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Mean–Field Driven Phase Transitions of the First Type

Joint work:

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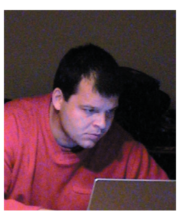


M. Biskup and L. Chayes, *Rigorous analysis of discontinuous phase transitions via mean-field bounds*, Commun. Math. Phys. **238**, no. 1-2, 53–93 (2003).

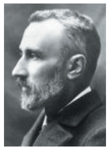
M. Biskup, L. Chayes and N. Crawford, *Mean-field driven first-order phase transitions in systems with long-range interactions*, to appear in J. Statist. Phys.

Talk Outline

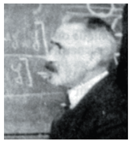
- Background & Review (MFT–101).
- Comparison to actual systems. (Also, models under consideration.)
- Allusion to technical tools (Infrared Bounds).
- More background (MFT–201).
- Description & statement of complete results.

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,

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

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

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

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

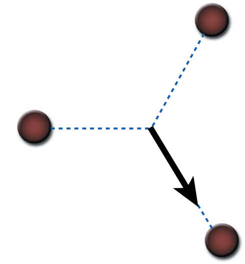
(1) $\beta_c J = 1$ (Curie temperature).

(2) $m(\beta) \approx K(\beta - \beta_c)^{1/2}$ (Critical behavior).

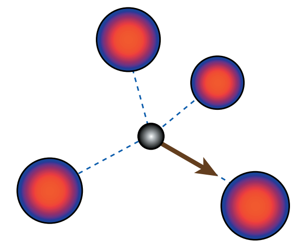
Now, look @ related spin–system

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

But S_r:



$(q = 3)$



$(q = 4)$

$\ldots$

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

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

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

(obviously same if $q = 2$).

$$\theta \propto m \qquad J \propto K$$

Now: do our "analysis".

$$\theta \ll 1 \qquad \theta = \frac{\beta K\theta + \frac{1}{2}(\beta K\theta)^2 + \ldots}{q + \beta K\theta + \ldots}$$

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

Note sign of coefficient.

(i) "$\frac{\beta_c K}{q} = 1$".

(ii) $\beta \gtrapprox \beta_c$; write $\beta K = q + \varepsilon$; ε small.

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

Predicts: θ slightly *negative*.

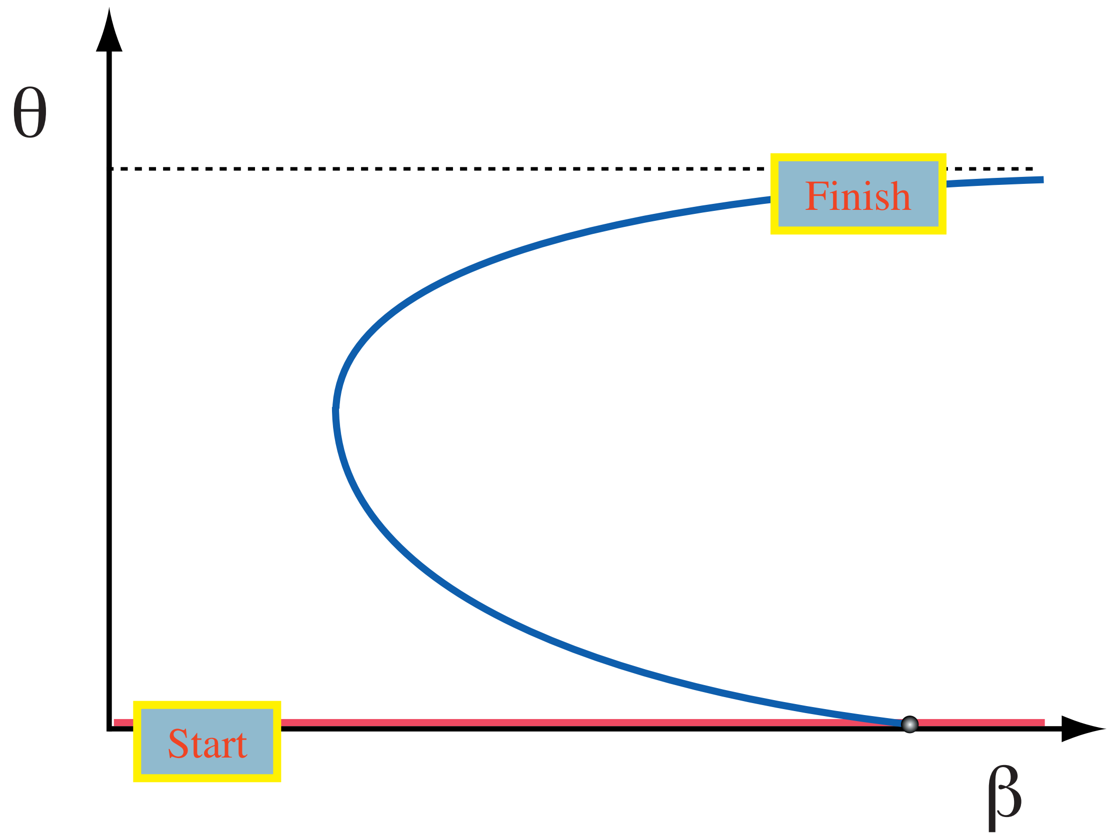
Impossible:

(a) On physical grounds.

(b) Probabilistic interpretation of θ.

No solutions of MFT ($q > 2$) with magnetization going continuously to zero.

Plot:



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 1^{st} order even if it "admits" continuous solutions? • Genuine discontinuous thermodynamics (e.g. energy density etc.)?

In some sense, MFT not such a wild "theory".

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

$$\mathfrak{M}_0 = \frac{1}{2d} \sum_{|r|=1} S_r$$

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

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

Then, given the value of $\mathfrak{M}_0$, the (random) magnetization @ origin, $\mathfrak{m}_0$ will be:

$$\mathfrak{m}_0 = Q(\mathfrak{M}_0).$$

Quantity $\mathfrak{m}_0$ is average value of magnetization *given* $\mathfrak{M}_0$.

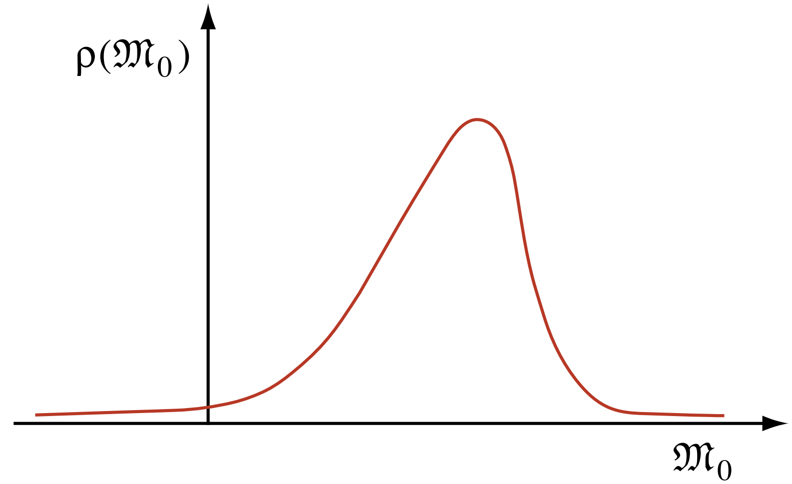
True (fully interacting) stat. mech. equations must be:

$$m(\beta) = \langle \mathfrak{m}_0 \,|\, \mathfrak{M}_0 \rangle_\beta = \langle Q(\mathfrak{M}_0) \rangle_\beta \,;$$

where $\langle - \rangle_\beta$ denotes thermal average @ inverse temperature β.

Generic random variables have to have some distribution or density.

If the RV was deterministic – i.e. if $\rho(\mathfrak{M}_0)$ were concentrated at a single value then mean field equations would be exact.



However: $\mathfrak{m}_0 = Q(\mathfrak{M}_0).$

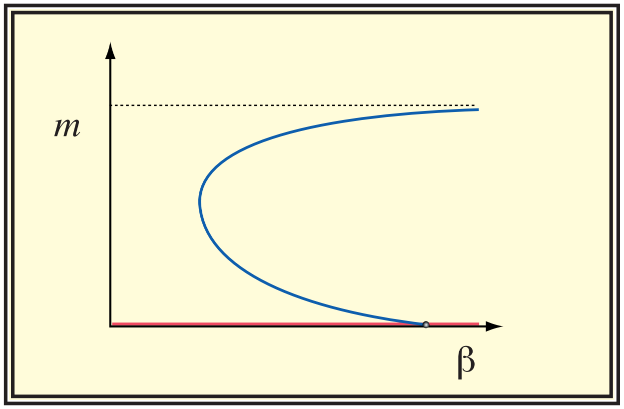
Continuous function

If $\mathfrak{M}_0$ is almost always close to its average value then $\mathfrak{m}_0$ must also be close to *its* average and they must both be close to *some* solution of the mean field equation.

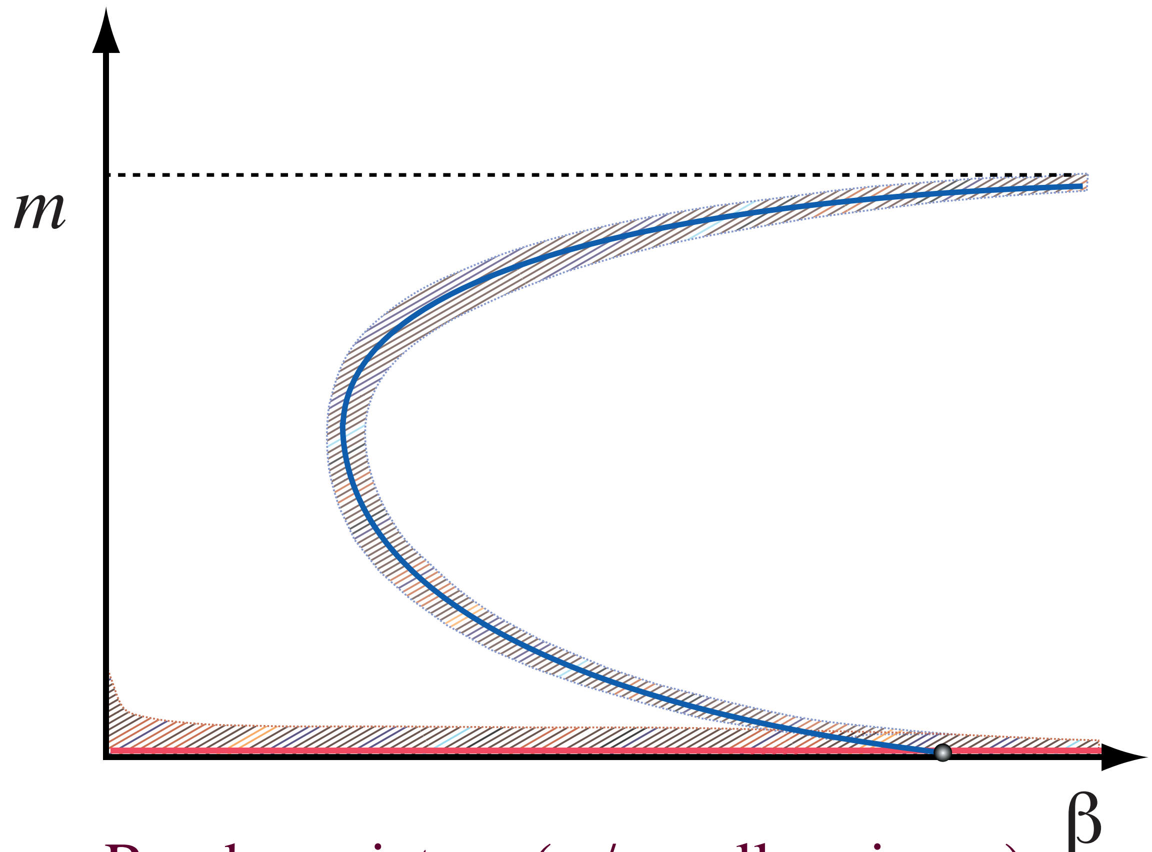
Q. How can we show this?

Ans. Show that variance is small.

If we can show that variance is small:



Deterministic picture



Random picture (w/ small variance)

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.

Systems under consideration:

(bad news)

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

Under these conditions, system is *reflection positive*.

May work with techniques of *Infrared Bounds*.

Good news:

S_r = 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.

Example: BEG model. Can emulate σ_r^2 by generating *new* component τ_r.

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

J. Fröhlich, B. Simon and T. Spencer, *Infrared bounds, phase transitions and continuous symmetry breaking*, Commun. Math. Phys. **50** (1976) 79–95.

J. Fröhlich, R. Israel, E.H. Lieb and B. Simon, *Phase transitions and reflection positivity. I. General theory and long-range lattice models*, Commun. Math. Phys. **62** (1978), no. 1, 1–34.

F.J. Dyson, E.H. Lieb and B. Simon, *Phase transitions in quantum spin systems with isotropic and nonisotropic interactions*, J. Statist. Phys. **18** (1978) 335–383.

J. Fröhlich, R. Israel, E.H. Lieb and B. Simon, *Phase transitions and reflection positivity. II. Lattice systems with short-range and Coulomb interactions*, J. Statist. Phys. **22** (1980), no. 3, 297–347.

Statement of infrared bounds:

Starting on torus of size L,

w_r any function with $\sum_r w_r = 0.$

Then

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

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:

$$\left|\hat{S}(k)\right|^2 \leq \frac{n}{\beta J} \frac{1}{\hat{D}(k)} \quad ; d \geq 3 \Rightarrow$$

condensation of spin–waves.

$(k \neq 0)$

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

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

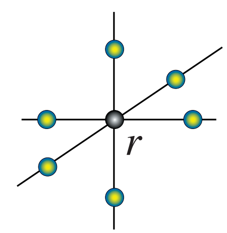
To do this we must assume (i.e. prove existence of) state – which is limit of torus states – where relevant observable, here the magnetization, is a sharp observable.

Has the effect of subtracting off background terms.

Get:

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

Now simply use v_r to explore neighborhood of r.



Result:

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

↑

This is exactly Var($\mathfrak{M}_r$).

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.)

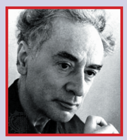
From perspective of MFT: Not the whole story.

E.g. when the transition is of the first type, where does it occur?

Define: Mean field free energy *function*.

$\Phi(m)$

$\Phi(m)$ = free energy that MFT *would* have if magnetization were constrained to equal m.

¿How? (0) Landau. 

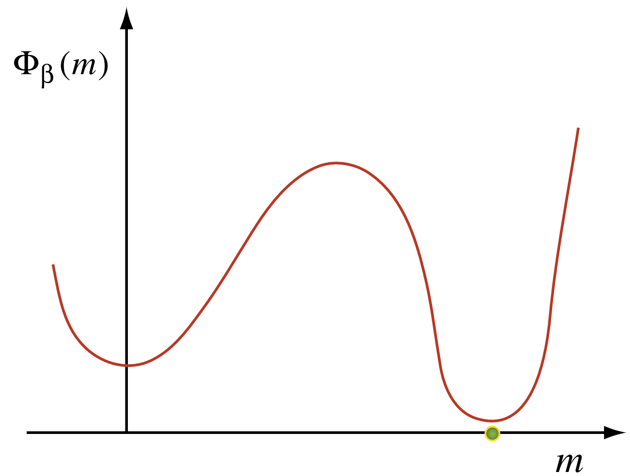
(1) $$-H^{(N)}_{\mathrm{MF}} = \frac{J}{N}\sum_{r,r'} S_r \cdot S_{r'}\,;$$

find (limiting) constrained free energy.

(2) $$G(\vec{h}) = \log \int_\Omega dS\, e^{S\cdot\vec{h}}$$

$\mathbf{S}(m)$ defined by Legendre transform.

$$\Phi_\beta(m) = -\tfrac{1}{2}\beta J m^2 - \mathbf{S}(m).$$

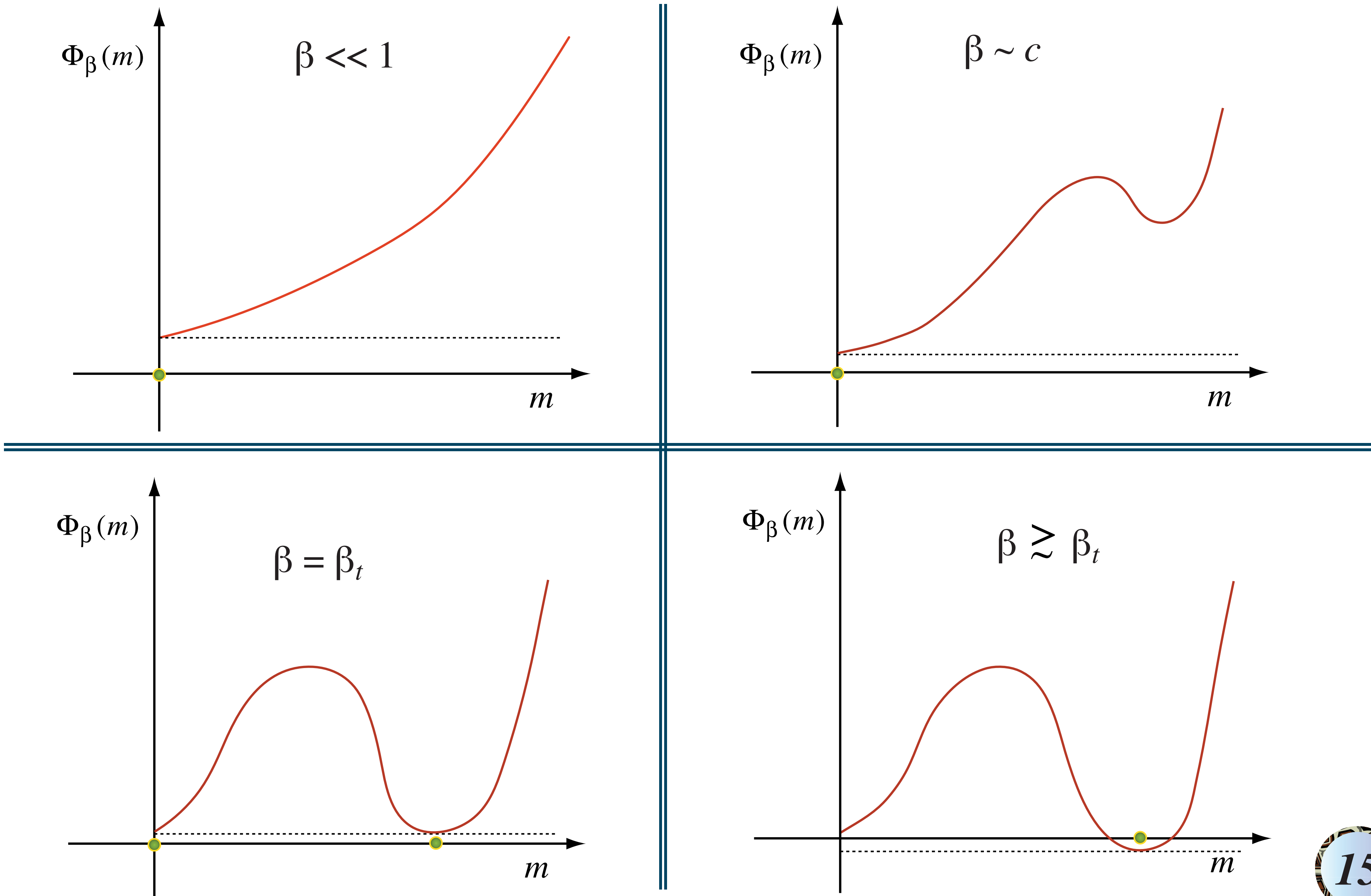


Find m which minimizes $\Phi_\beta(m)$; that is the MF magnetization. Φ_β evaluated @ minimizing m defines the *MF free energy*; entropy & energy make sense separately.

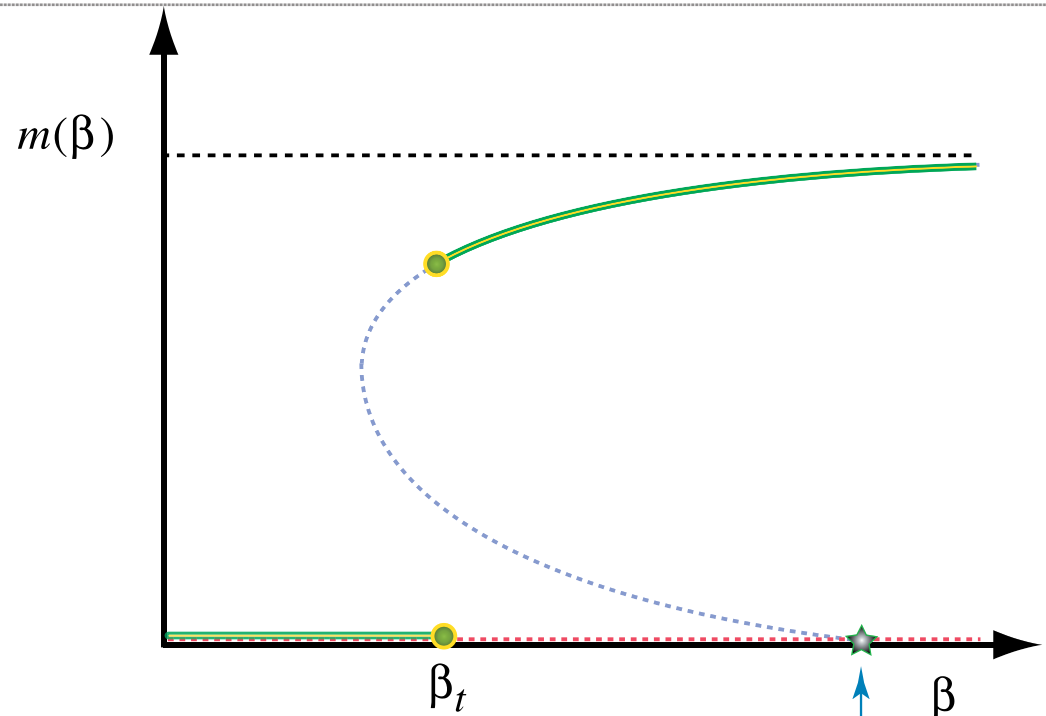
$$\Phi'_\beta(m) = 0$$

are exactly the mean field equations that were discussed in MFT–101.

Typical evolution of a MF 1st order transition.



And we get:



Point of false transition is place where high temperature minimum becomes unstable; merges with previous local maximum of $\Phi(m)$.

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.

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.
- $I_d = \int_{[-\pi,+\pi]^d} \frac{d^d k}{(2\pi)^d} \frac{[1-\hat{D}(k)]^2}{\hat{D}(k)}$; our small parameter.

$$F(\beta) = \min_m \Phi_\beta(m)$$ the mean field free energy.

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

And κ some constant that depends on the details of the spin–space.

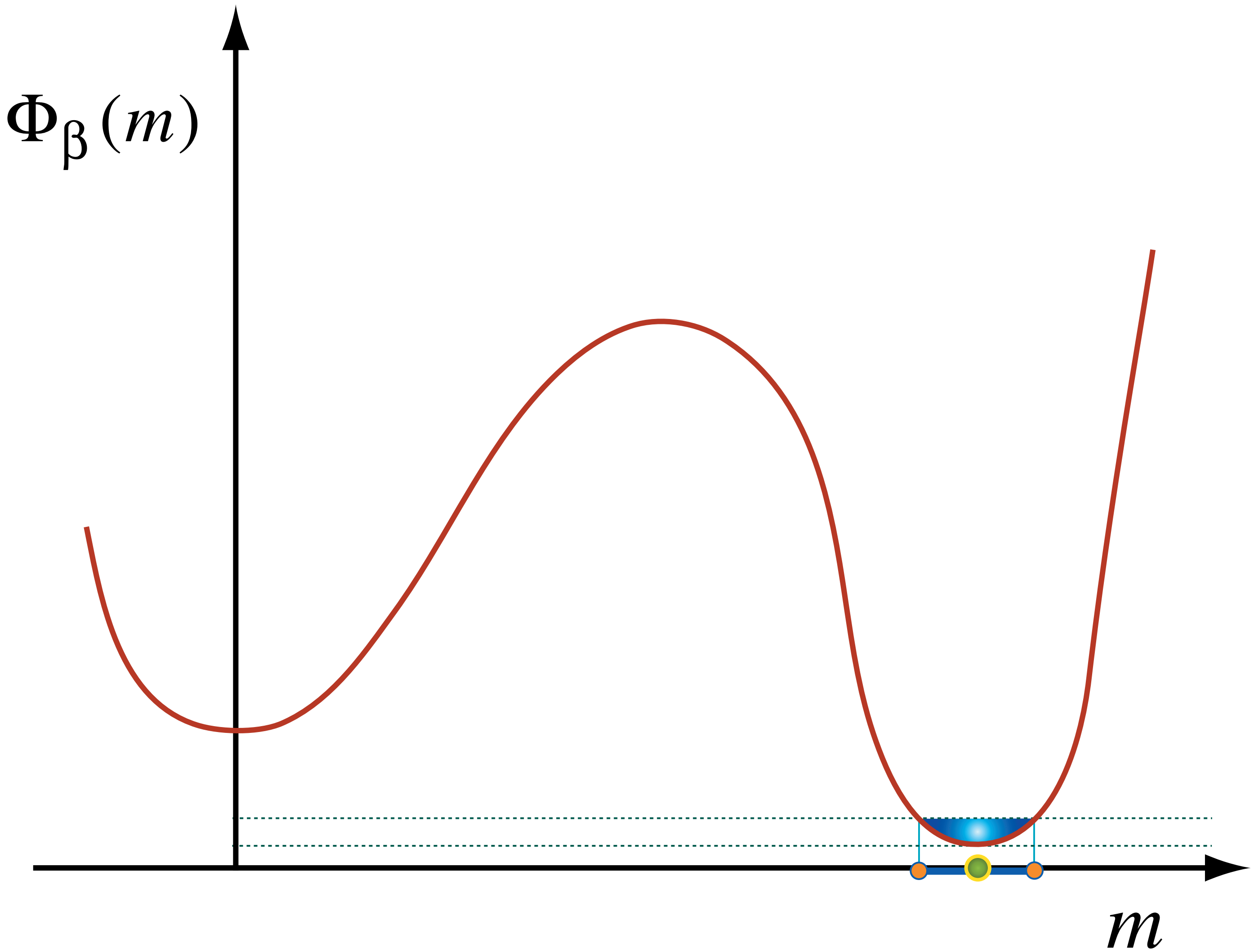
Then:

$$\left| \Phi_\beta(\mu) - F(\beta) \right| \leq \kappa I_d \, .$$

Has implications:

Main Result

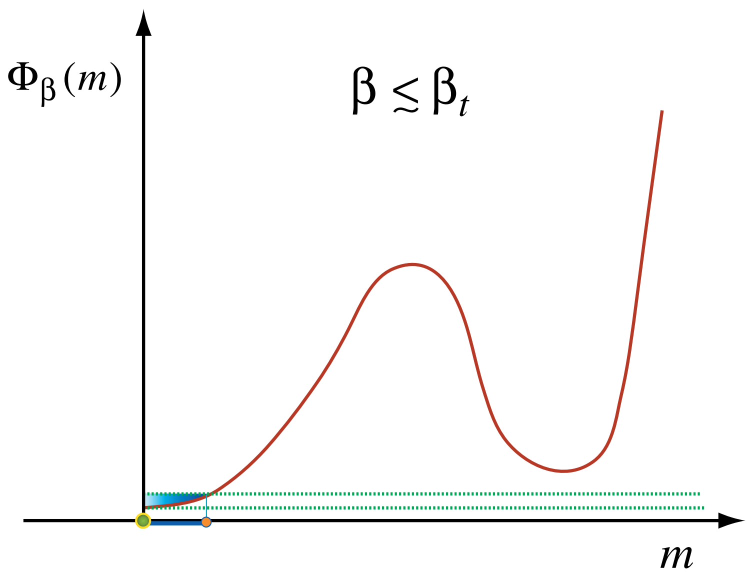
Typically, actual magnetization must follow mean field magnetization.

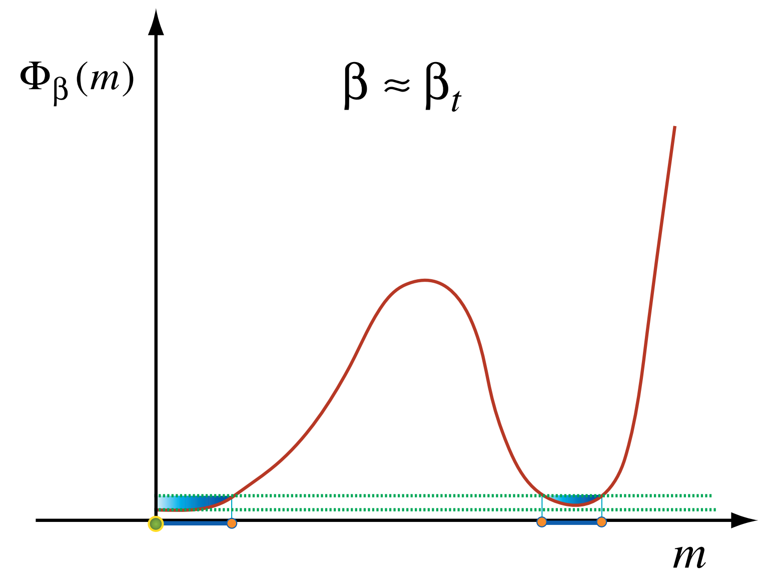


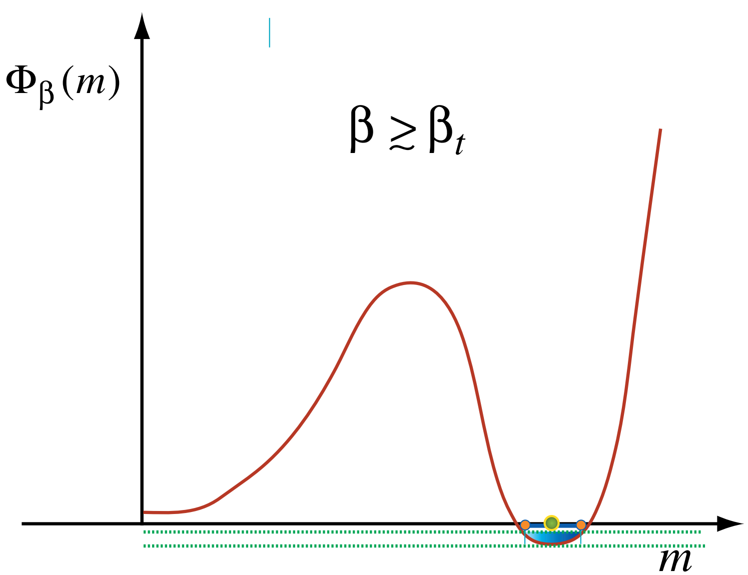
Not only do we learn that actual magnetization must be near *a* solution to the mean field equations, it must be near *the* solution to the mean field equations.

Main Result

At points of MF first order transition:

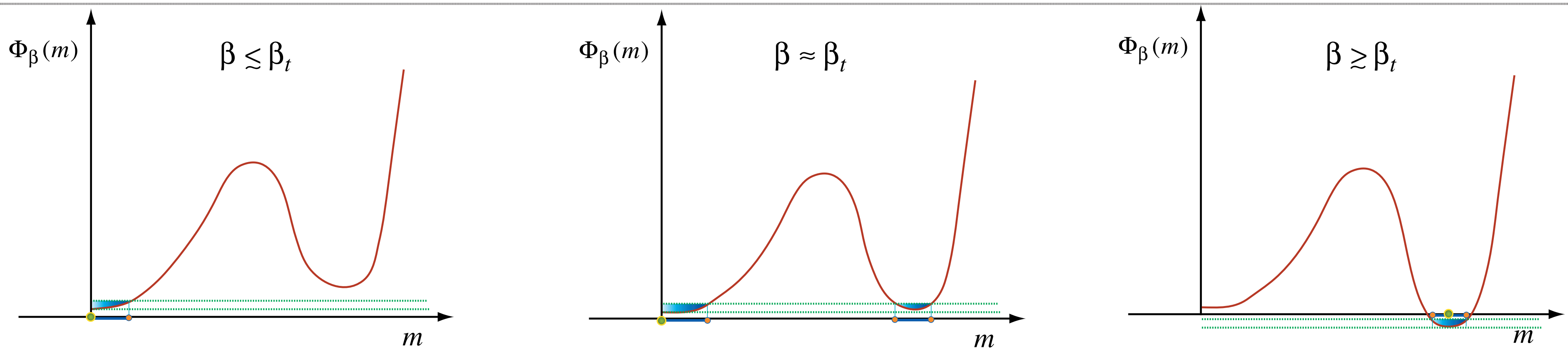


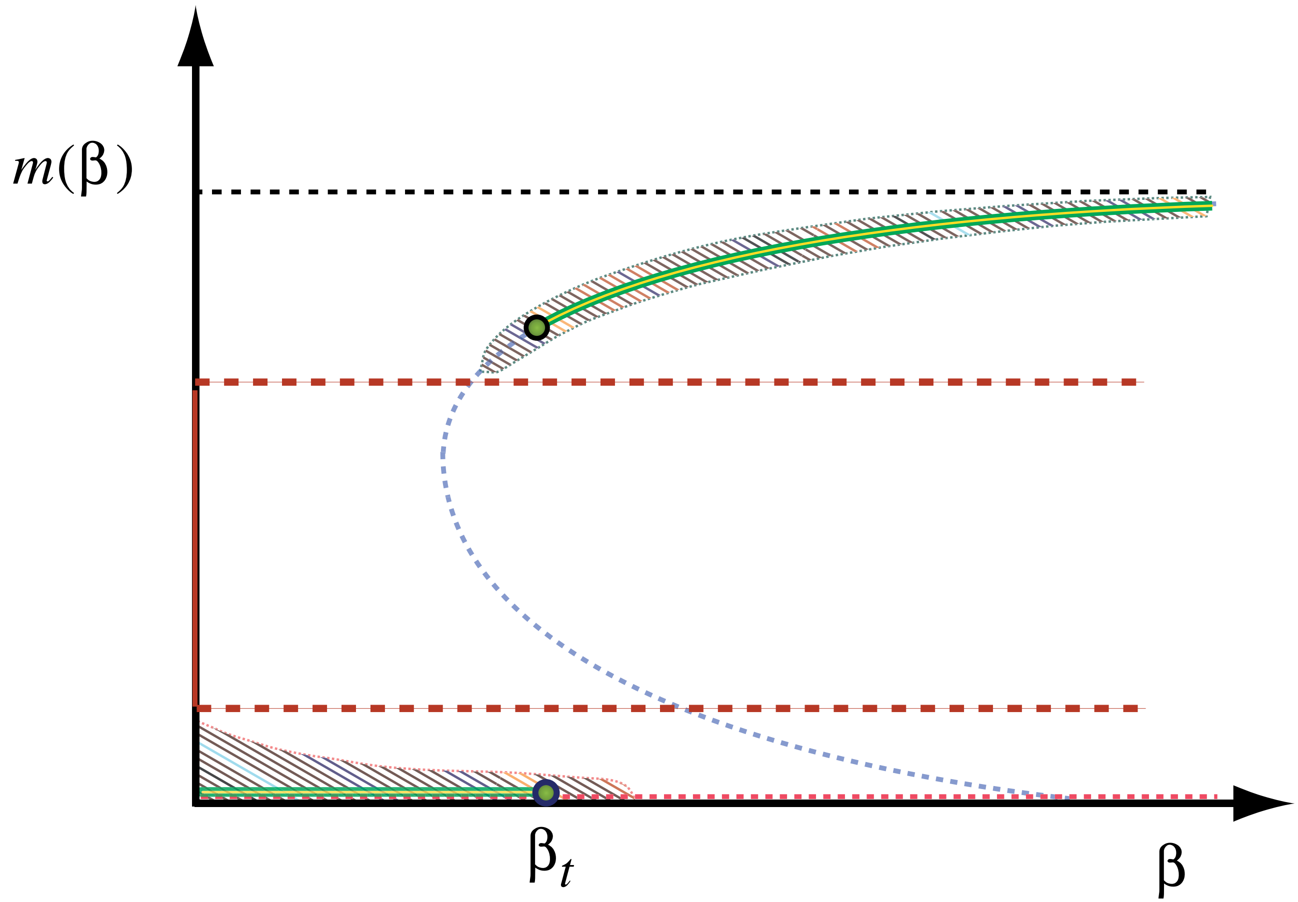




So if we plot (allowed values of) magnetization vs. β,

Main Result





- 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 λ sufficiently small.

A three dimensional 3–state Potts model.

(b) Power law couplings

can reduce requirement that $d > 2$.

(II) Quantum systems & Gauge systems.

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 λ small or ...

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

Then actual systems follows MF system:

1st order, with (asymptotically) correct gap, latent heat, ...

¿Continuous transitions? NO.