Mean–Field Driven
Phase Transitions of the First Type

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Talk Outline

• Background & Review (MFT–101).
• Comparison to actual systems.  (Also, models under consideration.)
• Allusion to technical tools (Infrared Bounds).
• More background (MFT–201).
• Description & statement of complete results.
Sort of analysis started from the outset:

Curie Theory of Magnetism

Weiss Molecular Field Theory

Start simple:  
\[-H = \frac{J}{2d} \sum_{r,r'} S_r S_{r'}\]

with \(r, r'\) nearest neighbors on \(d\)-dimensional lattice,  
and \(S_r\) an Ising spin (\(S_r = \pm 1\)).

"Too hard"

Look at situation from perspective of single spin.  
Effective field due to collective interaction.

\[
\frac{1}{2d} \sum_r S_r \approx m;
\]

Allows us to get (some sort of approximate)  
Mean Field Equation.
With effective “external” field frozen at $m$,

$$
\langle S_0 \rangle = \frac{\sum S_0 e^{\beta J m S_0}}{\sum e^{\beta J m S_0}} = \tanh(\beta J m).
$$

But $\langle S_0 \rangle$ should equal $m$:

$$
m = \tanh(\beta J m).
$$

Analysis: Expand; $m \ll 1$.  $m \approx \beta J m - \frac{1}{3} (\beta J m)^3 + \cdots$

(1) $\beta_c J = 1$ (Curie temperature).

(2) $m(\beta) \approx K (\beta - \beta_c)^{1/2}$ (Critical behavior).
Now, look @ related spin–system

\[ -H = \frac{J}{2d} \sum_{\langle r, r' \rangle} S_r \cdot S_{r'} \]

But \( S_r : \)

\[ (q = 3) \]

Same (elementary) mean field type perspective leads to following equation:

\[ \theta = \frac{e^{\beta K \theta} - 1}{e^{\beta K \theta} + (q - 1)} \]

\( \theta \propto m \quad J \propto K \)

Model can be defined for any \( q \geq 0 \); but here \( q \) = integer, \( q \geq 2 \).

\[ (q = 4) \]

(Obviously same if \( q = 2 \)).

Now: do our “analysis”.

...
\[ \theta \ll 1 \quad \theta = \frac{\beta K \theta + \frac{1}{2} (\beta K \theta)^2 + \ldots}{q + \beta K \theta + \ldots} \]

\[ \approx \frac{1}{q} \left[ \beta K \theta + \left(\frac{1}{2} - \frac{1}{q}\right)(\beta K \theta)^2 + \ldots \right] \]

(i) \( \frac{\beta_c K}{q} = 1 \)”.  

Note sign of coefficient.

(ii) \( \beta \geq \beta_c \); write \( \beta K = q + \varepsilon \); \( \varepsilon \) small.

\[ \theta \approx \theta + \frac{\varepsilon}{q} \theta + \left(\frac{q}{2} - 1\right) \theta^2 + \ldots \]

Predicts: \( \theta \) slightly negative.

Impossible:  
(a) On physical grounds.

(b) Probabilistic interpretation of \( \theta \).
No solutions of MFT ($q > 2$) with magnetization going continuously to zero.

**Fact:** Cannot get from start to finish without a discontinuity.

**Topics for discussion:**  
- Where (in the context of MFT) does the discontinuity actually occur? [MFT 201].  
- Does this sort of thing happen a lot? What does this say about the actual system?  
- Can system be 1st order even if it “admits” continuous solutions?  
- Genuine discontinuous thermodynamics (e.g. energy density etc.)?
Comparison to Real Systems

In some sense, MFT not such a wild “theory”.

Certainly, the average magnetization (spacial, of neighbors of origin)

\[ M_0 = \frac{1}{2d} \sum_{|r|=1} S_r \]

has to equal something. Of course, this something is random.

Express mean–field equations as \( m = Q(m) \).

Then, given the value of \( M_0 \), the (random) magnetization @ origin, \( m_0 \) will be:

\[ m_0 = Q(M_0) \]

Quantity \( m_0 \) is average value of magnetization given \( M_0 \).

True (fully interacting) stat. mech. equations must be:

\[ m(\beta) = \langle m_0 | M_0 \rangle_\beta = \langle Q(M_0) \rangle_\beta \]

where \( \langle \cdot \rangle_\beta \) denotes thermal average @ inverse temperature \( \beta \).
Comparison to Real Systems

Generic random variables have to have some distribution or density.

If the RV was deterministic – i.e. if $\rho(M_0)$ were concentrated at a single value then mean field equations would be exact.

However: $m_0 = Q(M_0)$.

If $M_0$ is almost always close to its average value then $m_0$ must also be close to its average and they must both be close to some solution of the mean field equation.

Q. How can we show this?
Ans. Show that variance is small.
Comparison to Real Systems

If we can show that variance is small:

Clear: Notwithstanding all the thermal randomness, $m(\beta)$ would always be "near" a solution of the mean field equations. If these equations do not admit continuous solutions, then the actual system must also exhibit a discontinuity.
Comparison to Real Systems

Systems under consideration: (bad news)

\[-H = \frac{J}{2d} \sum \langle r, r' \rangle S_r \cdot S_{r'}\]

\text{Under these conditions, system is reflection positive.}

\text{May work with techniques of Infrared Bounds.}

\textbf{Good news:}

\(S_r = \text{anything.}\)

- Magnetic (vector) spins Ising, Potts, \(O(N)\), ...
- Matrices – nematic models.
- Continuous fields (i.e. discrete field theories).

And: Dot product can also mean “anything”; simply has to be a positive definite inner product. Also, can add arbitrary external field or weigh the single –spin distribution in any fashion.

\textbf{Example:} BEG model. Can emulate \(\sigma_r^2\) by generating new component \(\tau_r\).

Includes many classical systems physical interest. More generalities, subject of [BCC]
Technical discussion

Statement of infrared bounds:

Starting on torus of size $L$, any function with $\sum_r w_r = 0$.

Then

$$\sum_{r,r'} w_r w_{r'} \left\langle S_r \cdot S_{r'} \right\rangle_\beta \leq \frac{n}{\beta J} \sum_{r,r'} w_r D^{-1}(r, r') w_{r'}$$

where $D^{-1}$ is the inverse of the lattice Laplacian

$$D^{-1}(r, r') = \int_{[-\pi, +\pi]^d} \frac{d^d k}{(2\pi)^d} \frac{e^{ik(r-r')}}{1 - \sum_{j=1}^d \cos k_j}.$$ 

Usually take $w_r$ to be plane waves with the result:

$$\left| \hat{S}(k) \right|^2 \leq \frac{n}{\beta J} \frac{1}{\hat{D}(k)} \quad ; \quad d \geq 3 \implies \text{condensation of spin–waves.}$$

\[(k \neq 0)\]
Technical discussion

Here: Don’t have the $w_r$ sum to zero. Write

$$w_r = v_r + \text{(constant)}$$

Has the effect of subtracting off background terms.

Get:

$$\sum_{r,r'} v_r v_{r'} \left\langle (S_r - \bar{m}) \cdot (S_{r'} - \bar{m}) \right\rangle_\beta \leq \frac{n}{\beta J} \sum_{r,r'} v_r D^{-1}(r, r') v_{r'}.$$

Now simply use $v_r$ to explore neighborhood of $r$.

Result:

$$\left| \frac{1}{2d} \sum_{r:|r|=1} \left\langle S_r - \bar{m} \right\rangle_\beta \right|^2 \leq \frac{n}{\beta J} \int_{[-\pi, +\pi]^d} \frac{d^d k}{(2\pi)^d} \frac{\left[ 1 - \hat{D}(k) \right]^2}{\hat{D}(k)}.$$

This is exactly $\text{Var}(M_r)$.

To do this we must assume (i.e. prove existence of) state – which is limit of torus states – where relevant observable, here the magnetization, is a sharp observable.

Conditions under which this is small:
Certainly need $d \geq 3$. Then, as $d \to \infty$ this gets smaller & smaller. (Prob. of R.W. returning to origin.)
From perspective of MFT: Not the whole story.
E.g. when the transition is of the first type, where does it occur?

Define: Mean field free energy function. \[ \Phi(m) \]

\[ \Phi(m) = \text{free energy that MFT would have if magnetization were constrained to equal } m. \]

¿How? (0) Landau.

1. \[ -H_{\text{MF}}^{(N)} = \frac{J}{N} \sum_{r,r'} S_r \cdot S_{r'}; \]
   find (limiting) constrained free energy.

2. \[ G(\vec{h}) = \log \int_{\Omega} dS e^{S \cdot \vec{h}} \]
   S(m) defined by Legendre transform.
   \[ \Phi_\beta(m) = -\frac{1}{2} \beta Jm^2 - S(m). \]

Find \( m \) which minimizes \( \Phi_\beta(m) \); that is the MF magnetization. \( \Phi_\beta \) evaluated @ minimizing \( m \) defines the MF free energy; entropy & energy make sense separately.

\( \Phi_\beta'(m) = 0 \)

are exactly the mean field equations that were discussed in MFT–101.
Typical evolution of a MF 1\textsuperscript{st} order transition.

- $\beta \ll 1$
- $\beta \approx c$
- $\beta = \beta_t$
- $\beta \geq \beta_t$
And we get:

Thus a definitive prediction for the transition temperature as well as other desirable features e.g. magnitude of the gap, latent heat, susceptibility, ...

In short, a full (albeit mean field) stat. mech., thermodynamic theory.

Clear:

Would like to implement these ideas in the context of real systems.
Main Result

Statement of Main Result (Theorem)

- \( -H = J \sum_{\langle r, r' \rangle} S_r \cdot S_{r'} \) on \( d \)-dimensional cubic lattice.
- \( \Phi_\beta(m) \) = associated mean field free energy function.
- \( I_d = \int_{[-\pi, +\pi]^d} \frac{d^d k}{(2\pi)^d} \left[ 1 - \hat{D}(k) \right]^2 \hat{\delta}(k) \); our small parameter.

\[
F(\beta) = \min_m \Phi_\beta(m) \quad \text{the mean field free energy.}
\]

- \( \mu = \mu(\beta) = \) actual magnetization of the real \( d \)-dimensional system.

And \( \kappa \) some constant that depends on the details of the spin–space.

Then:
\[
\left| \Phi_\beta(\mu) - F(\beta) \right| \leq \kappa I_d.
\]

Has implications:
Main Result

Typically, actual magnetization must follow mean field magnetization.

\[ \Phi_\beta(m) \]

Not only do we learn that actual magnetization must be near a solution to the mean field equations, it must be near the solution to the mean field equations.
At points of MF first order transition:

\[ m \approx m_0 \quad (m) \approx m_0 \]

\[ \beta \leq \beta_t \]

So if we plot (allowed values of) magnetization vs. \( \beta \),
Main Result

\[ \Phi_\beta(m) \]

- \[ \beta \leq \beta_t \]
- \[ \beta = \beta_t \]
- \[ \beta \geq \beta_t \]

\[ m(\beta) \]

- Forbidden region
- Transition temperature
- Other features
  - Energy, entropy, susceptibility, ...

All can be estimated (upper and lower bounds). Becomes exact as \( I_d \) tends to zero.
Current & Future Directions

(I) Get rid of assumption $d \gg 1$.

(a) Yukawa – type couplings

$$J_r = J_0 e^{-\lambda |r|}$$

requires $d \geq 3$ and $\lambda$ sufficiently small.

(b) Power law couplings

can reduce requirement that $d > 2$.

(II) Quantum systems & Gauge systems.

A three dimensional 3–state Potts model.
Talk Summary

- Write down $-H = \sum_{\langle r,r' \rangle} J_{r,r'} S_r \cdot S_{r'}$. (Interaction must be R.P.)

- Compute $\Phi_\beta(m)$ — see if transition is 1st order.

- Dimension large or $\lambda$ small or ...

$$\int_{[-\pi, +\pi]^d} \frac{1}{(2\pi)^d} \frac{[1 - \hat{J}(k)]^2}{\hat{J}(k)} d^d k \ll 1.$$  

Then actual systems follows MF system: 
1st order, with (asymptotically) correct gap, latent heat, ...

¿Continuous transitions? NO.