Ferromagnets and the classical Heisenberg model

Kay Kirkpatrick, UIUC

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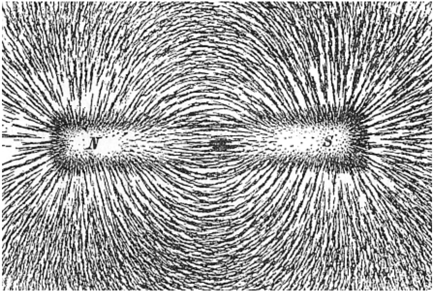
June 11, 2012



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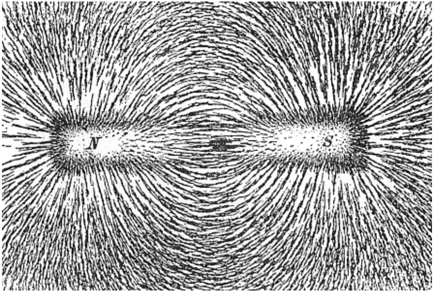
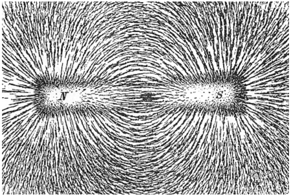


Joint with Elizabeth Meckes (Case Western Reserve University).

The classical physics models of ferromagnets



Simplest: Ising model on a periodic lattice of n sites has Hamiltonian energy for spin configuration $\sigma \in \{-1, +1\}^n$

$$H(\sigma) = -J \sum_{i=1}^{n} \sigma_i \sigma_{i+1}$$

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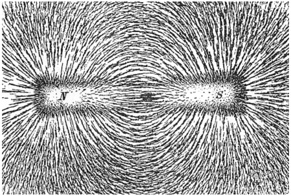

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Ising's 1925 solution in 1D. Onsager's 1944 solution in 2D.

Main goals for spin models

Gibbs measure

$$\frac{1}{Z(\beta)} e^{-\beta H(\sigma)}.$$

Partition function

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Fruitful approach: Mean-field spin models.

Work on the mean-field Ising model = Curie-Weiss model

Motivation: Curie-Weiss model is believed to approximate high-dimensional Ising model ($d \geq 4$).

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Also Curie-Weiss-Potts model with finitely many discrete spins.

The classical Heisenberg model of ferromagnetism

Spins are now in the sphere, and for spin configuration $\sigma \in (\mathbb{S}^2)^n$ the Hamiltonian energy is:

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Like Ising and Curie-Weiss models, two main cases:

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- Nearest-neighbor: $J_{i,j} = J$ for nearest neighbors i, j, $J_{i,j} = 0$ otherwise. Most interesting and challenging (and open) in 3D.
- Mean-field: averaged interaction $J_{i,j} = \frac{1}{2n}$ for all i, j. Can be viewed as either sending the dimension or the number of vertices in a complete graph to infinity.

(Mean-field theory is the starting point for phase transitions.)

Results for the mean-field Heisenberg model

Classical Heisenberg model on the complete graph with n vertices:

$$H_n(\sigma) = -\frac{1}{2n} \sum_{i,j=1}^{n} \langle \sigma_i, \sigma_j \rangle$$

- Previous work and set-up of Gibbs measures $e^{-\beta H_n}$.

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- CLTs for magnetization above and below critical temperature.
- Nonnormal limit theorem for magnetization at critical temperature.

Previous work on high-dimensional Heisenberg models

Nearest-neighbor (NN) Heisenberg model in d-dimensions:

$$H(\sigma) = -J \sum_{|i-j|=1} \langle \sigma_i, \sigma_j \rangle$$

Magnetization: normalized sum of spins

Kesten-Schonmann '88: approximation of the d-dimensional NN model by the mean-field behavior as dimension $d \to \infty$, with critical temperature $\beta_c = 3$

- Magnetization is zero for all $\beta < 3$ and all dimensions d.
- Magnetization converges to the mean-field magnetization as $d \to \infty$ for $\beta > 3$.

The set-up and Gibbs measure

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Gibbs measure $P_{n,\beta}$, or canonical ensemble, has density:

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Partition function: $Z = Z_n(\beta) = \int_{(\mathbb{S}^2)^n} e^{-\beta H_n(\sigma)} dP_n$.

The Cramèr-type LDP at $\beta = 0$ (i.i.d. case)

Empirical magnetization: $M_n(\sigma) = \frac{1}{n}\sum_{i=1}^{n} \sigma_i$.

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Theorem (K.-Meckes '12): For i.i.d. uniform random points $\{\sigma_i\}_{i=1}^{n}$ on $\mathbb{S}^2 \subseteq \mathbb{R}^3$, the magnetization laws $\mu_n := \mathcal{L}(M_n)$ satisfy an LDP (large deviations principle):

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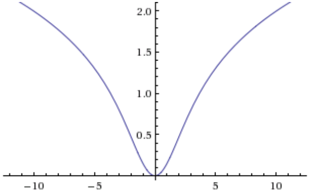

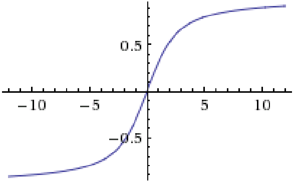

$I(c) = cg(c) - \log\left(\frac{\sinh(c)}{c}\right)$, $\qquad g(c) = \coth(c) - \frac{1}{c} = |x|$.

The Sanov-type LDP at $\beta = 0$

Empirical measure of spins:

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$$P_n\{\mu_{n,\sigma} \in B\} \simeq \exp\{-n \inf_{\nu \in B} H(\nu|\mu)\}$$

where

$$H(\nu \mid \mu) := \begin{cases} \int_{\mathbb{S}^2} f \log(f) d\mu, & f := \frac{d\nu}{d\mu} \textit{ exists}; \\ \infty, & \textit{otherwise}. \end{cases}$$

Here μ is uniform measure and B is a Borel subset of $M_1(\mathbb{S}^2)$.

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Now, how do the LDPs depend on temperature?

LDPs for arbitrary temperature

Equivalence of ensembles approach (Ellis-Haven-Turkington '00): find hidden space, hidden process, interaction representation.

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Theorem (K.-Meckes '12): : LDP with respect to the Gibbs measures:

$$P_{n,\beta}\{\mu_{n,\sigma} \in S\} \simeq \exp\{-n \inf_{\nu \in S} I_\beta(\nu)\},$$

where

$$I_\beta(\nu) = H(\nu \mid \mu) - \frac{\beta}{2} \left| \int_{\mathbb{S}^2} x d\nu(x) \right|^2 - \varphi(\beta),$$

and free energy

$$\varphi(\beta) := -\lim_{n\to\infty} \frac{1}{n} \log Z_n(\beta) = \inf_\nu \left[H(\nu \mid \mu) - \frac{\beta}{2} \left| \int_{\mathbb{S}^2} x d\nu(x) \right|^2 \right]$$

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$$= \frac{1}{2} \int_{-1}^{1} g(x) \log[g(x)] dx - \frac{\beta}{2} \left(\int_{-1}^{1} \frac{x g(x)}{2} dx \right)^2$$

$$= -h\left(\frac{g}{2}\right) + \log(2) - \frac{\beta}{2} \left(\int_{-1}^{1} \frac{x g(x)}{2} dx \right)^2$$

for increasing $g : [-1, 1] \to \mathbb{R}_+$ with $\frac{1}{2} \int_{-1}^{1} g(x) dx = 1$.

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Usual entropy h, so constrained entropy optimization...

Free energy and phase transition

… gives optimizing densities $g(z) = ce^{kz}$, and the free energy $\varphi(\beta) = \inf_{k\in[0,\infty)} \Phi_\beta(k)$, where

$$\Phi_\beta(k) := \log\left(\frac{k}{\sinh k}\right) + k\coth k - 1 - \frac{\beta}{2}\left(\coth k - \frac{1}{k}\right)^2$$

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Calculus: optimized at 0 for $\beta \le \beta_c := 3$, and is given implicitly for $\beta > 3$ by $\gamma(k) = \frac{k}{\coth k - \frac{1}{k}} = \beta$:

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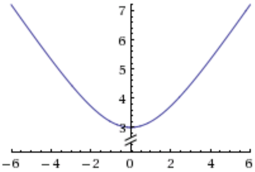

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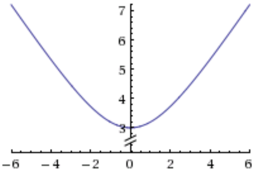

2nd-order phase transition: φ and φ' are continuous at $\beta = 3$.

The canonical macrostates across the phase transition

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Now, what about asymptotics of the magnetization in each phase? Central and non-central limit theorems...

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$$\sup_{h: M_1(h), M_2(h) \leq 1} \left| \mathbb{E} h(W) - \mathbb{E} h(Z) \right| \leq \frac{c_\beta \log(n)}{\sqrt{n}}$$

- $M_1(h)$ is the Lipschitz constant of h
- $M_2(h)$ is the maximum operator norm of the Hessian of h
- Z is a standard Gaussian random vector in $\mathbb{R}^3$.

The supercritical (ordered) phase, $\beta > 3$

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where Z is a centered Gaussian random variable with variance

$$\sigma^2 := \frac{4\beta^2}{(1-\beta g'(k))\,k^2}\left[\frac{1}{k^2} - \frac{1}{\sinh^2(k)}\right],$$

for $g(x) = \coth x - \frac{1}{x}$.

At the critical temperature $\beta = 3$

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where X has density

$$p(t) = \begin{cases} \frac{1}{z} t^5 e^{-3ct^2} & t \ge 0; \\ 0 & t < 0, \end{cases}$$

with $c = \frac{1}{5c_3}$ and z a normalizing factor.

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- The mean-field Heisenberg model is exactly solvable.
- Asymptotics for magnetization above, below, and at (non-Gaussian) the critical temperature.

What's next

- 3D nearest-neighbor Heisenberg model is the big challenge.
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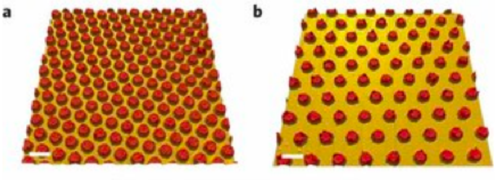
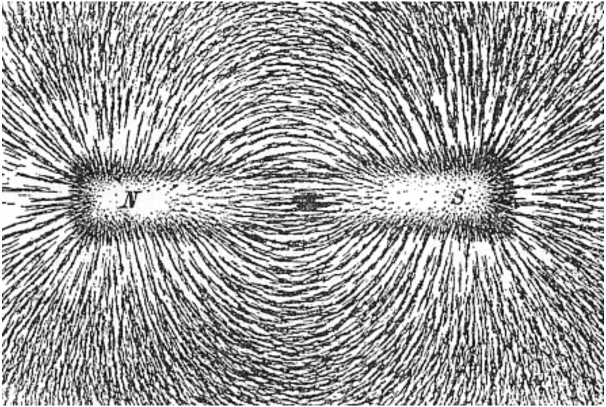


Figure: Arrays of 87-nm-thick Nb islands (red) on 10-nm-thick Au layer (yellow). Edge-to-edge spacing of 140nm (a) and 340nm (b). Courtesy of N. Mason at UIUC.

Thank you



arXiv:1204.3062