle \vec{S}_0 \cdot \vec{S}_0 \rangle}_{=3/4} - \underbrace{\langle \vec{S}_0 \cdot \vec{S}_x \rangle}_{\leqslant 1/4} \geqslant \tfrac{1}{2}$$

However, assuming the infrared bound to hold,

$$\begin{aligned} \big| \langle \vec{S}_0 \cdot \vec{S}_0 \rangle - \langle \vec{S}_0 \cdot \vec{S}_x \rangle \big| &= \frac{1}{|\Lambda|} \Big| \sum_{k \in \Lambda^*} (1 - \mathrm{e}^{\mathrm{i}kx}) \widehat{\kappa}(k) \Big| \\ &\leqslant \frac{1}{|\Lambda|} \frac{\mathrm{const}}{\beta} \sum_{k \in \Lambda^* \setminus \{0\}} \frac{|1 - \mathrm{e}^{\mathrm{i}kx}|}{\varepsilon(k)} \end{aligned}$$

which goes to 0 as $\beta \to \infty$, contradiction

Extension to quantum systems

Theorem **[Dyson, Lieb, Simon '78]** Assume that $u \in [-1, 0]$. Then

$$\frac{1}{|\Lambda|^2} \sum_{x,y \in \Lambda} \langle S_x^3 S_y^3 \rangle \geqslant \tfrac{1}{3} S(S+1) - \frac{1}{\sqrt{2}|\Lambda|} \sum_{k \in \Lambda^* \setminus \{0\}} \sqrt{\frac{\varepsilon_u(k)}{\varepsilon(k)}} - \frac{1}{2\beta|\Lambda|} \sum_{k \in \Lambda^* \setminus \{0\}} \frac{1}{\varepsilon(k)}$$

where $\varepsilon_u(k) = \sum_{i=1}^d \big((1 - u \cos k_i) \langle S_0^1 S_{e_i}^1 \rangle + (u - \cos k_i) \langle S_0^2 S_{e_i}^2 \rangle \big)$

Since $\varepsilon_u(k) \leqslant S(S+1)$, 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:

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

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

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

$$\frac{2\langle A^* A + A A^* \rangle}{\langle [A^*, [H, A]] \rangle} \leqslant \Phi\Big(\frac{4(A, A)}{\langle [A^*, [H, A]] \rangle} \Big)$$

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 $\mathcal{H}_1 \simeq \mathcal{H}_2$.
Matrices A, B, C_i, D_i in small space $\mathcal{H}_1$. Then

$$\left|\mathrm{Tr}_{\mathcal{H}}\, \mathrm{e}^{A\otimes\mathbb{1}+\mathbb{1}\otimes B-\sum^k (C_i\otimes\mathbb{1}-\mathbb{1}\otimes D_i)^2}\right|^2 \leqslant \mathrm{Tr}_{\mathcal{H}}\, \mathrm{e}^{A\otimes\mathbb{1}+\mathbb{1}\otimes\bar{A}-\sum^k (C_i\otimes\mathbb{1}-\mathbb{1}\otimes\bar{C}_i)^2}$$
$$\cdot\, \mathrm{Tr}_{\mathcal{H}}\, \mathrm{e}^{\bar{B}\otimes\mathbb{1}+\mathbb{1}\otimes B-\sum^k (\bar{D}_i\otimes\mathbb{1}-\mathbb{1}\otimes D_i)^2}$$

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]**

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- Gives interesting results for quantum systems in 2D **[Neves, Perez '86]**
- 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!

THANK YOU!