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Statistical Physics with Continuous Symmetries

I. Warming Up

The object of equilibrium statistical physics:

Understand macroscopic equilibrium behaviour of large systems consisting of many identical, interacting microscopic constituent elements/particles.

- macroscopic: described by a small number of characteristic global parameters.
- equilibrium: steady in time, "balanced" with no flows
- large, many: limit of system size $\to \infty$.

Mathematical description (lattice models):

- system size: $\Lambda \nearrow \mathbb{Z}^d$
- state space: $\Omega_\Lambda := S^\Lambda$, a (locally) compact complete separable metric space. $\omega \in \Omega_\Lambda$ encodes the states of the system.

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- <u>reference measure</u>: $\nu_\Lambda(d\omega)$, "uniform" measure on Ω_Λ given by some natural symmetries.
- <u>Hamiltonian</u>: $H_\Lambda : \Omega_\Lambda \to \mathbb{R}$
  $H_\Lambda(\omega)$ is the "energy" of the system in state ω.
  May have parameters.
  States with lower energy are more stable.
  Ground state(s): minimiser(s) of H_Λ.
- <u>Gibbs state</u>: Probability measure on Ω_Λ which captures the distribution of states at
  inverse temperature $\beta = T^{-1} \geq 0$:

$$\mu_{\Lambda,\beta}(d\omega) := \frac{1}{Z_{\Lambda,\beta}} e^{-\beta H_\Lambda(\omega)} \nu_\Lambda(d\omega)$$

Why exactly this formula? We'll see soon.

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- Free energy:

$$f_\Lambda(\beta) := -|\Lambda|^{-1} \log Z_{\Lambda,\beta}$$

It inherits the parameters of H_Λ

- Thermodynamic limit: $\Lambda \nearrow \mathbb{Z}^d$.

Wanted:

(1) Probabilistic objects: expectations, variances, etc. of relevant "observables", in the thermodynamic limit

(2) Analytic features of of the thermodynamic functions, e.g.,

$$f(\beta) := \lim_{\Lambda \nearrow \mathbb{Z}^d} f_\Lambda(\beta)$$

These are intimately related.

The Holy Trinity of Classical Probability Theory

Let $\xi_1, \xi_2. \ldots, \xi_n$ be i.i.d. random variables whose exponential moment generating function is finite. Denote

$$m := \mathbf{E}\big(\xi\big), \qquad \sigma^2 := \mathbf{Var}\big(\xi\big) = \mathbf{E}\big(\xi^2\big) - \mathbf{E}\big(\xi\big)^2$$

and

$$S_n := \xi_1 + \cdots + \xi_n$$

WLLN:

$$\frac{S_n}{n} \xrightarrow{\mathbf{P}} m$$

Proof: Chebyshev/Markov inequality

$$\mathbf{P}\Big(|S_n - nm| > n\varepsilon \Big) \leq \frac{\mathbf{E}\Big(|S_n - nm|^2 \Big)}{n^2 \varepsilon^2} = \frac{n\sigma^2}{n^2\varepsilon^2} \to 0$$

. . . $\square$

CLT: $$\frac{S_n - nm}{\sqrt{n}} \Rightarrow \texttt{GAU}(0, \sigma^2)$$

Proof: Characteristic function.
W.l.o.g. assume $m = 0$ and let $\varphi : \mathbb{R} \to \mathbb{C}$

$$\varphi(u) := \mathbf{E}\Big(e^{iu\xi}\Big) = \cdots = 1 + 0 \cdot u - \frac{\sigma^2 u^2}{2} + o(u^2)$$

Then

$$\mathbf{E}\Big(e^{iuS_n/(\sigma\sqrt{n})}\Big) = \varphi(\frac{u}{\sigma\sqrt{n}})^n = (1 - \frac{u^2}{2n} + o(n^{-1}))^n \to e^{-\frac{u^2}{2}}$$

$\square$

. . .

Further, denote, and assume $\forall \lambda \in \mathbb{R}: \quad Z(\lambda) < \infty$

$$Z(\lambda) := \mathbf{E}\Big(e^{\lambda \xi_j}\Big), \quad \widehat{I}(\lambda) := \log Z(\lambda), \quad I(x) := \sup_{\lambda} \Big(\lambda x - \widehat{I}(\lambda)\Big)$$

Facts:

- $\widehat{I} : \mathbb{R} \to \mathbb{R}$ is C^∞ and strictly convex.

$$\widehat{I}'(\lambda) = \frac{\mathbf{E}\Big(\xi e^{\lambda\xi}\Big)}{\mathbf{E}\Big(e^{\lambda\xi}\Big)} \qquad \widehat{I}''(\lambda) = \frac{\mathbf{E}\Big(\xi^2 e^{\lambda\xi}\Big)}{\mathbf{E}\Big(e^{\lambda\xi}\Big)} - \left(\frac{\mathbf{E}\Big(\xi e^{\lambda\xi}\Big)}{\mathbf{E}\Big(e^{\lambda\xi}\Big)}\right)^2$$

- $I : \mathbb{R} \to \mathbb{R}_+$ is C^∞ and strictly convex.

Cramér's LDP:

$$-\lim_{n\to\infty} n^{-1} \log \mathbf{P}\Big(\frac{S_n}{n} \in (a,b)\Big) = \inf_{a<x<b} I(x)$$

$$-\lim_{\varepsilon\to 0}\lim_{n\to\infty} n^{-1} \log \mathbf{P}\Big(\frac{S_n}{n} \in (x-\varepsilon, x+\varepsilon)\Big) = I(x)$$

In plain terms: $\mathbf{P}\Big(\frac{S_n}{n} \approx x\Big) \approx e^{-nI(x)}$

Proof: Exponential tilting: Define the *tilted* distribution, with parameter $\lambda \in \mathbb{R}$,

$$\mathbf{E}\Big(f(\xi^{\lambda})\Big) := \frac{\mathbf{E}\Big(f(\xi)e^{\lambda\xi}\Big)}{\mathbf{E}\Big(e^{\lambda\xi}\Big)}$$

Upper/Lower bounds: Subtle "turbo-Markov-inequalities" for the tilted variables and optimisation for λ. $\square$

Exercise (HW): Compute the functions $\widehat{I}(\lambda)$ and $I(x)$ for specific distributions of ξ:
$\mathtt{BERN}$, $\mathtt{BIN}$, $\mathtt{GEOM}$, $\mathtt{NEGGEOM}$, $\mathtt{POI}$, $\mathtt{UNI}$, $\mathtt{GAU}$, $\mathtt{EXP}$, $\mathtt{GAMMA}$, $\mathtt{BETA}$, $\dots$,

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We'll look for these phenomena holding or failing to hold for sums of <u>dependent</u> random variables (under Gibbs measures) naturally showing up in statistical physical models.

Why the Gibbs measure?

Exercise (HW): Let $\vec{X}_n = (X_{n,1}, \ldots, X_{n,n})$ be a random vector sampled uniformly from the sphere

$$\{(x_1, \ldots, x_n) \in \mathbb{R}^n : x_1^2 + \cdots + x_n^2 = En\}.$$

Prove that

$$X_{n,1} \Rightarrow \mathtt{GAU}(0, E), \qquad \text{as } n \to \infty.$$

Exercise (HW): Let $\vec{X}_n = (X_{n,1}, \ldots, X_{n,n})$ be a random vector sampled uniformly from the simplex

$$\{(x_1, \ldots, x_n) \in \mathbb{R}_+^n : x_1 + \cdots + x_n = En\}.$$

Prove that

$$X_{n,1} \Rightarrow \mathtt{EXP}(E^{-1}), \qquad \text{as } n \to \infty.$$

Gibbs Sampling Principle:
Let $\xi_1, \xi_2. \ldots, \xi_n$ be i.i.d. random variables whose exponential moment generating function is finite

$$\forall \lambda \in \mathbb{R}: \qquad Z(\lambda) := \mathbf{E}\Big(e^{\lambda \xi_j}\Big) < \infty.$$

Then (under reasonable regularity conditions)

$$\lim_{\varepsilon \to 0} \lim_{n \to \infty} \mathbf{P}\Big(\xi_1 < x \Big| E - \varepsilon < \frac{\xi_1 + \cdots + \xi_n}{n} < E + \varepsilon\Big) = Z(\lambda^*)^{-1} \mathbf{E}\Big(e^{\lambda^* \xi_1} \mathbb{1}_{\{\xi_1 < x\}}\Big),$$

where $\lambda^* = \lambda^*(E)$ is the unique $\lambda \in \mathbb{R}$ for which

$$Z(\lambda^*)^{-1} \mathbf{E}\Big(e^{\lambda^* \xi_1} \xi_1\Big) = E$$

Exercise (HW): Another probabilistic characterisation of the Gibbs measure.
Let ν_i be a reference measure on the set $\{E_i : i \in I\}$,

$$\mathbf{P}\Big(\xi = E_i\Big) = p_i, \qquad \sum_i p_i = 1$$

and

$$S := -\sum_i p_i \ln \frac{p_i}{\nu_i} \qquad U := \sum_i p_i E_i \qquad F := U - \beta^{-1} S$$

In physical terms: S is the *entropy*, U is the *internal energy*, F is the *free energy*.

Prove that (given β) the unique probability measure which maximises F is

$$p_i^*(\beta) := Z(\beta)^{-1} e^{-\beta E_i} \nu_i$$

Hint: Use Lagrange multipliers.

The Ising Model:

$\Lambda := (\mathbb{Z}/L)^d,$ periodic boundary conditions

$\Omega_\Lambda = \{-1, +1\}^\Lambda, \qquad \underline{\sigma} := \big(\sigma(x)\big)_{x\in\Lambda} \in \Omega_\Lambda$

$\nu_\Lambda =$ counting measure on Ω_Λ

The Hamiltonian and the Gibbs measure:

$$H_\Lambda(\underline{\sigma}) := \underbrace{-\frac{1}{2}\sum_{x\sim y\in\Lambda}\sigma(x)\sigma(y)}_{\mathbb{Z}_2\text{-symmetry}} \underbrace{-h\sum_{x\in\Lambda}\sigma(x)}_{\text{symm. breaking}}$$

$$Z_{\Lambda,\beta,h} := \sum_{\underline{\sigma}\in\Omega_\Lambda} e^{-\beta H_\Lambda(\underline{\sigma})}$$

$$\mu_{\Lambda,\beta,h}(\underline{\sigma}) := \frac{\exp\{-\beta H_\Lambda(\underline{\sigma})\}}{Z_{\Lambda,\beta,h}}$$

Under the probability measure $\mu_{\Lambda,\beta,h}$, $\big(\sigma(x)\big)_{x\in\Omega_\Lambda}$ are identically distributed, <u>dependent</u> random variables. One expects that

- ∘ for small β their qualitative behaviour is close to i.i.d.: WLLN, CLT, LDP hold.
- ∘ for large β their qualitative behaviour may differ from i.i.d.

Main question: Existence of *spontaneous symmetry breaking* and/or *long range order* at low positive temperatures, large values of β?

The <u>*spontaneous magnetisation:*</u> (mind the order of the limits!)

$$m_\Lambda(\beta,h) := \left\langle |\Lambda|^{-1} \sum_{x\in\Lambda} \sigma(x) \right\rangle_{\Lambda,\beta,h} \overbrace{=}^{\text{per. b.c.}} \langle \sigma(0) \rangle_{\Lambda,\beta,h}$$

$$m(\beta,h) := \lim_{\Lambda\nearrow\mathbb{Z}^d} m_\Lambda(\beta,h)$$

$$m(\beta) := \lim_{h\to 0} m(\beta,h) \quad \left\{ \begin{matrix} = \\ \neq \end{matrix} \right\} \; 0 \qquad \mathbf{?}$$

The <u>*long range order parameter:*</u> $h = 0$,

$$r_\Lambda(\beta)^2 := \left\langle \left(|\Lambda|^{-1} \sum_{x\in\Lambda} \sigma(x) \right)^2 \right\rangle_{\Lambda,\beta} \overbrace{=}^{\text{per. b.c.}} |\Lambda|^{-1} \sum_{x\in\Lambda} \langle \sigma(0)\sigma(x) \rangle_{\Lambda,\beta}$$

$$r(\beta)^2 := \lim_{\Lambda\nearrow\mathbb{Z}^d} r_\Lambda(\beta)^2 \quad \left\{ \begin{matrix} = \\ \neq \end{matrix} \right\} \; 0 \qquad \mathbf{?}$$

Fact: $r > 0 \Rightarrow m > 0$.

The Main Mathematical Results about Ising:

∘ [R Peierls (1936)], [TD Lee, CN Yang (1952)], [JG Kirkwood, ZW Salsburg (1953)], . . .

$d \geq 2$:: there exists $\beta_c \in (0, \infty)$ such that

(i) $\beta \in [0, \beta_c)$:: $m = 0$, $r = 0$.

(ii) $\beta \in (\beta_c, \infty)$:: $m > 0$, $r > 0$.

∘ [L Onsager (1944)]

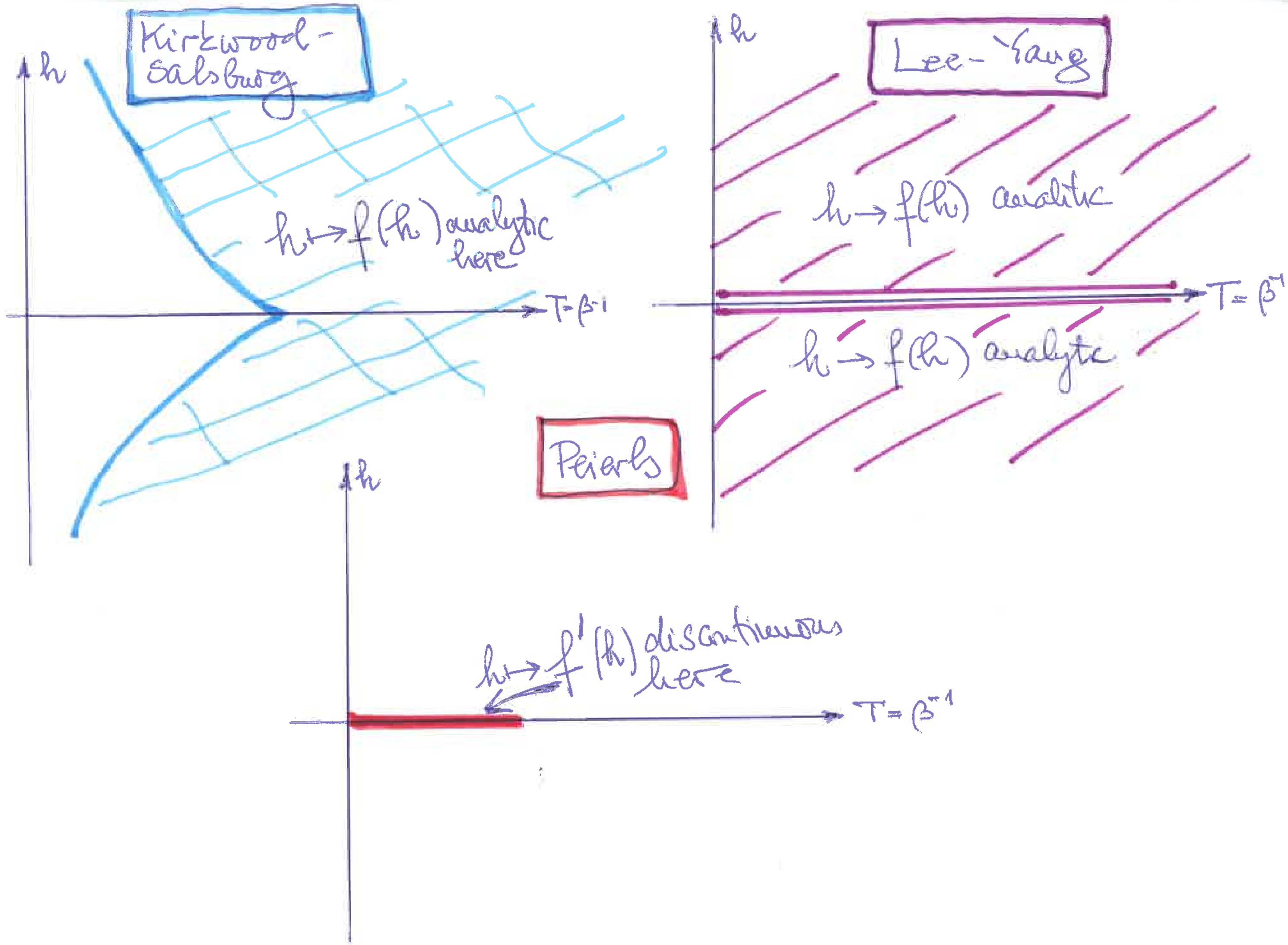
$d = 2$, $h = 0$: Full solution: $f(\beta) := \lim_{\Lambda \nearrow \mathbb{Z}^d} |\Lambda|^{-1} \log Z_{\Lambda,\beta}$ ✓.

The main ideas and technical ingredients:

(i) Convergent expansions ("cluster expansions")

& The Lee-Yang circle theorem.

(ii) Peierls's contour method


Kirkwood-Salsburg
h
h ↦ f(h) analytic here
T = β⁻¹
Lee-Yang
h
h → f(h) analytic
T = β⁻¹
h → f(h) analytic
Peierls
h
h ↦ f'(h) discontinuous here
T = β⁻¹

Sketch of Peierls's contour argument

This is important for understanding the key difference between discrete and continuous symmetry breaking.

Let $\Lambda = [0, L]^2 \cap \mathbb{Z}^2$ and consider the Ising Hamiltonian with $h = 0$ and $+$-boundary condition (rather than periodic):

$$H_\Lambda(\underline{\sigma}) = \underbrace{-\frac{1}{2} \sum_{x \sim y \in \Lambda} \sigma(x)\sigma(y)}_{\text{bulk terms}} \underbrace{- \sum_{x \in \partial^- \Lambda} \sigma(x)}_{\text{boundary terms}}$$

We prove

$$m_\Lambda(\beta) \geq \alpha > 0$$

uniformly in $\Lambda \nearrow \mathbb{Z}^2$.

Denote

$$\Lambda_{\pm}(\underline{\sigma}) := \{x \in \Lambda : \sigma(x) = \pm 1\}.$$

Then

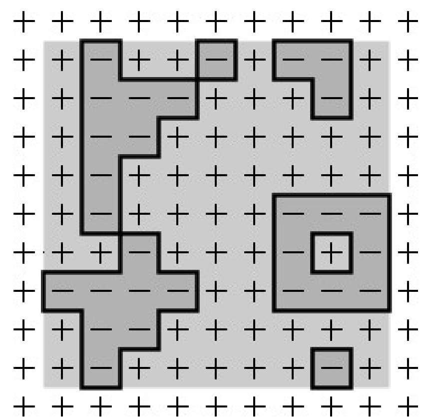
$$|\Lambda| = \Big|\Lambda_{+}(\sigma)\Big| + |\Lambda_{-}(\sigma)| \qquad \sum_{x\in\Lambda} \sigma(x) = \Big|\Lambda_{+}(\sigma)\Big| - |\Lambda_{-}(\sigma)|$$

and hence

$$m_{\Lambda}(\beta) = \frac{\Big\langle \Big|\Lambda_{+}\Big| - |\Lambda_{-}| \Big\rangle^{+}_{\Lambda,\beta}}{|\Lambda|} = 1 - 2\frac{\langle |\Lambda_{-}| \rangle^{+}_{\Lambda,\beta}}{|\Lambda|}$$

Let

$$\mathcal{C}_{\Lambda} := \{\text{simple contours in } \underbrace{\Lambda^{*}}_{\text{Whittney dual of } \overline{\Lambda}}\}$$



For $\gamma \in \mathcal{C}_\Lambda$

$$\chi_\gamma(\underline{\sigma}) = \begin{cases} 1 & \text{if } \gamma \text{ is a countour of } \underline{\sigma} \\ 0 & \text{otherwise} \end{cases}$$

By isoperimetry

$$|\Lambda_-(\underline{\sigma})| \le \sum_{\gamma \in \mathcal{C}_\Lambda} \frac{|\gamma|^2}{16} \chi_\gamma(\underline{\sigma})$$

and, thus

$$\langle |\Lambda_-| \rangle^+_{\Lambda,\beta} \le \sum_{\gamma \in \mathcal{C}_\Lambda} \frac{|\gamma|^2}{16} \langle \chi_\gamma \rangle^+_{\Lambda,\beta}$$

This is a very generous upper bound!

Next, let

$$\Delta_{\Lambda,\gamma} := \{\underline{\sigma} \in \Omega_\Lambda : \gamma \text{ is a countour of } \underline{\sigma}\}$$

$$\Delta^*_{\Lambda,\gamma} := \{\underline{\sigma} \in \Omega_\lambda : \gamma \text{ is edge-disjoint of all countours of } \underline{\sigma}\}$$

$$R_\gamma : \Omega_\Lambda \to \Omega_\Lambda, \qquad (R_\gamma\underline{\sigma})(x) := \begin{cases} -\sigma(x) & \text{if } \gamma \text{ surrounds } x \\ +\sigma(x) & \text{otherwise} \end{cases}$$

Note that

- R_γ is a *bijection* between $\Delta_{\Lambda,\gamma}$ and $\Delta^*_{\Lambda,\gamma}$
- For $\underline{\sigma} \in \Delta_{\Lambda,\gamma}$

$$H_\Lambda(\sigma) - H_\Lambda(R_\gamma\sigma) = 2\,|\gamma|\,.$$

Hence

$$\langle \chi_\gamma \rangle^+_{\Lambda,\beta} = \frac{\sum_{\underline{\sigma} \in \Delta_{\Lambda,\gamma}} e^{-\beta H_\Lambda(\underline{\sigma})}}{\sum_{\underline{\sigma} \in \Omega_\Lambda} e^{-\beta H_\Lambda(\underline{\sigma})}} \le \frac{\sum_{\underline{\sigma} \in \Delta_{\Lambda,\gamma}} e^{-\beta H_\Lambda(\underline{\sigma})}}{\sum_{\underline{\sigma} \in \Delta^*_{\Lambda,\gamma}} e^{-\beta H_\Lambda(\underline{\sigma})}} = e^{-2\beta|\gamma|}$$

and

$$\langle |\Lambda_-(\underline{\sigma})| \rangle^+_{\Lambda,\beta} \le \sum_{\gamma \in \mathcal{C}_\Lambda} \frac{|\gamma|^2}{16} e^{-2\beta|\gamma|}$$

Since

$$\#\{\gamma \in \mathcal{C}_\Lambda : |\gamma| = r\} \le |\Lambda|\, 4^r$$

it follows that

$$\frac{\langle |\Lambda_-| \rangle^+_{\Lambda,\beta}}{|\Lambda|} \le \frac{1}{16} \sum_{r=4}^{\infty} r^2 e^{(\log 4 - 2\beta) r}$$

uniformly as $\Lambda \nearrow \mathbb{Z}^2$.

The $O(\nu)$, or Classical Heisenberg Model: $\nu \geq 2$,

$$\Lambda := (\mathbb{Z}/L)^d, \qquad \Omega_\Lambda = (S^{\nu-1})^\Lambda, \qquad \nu_\Lambda(d\underline{\sigma}) = \prod_{x\in\Lambda} \underbrace{d\,\sigma(x)}_{\text{Haar}}$$

The Hamiltonian and the Gibbs measure:

$$H_\Lambda(\underline{\sigma}) := \underbrace{-\frac{1}{2}\sum_{x\sim y\in\Lambda}\sigma(x)\cdot\sigma(y)}_{O(\nu)\text{-symmetry}} \underbrace{-\varepsilon\sum_{x\in\Lambda}\sigma_1(x)}_{\text{symm. breaking}}$$

$$\mu_{\Lambda,\beta,\varepsilon}(d\underline{\sigma}) := (Z_{\Lambda,\beta,\varepsilon})^{-1}\,\text{exp}\{-\beta H_\Lambda^{(\varepsilon)}(\underline{\sigma})\}\prod_{x\in\Lambda}\underbrace{d\,\sigma(x)}_{\text{Haar}}$$

$$Z_{\Lambda,\beta,\varepsilon} = \int_{(S^{\nu-1})^\Lambda}\text{exp}\{-\beta H_\Lambda^{(\varepsilon)}(\underline{\sigma})\}\prod_{x\in\Lambda} d\,\sigma(x)$$

The *spontaneous magnetisation:*

$$m_\Lambda(\beta,\varepsilon) := \left\langle |\Lambda|^{-1} \sum_{x\in\Lambda} \sigma_1(x) \right\rangle_{\Lambda,\beta,\varepsilon} \overbrace{=}^{\text{per. b.c.}} \langle \sigma_1(0) \rangle_{\Lambda,\beta,\varepsilon}$$

$$m(\beta,\varepsilon) := \lim_{\Lambda \nearrow \mathbb{Z}^d} m_\Lambda(\beta,\varepsilon)$$

$$m(\beta) := \lim_{\varepsilon\to 0} m(\beta,\varepsilon) \quad \begin{Bmatrix} = \\ \neq \end{Bmatrix} \; 0 \qquad \textbf{?}$$

The *long range order parameter:* $\varepsilon = 0$,

$$r_\Lambda(\beta)^2 := \left\langle \left(|\Lambda|^{-1} \sum_{x\in\Lambda} \sigma(x) \right)^2 \right\rangle_{\Lambda,\beta} \overbrace{=}^{\text{per. b.c.}} |\Lambda|^{-1} \sum_{x\in\Lambda} \langle \sigma(0)\cdot\sigma(x) \rangle_{\Lambda,\beta}$$

$$r(\beta)^2 := \lim_{\Lambda \nearrow \mathbb{Z}^d} r_\Lambda(\beta)^2 \quad \begin{Bmatrix} = \\ \neq \end{Bmatrix} \; 0 \qquad \textbf{?}$$

Fact: $r > 0 \Rightarrow m > 0$.

Essential difference between Ising and $O(\nu)$:

discrete vs. continuous symmetry

No sharp contours $\Rightarrow$ No Peierls argument

The Main Results about $O(\nu)$:

[ND Mermin, H Wagner (1966)],
[RL Dobrushin, S Shlosman (1975)]:

- $d = 2$:: at any $\beta \in [0, \infty)$, $m = 0$ (and also $r = 0$).

[V Berezinski (1971-72)], [JM Kosterlitz, DJ Thouless (1972)],
[J Fröhlich, T Spencer (1981)]

- $d = 2$, $\nu = 2$:: $\exists \beta^* < \infty$ s.t. $\beta > \beta^* \Rightarrow$
  so-called topological vortex-binding phase (BKT phase)

[J Fröhlich, B Simon, T Spencer (1976)]:

- $d \geq 3$:: there exists $\beta_* < \infty$, such that
  $\beta > \beta_* \Rightarrow r > 0$ (and also $m > 0$).

The Classical XXZ Model:

$$\Omega_\Lambda = (S^2)^\Lambda \qquad \sigma(x) = (\sigma_1(x), \sigma_2(x), \sigma_3(x))$$

The Hamiltonian:

$$H_\Lambda^{(\varepsilon)}(\underline{\sigma}) := -\frac{1}{2} \sum_{x \sim y \in \Lambda} \Big(\underbrace{\sigma_1(x)\sigma_1(y) + \sigma_2(x)\sigma_2(y)}_{O(2)\text{-symmetry}} + u \underbrace{\sigma_3(x)\sigma_3(y)}_{\mathbb{Z}_2\text{-symmetry}} \Big)$$

$+$ symmetry breaking terms

Main Results:

- $|u| > 1$:: the Ising-behaviour of σ_3 prevails.
- $|u| = 1$:: this is exactly the $O(3)$-model.
- $|u| < 1$:: $O(2)$-behaviour of (σ_1, σ_2) prevails.