Ferromagnets and superconductors

Kay Kirkpatrick, UIUC

Ferromagnet and superconductor models: Phase transitions and asymptotics

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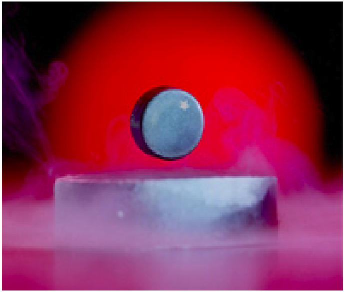
October 2012



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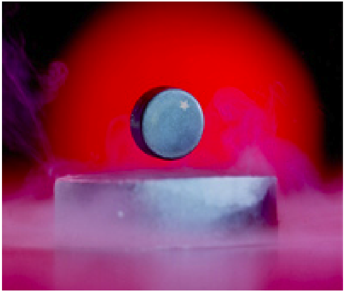

Joint with Elizabeth Meckes (Case Western), Enzo Marinari (Sapienza Roma), S. Olla (Paris IX), and Jack Weinstein (UIUC).

History of superconductivity (SC)

1911: Onnes discovered zero resistivity of mercury at 4.2 K. (Also superfluid transition of helium at 2.2 K.)

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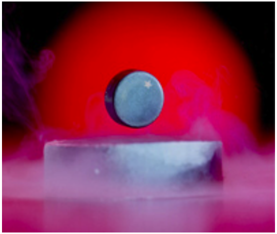

Figure : Magnetic fields bend around superconductors, allowing levitation (courtesy Argonne).

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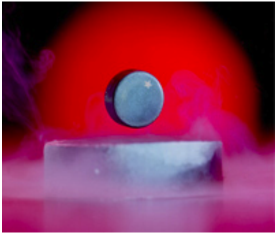

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Applications: SC magnets in MRIs and particle accelerators, measuring the Planck constant, etc.

Phenomenology of superconductivity (SC)

1950: Macroscopic Ginzburg-Landau theory, Schrödinger-like PDE.

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1959: From BCS to Ginzburg-Landau at transition temperature.

1960s: From BCS theory to Bose-Einstein condensation at zero temperature.

Mathematics of superconductivity (SC), 2005–

Serfaty et al: Ginzburg-Landau asymptotics, vortex lattices.

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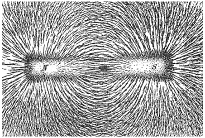
Problem: defining SC microscopically. Often SC phase is ferromagnetic phase...

The outline

The classical mean-field Heisenberg model of ferromagnets



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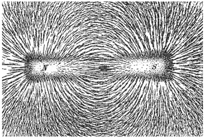
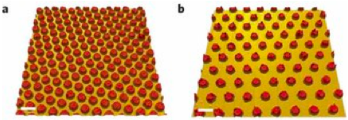
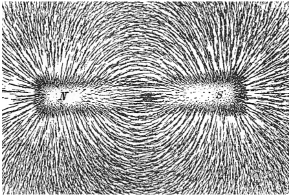


XY models and spin models of superconductors (in progress)



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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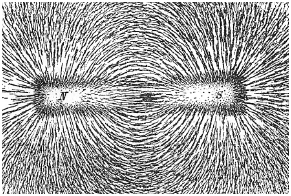

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Ising's 1925 solution in 1D. Onsager's 1944 solution in 2D.

Main goals for spin models

Gibbs measure

$$\frac{1}{Z_n(\beta)} e^{-\beta H_n(\sigma)}.$$

Partition function

$$Z_n(\beta) = \sum_{\sigma} e^{-\beta H_n(\sigma)}.$$

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Look for a phase transition via the free energy

$$\varphi(\beta) = -\lim_{n\to\infty} \frac{1}{\beta n} \log Z_n(\beta).$$

Fruitful approach: Mean-field spin models.

Mean-field Ising model = Curie-Weiss model

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

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Ellis and Newman '78: Magnetization $M_n(\sigma) = n^{-1} \sum_i \sigma_i$ of CW model has Gaussian law away from criticality, and at the critical temperature non-Gaussian law like $e^{-x^4/12}$.

Eichelsbacher and Martschink '10, Chatterjee and Shao '11: Rate of convergence and Berry-Esseen type error bound for magnetization at critical temperature.

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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:

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

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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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Our results:

- LDPs for the magnetization and empirical spin distribution, for any inverse temperature β.
- Free energy, macrostates, second-order phase transition.
- 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 in d-dimensions, $M^{(d)}$

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 $M^{(d)} = 0$ for all $\beta < 3$ and all dimensions d.
- $M^{(d)} \xrightarrow{d\to\infty} M$, the mean-field magnetization for all $\beta > 3$.

Our set-up and Gibbs measure

Classical Heisenberg model on the complete graph with n vertices:

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

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

$$\frac{1}{Z} \exp\left(\frac{\beta}{2n} \sum_{i,j=1}^{n} \langle \sigma_i, \sigma_j \rangle \right) = \frac{1}{Z} e^{-\beta H_n(\sigma)}.$$

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

The Cramér-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 satisfy a large deviations principle (LDP):

$$P_n\left(M_n \simeq x\right) \simeq e^{-nI(x)},$$

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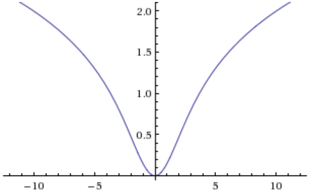

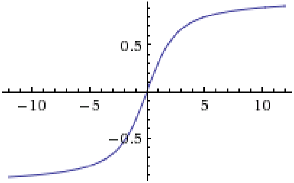

$$I(c) = cg(c) - \log\left(\frac{\sinh(c)}{c}\right), \qquad g(c) = \coth(c) - \frac{1}{c} = |x|.$$

Sanov's theorem, LDP at $\beta = 0$ (i.i.d.)

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

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Theorem (K.-Meckes '12):

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

where

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

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?

Transforming to Sanov LDPs at any β

Equivalence of ensembles approach (Ellis-Haven-Turkington '00).

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

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

where

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

and free energy

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

The free energy comes from optimizing

Densities symmetric about the north pole maximize $\left|\int_{\mathbb{S}^2} x d\nu(x)\right|$.

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So consider ν_g with density $f(x, y, z) = g(z)$ increasing in z:

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

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

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

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

Usual entropy h, so constrained entropy optimization...

The free energy and the phase transition

... gives optimizing densities $g(z) = ce^{kz}$ and free energy

$$\varphi(\beta) = \inf_{k \geq 0} \left\{ \log\left(\frac{k}{\sinh k}\right) + k \coth k - 1 - \frac{\beta}{2}\left(\coth k - \frac{1}{k}\right)^2 \right\}.$$

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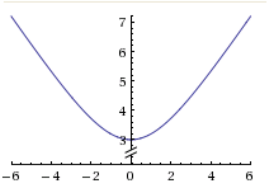
Calculus: inf at $k = 0$ for $\beta \leq \beta_c := 3$, and inf given implicitly for $\beta > 3$ by $\gamma(k) = \frac{k}{\coth k - \frac{1}{k}} = \beta$:



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

Transition temperature $\beta_c = 3$ matches Kesten-Schonmann.

The canonical macrostates across the phase transition

In the subcritical phase, $\beta < 3$, the canonical macrostates (zeroes of rate function I_β) are uniform on the sphere. Disordered.

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

In particular, as $\beta \to \infty$, these densities converge to delta functions (full alignment of the spins).

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

The subcritical (disordered) phase, $\beta < 3$

Scaling of magnetization:

$$W := \sqrt{\frac{3-\beta}{n}} \sum_{i=1}^{n} \sigma_i .$$

Theorem (K.-Meckes '12): There exists c_β such that

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

- $M_1(h)$ 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, $\beta > 3$

Scaled magnetization:

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

Theorem (K.-Meckes '12): There exists c_β such that

$$\sup_{h:\|h\|_\infty \le 1, \|h'\|_\infty \le 1}\left|\mathbb{E}h(W) - \mathbb{E}h(Z)\right| \le c_\beta\left(\frac{\log(n)}{n}\right)^{1/4},$$

where Z is Gaussian with mean 0 and variance

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

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

Interesting at the critical temperature $\beta = 3$

$$W := \frac{c_3 \left| \sum_{j=1}^{n} \sigma_j \right|^2}{n^{3/2}}, \text{ where } c_3 \text{ is s.t. } \mathbb{E}W = 1.$$

Theorem (K.-Meckes '12): There exists C such that

$$\sup_{\substack{\|h\|_\infty \le 1, \|h'\|_\infty \le 1 \\ \|h''\|_\infty \le 1}} \left| \mathbb{E}h(W) - \mathbb{E}h(X) \right| \le \frac{C \log(n)}{\sqrt{n}},$$

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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.

The main ideas of the proofs and the upshot

- LDP methods.
- Stein's method and special non-normal version of Stein's method. (Exchangeable pair via Glauber dynamics.)

- The mean-field Heisenberg model is exactly solvable.
- Asymptotics for magnetization above, below, and (non-Gaussian) at the critical temperature.
- 3D nearest-neighbor Heisenberg model?

What's next: phase transitions to superconductivity

With E. Marinari, E. Meckes, S. Olla, J. Weinstein...

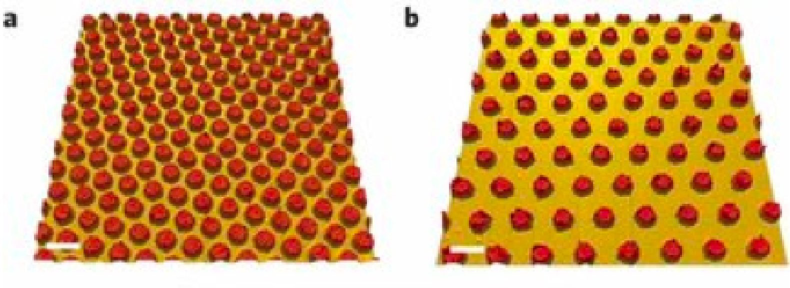

Figure : Arrays of Nb islands (red) on gold substrate (yellow). Edge-to-edge spacing of 140nm (a) and 340nm (b). Courtesy of Nadya Mason, UIUC physics.

Metastability in spin models

Hysteresis and metastability for the Ising model (Bodineau, Picco, et al):

(movies courtesy of J. Weinstein, using Metropolis)

Metastability in spin models

Hysteresis and metastability for the Ising model (Bodineau, Picco, et al):

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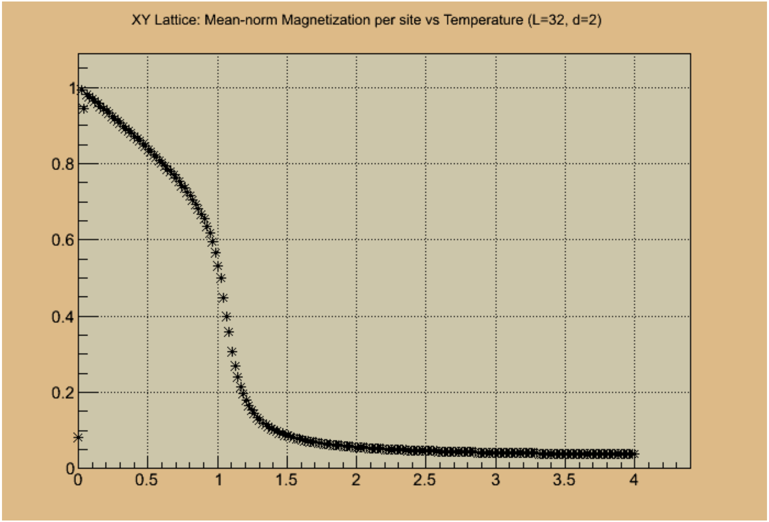
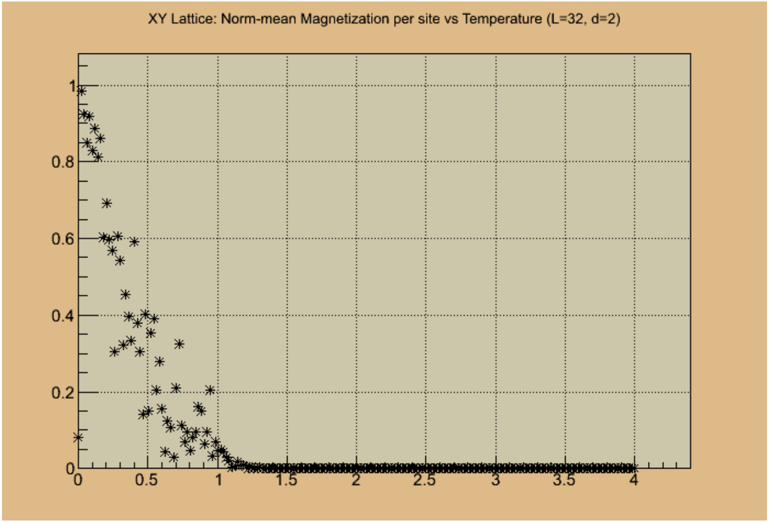
Hysteresis and metastability for the XY model, with spins in $\mathbb{S}^1$? (More general $O(n)$ or n-vector model: Ising is $n = 1$, XY is $n = 2$, and Heisenberg is $n = 3$.)

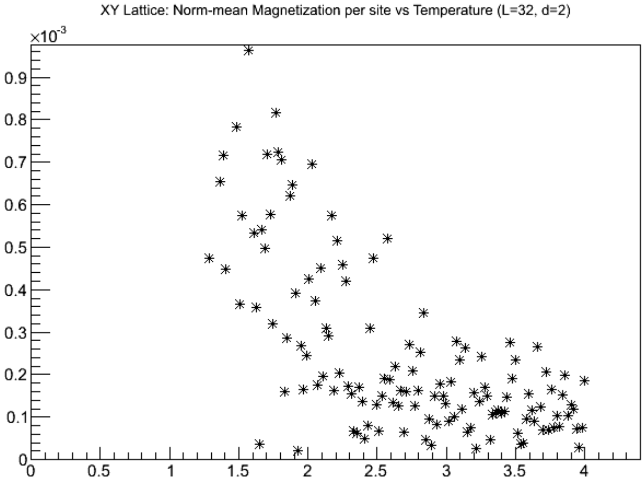
Graph of $\langle | \frac{1}{N} \sum \sigma_i | \rangle$ for XY model, courtesy of J. Weinstein



But randomness of $|\frac{1}{N}\langle\sum \sigma_i\rangle|$



And for high temperature, scaling by $\frac{1}{\sqrt{N}}$



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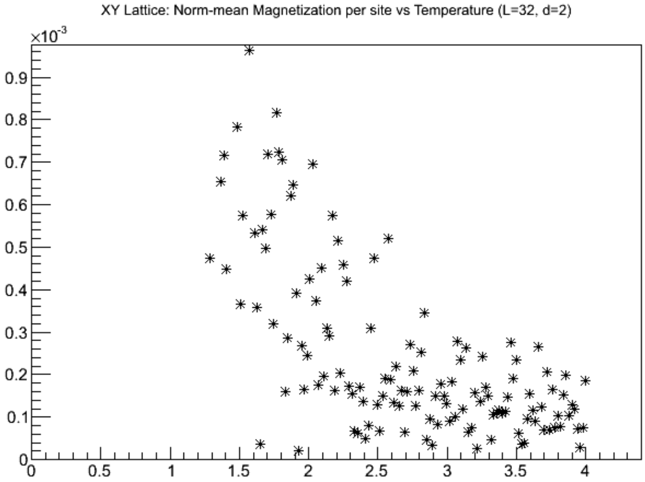


What's happening is "migration" of the ordered phase.

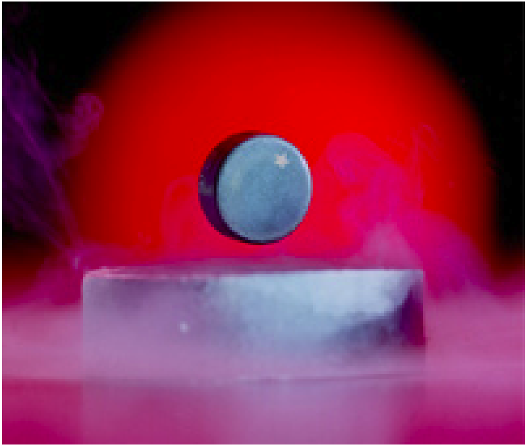
Spin models for superconductors

Working on a chain of XY models to reproduce the two-step phase transition in SC arrays (experiments by Nadya Mason's group at UIUC).

Want to add spin-glass-type disorder and prove rigorous results.

Guidance for SC spin model theory and for SC experiments...

Thank you



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