# Abnormal behavior of the mean-field Heisenberg model: superconductors and magnets

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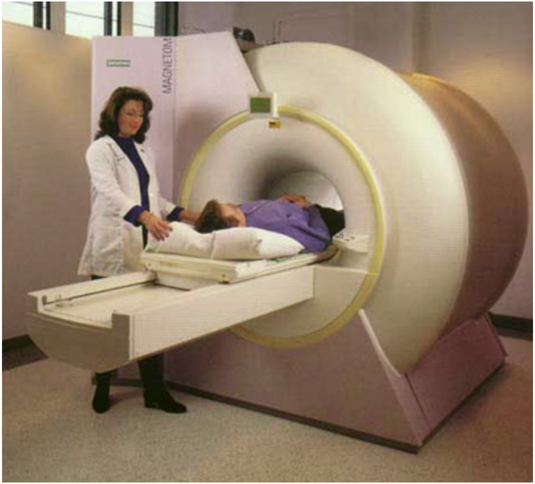
Joint with Elizabeth Meckes (Case Western)

# The big challenge

Hilbert's 6th problem: making physics rigorous.

Derive macro theories of superconductors and magnets (Ginzburg-Landau and Landau-Lifshitz-Gilbert equations) from microscopic models.

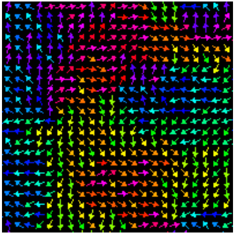
# Superconducting magnets in MRI machines



# Spin models of superconductors and magnets

Ising model, spins $\sigma_i \in \{\pm 1\}$

XY model, $\sigma_i \in \mathbb{S}^1$



Heisenberg model, $\sigma_i \in \mathbb{S}^2$

# More realistic models

# Higher spin dimension

$N$-vector model: graph $(V, E)$ with $n = |V|$ spins

spin configuration $\sigma \in (\mathbb{S}^{N-1})^n$

Hamiltonian energy

$$H_n(\sigma) = -\sum_{(i,j)\in E} J_{ij} \langle \sigma_i, \sigma_j \rangle$$

$N = 1$: Ising model
$N = 2$: XY model
$N = 3$: Heisenberg model

# Higher lattice dimension

Mean-field model on graph $G = (V, E)$ with $|V| = n$ has spin configuration $\sigma = (\sigma_i)_{i=1}^n \in (\mathbb{S}^{N-1})^n$ and Hamiltonian energy:

$$H_n(\sigma) = -\sum_{i,j} J_{ij} \langle \sigma_i, \sigma_j \rangle .$$

1. Send $n \to \infty$ in complete graph $G = K_n$: mean-field interaction $J_{ij} = \frac{1}{2n} \; \forall i, j$.

2. Send $d \to \infty$ in the $d$-dimensional lattice:

$$J_{ij} = \begin{cases} J, & \textit{if} \quad i, j \quad \textit{neighbors} \\ 0, & \textit{else}. \end{cases}$$

# The mean-field Ising (Curie-Weiss) model

Ellis-Newman '78 ... Chatterjee-Shao '11: phase transition

- $\beta < 1$: average spin goes to zero (LLN), with a CLT
- $\beta > 1$: average spin has normal asymptotics around two states
- At critical $\beta = 1$: non-normal limiting density $\propto e^{-x^4/12}$

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Mean-field $N$-vector models have phase transition at $\beta_c(N) = N$.

- For $\beta < \beta_c$, the average spin decays (Kesten-Schonmann '88)

# The mean-field Heisenberg results with E. Meckes

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

- For the average spin $\frac{1}{n}\sum_{i=1}^{n}\sigma_i$, we have large deviations principles (LDPs) at any $\beta$.
- We analyze the free energy and recover the phase transition at $\beta_c = 3$.
- We have limit theorems for the average spin above, below, and at $\beta_c = 3$.
- We find non-normal critical limiting density $\propto t^5 e^{-3ct^2}$

# We start with independent spins, $\beta = 0$

$P_n$ is product/uniform measure on $(\mathbb{S}^2)^n$.

Average spin $\frac{1}{n}\sum_{i=1}^n \sigma_i \xrightarrow{n\to\infty} 0$, with LLN and CLT.

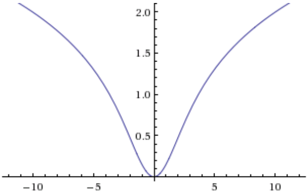
**Theorem (K.-Meckes '13):** Uniform random points $\{\sigma_i\}_{i=1}^n$ have a large deviations principle:

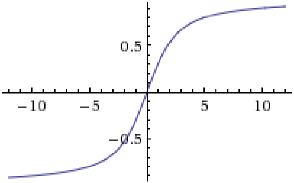
$$P_n\left(\frac{1}{n}\sum_{i=1}^n \sigma_i \simeq x\right) \simeq e^{-nI(x)},$$

where the rate function $I$ is ...

# The rate function is obnoxious

$I$ is implicitly




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

Macrostates $x$ are zeros of $I$: only $x = 0$ here. Disordered.

# We go up to LDP level 2, $\beta = 0$

Empirical measure of spins: $\mu_{n,\sigma} = \frac{1}{n}\sum_{i=1}^{n}\delta_{\sigma_i}$

**Theorem (K.-Meckes '13):** We have a Sanov LDP:

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

where

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

Uniform measure $\mu$ and Borel subset $B$ in $M_1(\mathbb{S}^2)$.

The only macrostate is $\mu$.

# Extend level 2 to $\beta > 0$ by Ellis-Haven-Turkington

Gibbs measures $P_{n,\beta}$ have densities $Z^{-1}e^{-\beta H_n(\sigma)}$.

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

**Theorem (K.-Meckes '13):** LDP w.r.t. Gibbs measures:

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

where

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

Zeros of $I_\beta$? Free energy $\varphi(\beta)$?

# The free energy is obnoxious

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

We discover

$$\varphi(\beta) = \begin{cases} 0, & \text{if } \beta < 3, \\ \Phi_\beta(\gamma^{-1}(\beta)), & \text{if } \beta \geq 3, \end{cases}$$

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

$$\gamma(k) := \frac{k}{\coth k - 1/k} = \beta$$

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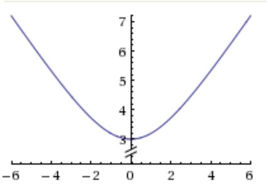
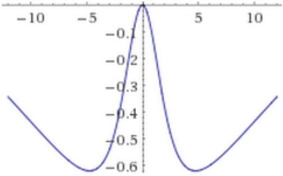



$\Phi_6$



# The phase transition and the macrostates

$\varphi$ and $\varphi'$ are continuous at $\beta_c = 3$ (2nd order phase transition)

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If $\beta < 3$, the macrostate (zero of $I_\beta$) is uniform.

If $\beta > 3$, the macrostates are rotations of the density

$$(x, y, z) \mapsto ce^{kz}, \text{ where } c = \frac{k}{2 \sinh k}, \; k = \gamma^{-1}(\beta).$$

If $\beta \to \infty$, then $ce^{kz} \to \delta_{(0,0,1)}$, consistent with heuristic.

# The average spin has a CLT below $\beta_c$

**Theorem (K.-Meckes '13):** For $\beta < 3$, and $Z$ standard normal random vector in $\mathbb{R}^3$,

$$W_n := \sqrt{\frac{3-\beta}{n}} \sum_{i=1}^{n} \sigma_i \xrightarrow{distr.} Z.$$

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We show there exists $c_\beta$ such that

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

- $M_1$ is Lipschitz constant, $M_2$ maximum op norm of Hessian
- L. A. Ross has refined this rate of convergence.

# The average spin has a CLT above $\beta_c$

**Theorem (K.-Meckes '13):** In the ordered phase, $\beta > 3$,

$$W_n := \sqrt{n} \left[ \frac{\beta^2}{n^2 k^2} \left| \sum_{j=1}^{n} \sigma_j \right|^2 - 1 \right] \xrightarrow{distr.} Y,$$

where $Y$ is Gaussian with mean 0 and variance

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

(Bounded-Lipschitz distance with explicit rate of convergence.)

# The limit is non-normal at $\beta_c = 3$

**Theorem (K.-Meckes '13):**

$$W_n := \frac{C}{n^{3/2}} \left| \sum_{j=1}^{n} \sigma_j \right|^2 \xrightarrow{distr.} X,$$

where $X$ has density

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

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

# Key ideas of the proof

- LDP methods, Ellis-Haven-Turkington method for $\beta > 0$
- Stein's method and a special non-normal version at $\beta_c$ (Exchangeable pair via Glauber dynamics.)
- Next: asymptotics for mean-field XY model, dynamics of Heisenberg

# What my students are working on

- Tayyab Nawaz: Critical asymptotics for mean-field XY and $O(n)$ models.
- Leslie Ann Ross: Dynamics of the average spin for mean-field Heisenberg and process-level Stein's method.

# What's next

- Dynamics between metastable states in XY and description of saddle points (with L. DeVille)

- Micro Heisenberg model to Macro Landau-Lifshitz-Gilbert equation (with J. Marzuola and J. Mattingly)

- 3D Heisenberg model
- XY and Heisenberg spin glasses
- Quantum $O(n)$ models

# Nadya Mason has found other cool features

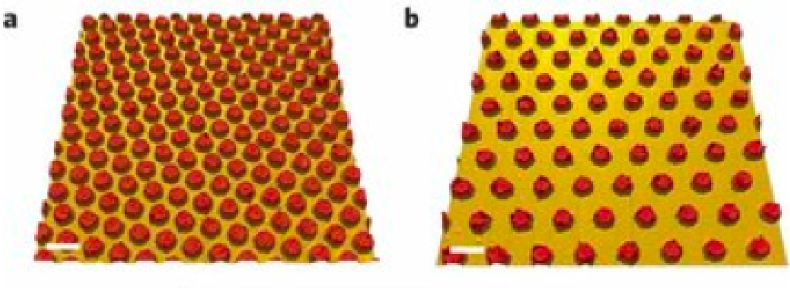


Figure : Red Nb islands on gold substrate, spaced 140nm & 340nm.

There's a two-step transition to superconductivity and a zero-temperature metallic state. Is the latter a spin glass?

# Thanks

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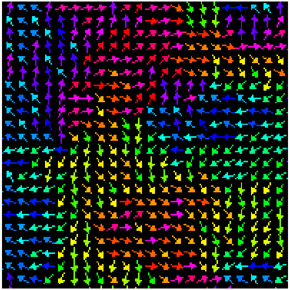
Figure : Courtesy of Mike Jory.

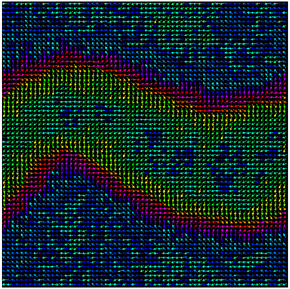
arXiv 1204.3062 (JSP), and forthcoming

# The 2D XY model has hysteresis and metastability

On a torus, the Hamiltonian is:

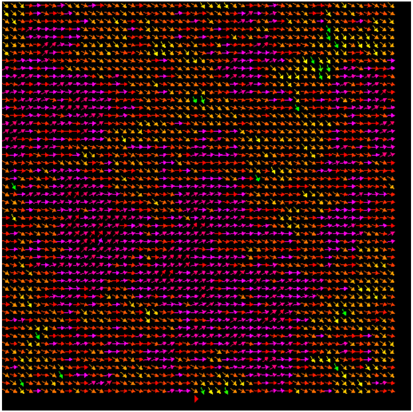
$$H(\sigma) = -\sum_{(i,j)\in E} \cos(\theta_i - \theta_j) - h\sum_{i\in V} \cos(\theta_i).$$





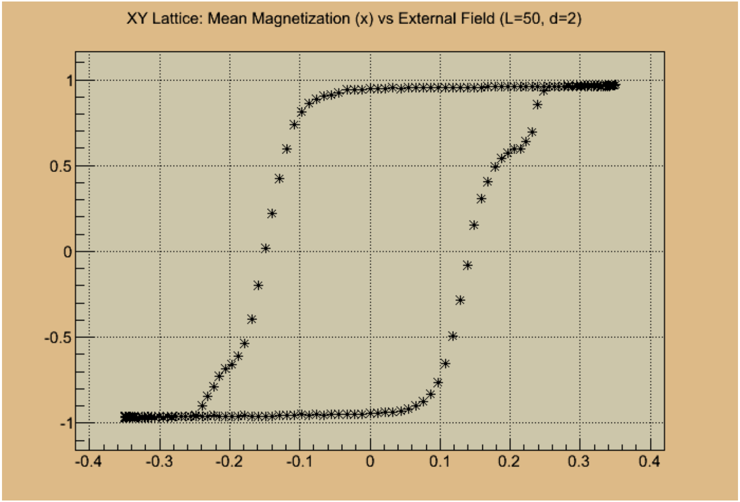
Batrouni '04 described “twisted” states like this.

# We found more metastable states for the XY model



Topological classification of metastable states (J. Weinstein)

# A funny hysteresis curve for the XY model




Bumps correspond to loops or twisted states that a strong enough external field overcomes.

# Superconductors are understood imperfectly

1911: Liquifying helium, Onnes saw resistivity of mercury vanish

1930s: Meissner effect causes levitation

60s heuristics: Bardeen-Cooper-Schrieffer (BCS) theory to Ginzburg-Landau (GL) and to Bose-Einstein condensation (BEC)

2000s: Erdős, K., Schlein, Staffilani, . . . : quantum systems to BEC; BCS to static GL. . . .

micro models $\rightsquigarrow$ $\rightsquigarrow$ MACRO Ginzburg-Landau, BEC

$\searrow$ $\nearrow$

MESO BCS