Phase Transitions in Infinitely Coordinated Models

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1 Motivation

- Systems are hard to solve! Even "simple" models like Ising (in 3D), Hubbard (in 2D) escape exact solutions...
- Going to infinite coordination can give us a better mathematical handle, and could give us intuition/insight about what happens in "real" models (more realistic coordination matters), insights into the nature of phase transitions.
- Many realms of application:
  - Superconductors (very long coherence length/cooper pair width on the lengthscale of atoms)
  - Modelling of nuclei (Lipkin model of nucleus)
  - Van der Waals gases
  - Long range interactions $\sim r^{-p}$ for sufficiently small p, e.g. 1-D Ising model with $p < p_c = 2$ behaves like Infinite coordinated version.
  - Fireflies and syncing of light phases; all-to-all Kuramoto model (https://home.iscte-iul.pt/~jaats/myweb/papers/new_kuras.pdf https://heptar.ch/6IT1/#sec-5) of:

$$\dot{\theta}_i = \omega_i + \frac{K}{N}\sum_{j=1}^{N}\sin(\theta_j - \theta_i) \tag{1.1}$$

  - Mean field (Sherrington-Kerrpatrick) model for spin glases (first solvable model! and confusions about negative entropy lead to RSB, Parisi's nobel prize) - mean field solutions can be complicated/rich!
  - Superradiance (N atoms coherently interacting with light to emit a high intensity pulse).
- Personal motivations; studying quantum dynamics and phase transitions on a hyperbolic lattice. There there is a sense of "infinite dimensionality" - if we take one definition of dimensionality for hypercubic lattices:

$$\lim_{N\to\infty}\frac{\ln c_N}{\ln N} = d \tag{1.2}$$

  with c_N the number of sites that are N steps from a given site, for a Bethe lattice/infinite Cayley tree we have $c_N = q\frac{(q-1)^N-1}{q-2} \sim q^N$ for coordination number q, which is faster than N^d (so "infinite dimensional") - even though the coordination number q is finite in this case (so not quite the same limit we are taking of $q \to \infty$ in the models we consider in this talk), is there perhaps something we can learn about our system from these mathematically tractable models?

2 Warm-Up: Mean Field Theory and Ising Models

2.1 What is MFT?

What is mean field theory? In condensed matter we think of it often as replacing an interaction term with an average/molecular field to replace a many-body problem into a solvable single body problem

(heuristic sketch)

In Landau-Ginzberg theory, we write down some expression for the free energy as dependent on an order parameter (as opposed to microscopic details), e.g. magnetization. Mean field theory is obtained by looking at the minima of such free energy (saddle point approximation), neglecting fluctuations of the order parameter.

2.2 Mean-Field Solutions to Ising

For example consider the Ising model with energy:

$$H = -J \sum_{\langle ij \rangle} s_i s_j - B \sum_i s_i \tag{2.1}$$

Replace $s_i s_j$ using deviation from average $m = \langle s_i \rangle$:

$$s_i s_j = [(s_i - m) + m][(s_j - m) + m] = (s_i - m)(s_j - m) + m(s_j - m) + m(s_i - m) + m^2 \approx m(s_i + s_j) - m^2 \tag{2.2}$$

so:

$$H_{mf} = -J \sum_{\langle ij \rangle} [m(s_i + s_j) - m^2] - B \sum_i s_i = \frac{1}{2} JNqm^2 - (Jqm + B) \sum_i s_i \tag{2.3}$$

Replaced the interactions with an effective single-spin interaction $B_{\text{eff}} = (Jqm + B)$.

Partition function:

$$Z = \sum_{\{s_i\}} e^{-\beta E[s_i]} = \sum_m e^{-\beta F(m)} = \int dm e^{-\beta N f(m)} \tag{2.4}$$

Replace spins with mean value $\langle s \rangle = m$:

$$E = -J \sum_{\langle ij \rangle} m^2 - B \sum_i m \implies \frac{E}{N} = -\frac{1}{2} Jqm^2 - Bm \tag{2.5}$$

with q the coordination number. Magnetization of configuration is:

$$m = \frac{N_\uparrow - N_\downarrow}{N} = \frac{2N_\uparrow - N}{N} \tag{2.6}$$

So:

$$\log \Omega = \log \frac{N!}{N!(N - N_\uparrow)!} \implies \frac{\log \Omega}{N} \overset{\approx}{\text{Stirling}} \log 2 - \frac{1}{2}(1+m)\log(1+m) - \frac{1}{2}(1-m)\log(1-m) \tag{2.7}$$

So:

$$f(m) \approx E - TS = -Bm - \frac{1}{2} Jqm^2 - T\left(\log 2 - \frac{1}{2}(1+m)\log(1+m) - \frac{1}{2}(1-m)\log(1-m)\right) \tag{2.8}$$

Minimizing:

$$\frac{\partial f}{\partial m} = 0 \implies m = \tanh(\beta B + \beta Jqm) \tag{2.9}$$

Self-consistency condition for m.

Taylor expanding for small m:

$$f(m) \approx -T\log 2 - Bm + \frac{1}{2}(T - Jq)m^2 + \frac{1}{12}Tm^4 \tag{2.10}$$

Sign of quadratic term tells us whether we have one minima at $m = 0$ or degenerate minima $\pm m_0$, giving gritical temperature:

$$T_c = Jq \tag{2.11}$$

with:

$$m_0 = \sqrt{\frac{3(T_c - T)}{T}} \tag{2.12}$$

(c.f. $v_g - v_l \sim (T_c - T)^{1/2}$ in Van der Waals)

Heat Capacity:

$$c = \frac{1}{N}\beta^2 \frac{\partial^2}{\partial \beta^2}\log Z = \begin{cases} 0 & T \to T_c^+ \\ 3/2 & T \to T_c^- \end{cases} \tag{2.13}$$

Introducing external magnetic field:

$$f(m) \approx -Bm + \frac{1}{2}(T - Jq)m^2 + \frac{1}{12}Tm^4 \tag{2.14}$$

at $T = T_c$ we have:

$$m \sim B^{1/3} \tag{2.15}$$

(c.f. $v_g - v_l \sim (p - p_c)^{1/3}$ in van der waals)

and for $T \geq T_c$ but close we have:

$$f(m) \approx -Bm + \frac{1}{2}(T - T_c)m^2 \implies m \approx \frac{B}{T - T_c} \implies \chi = \frac{\partial m}{\partial B} = \frac{1}{T - T_c} \tag{2.16}$$

and approaching from other side we see:

$$\chi \sim |T - T_c|^{-1} \tag{2.17}$$

In Landau-Ginzberg theory, we write down the free energy:

$$F[m(\mathbf{x})] = \int d^d x f[\phi(\mathbf{x})] = \int d^d x \left[\frac{1}{2}\alpha\phi^2 + \frac{1}{4}u\phi^4 + \frac{1}{2}K(\boldsymbol{\nabla}\phi)^2 + \dots\right] \tag{2.18}$$

and solve/approximate the functional integral:

$$Z = \int \mathcal{D}\phi e^{-\beta F[\phi(\mathbf{x})]} \tag{2.19}$$

Looking at functional derivative/saddle point approximation:

$$\frac{\delta F}{\delta \phi(\mathbf{x})} = \alpha\phi + u\phi^3 - \gamma\boldsymbol{\nabla}^2\phi \tag{2.20}$$

Setting to zero, we get:

$$\gamma\boldsymbol{\nabla}^2\phi = \alpha\phi + \beta\phi^3 \tag{2.21}$$

Gives rise to same structure as previous mean field theory approach.

2.3 Comparison with Infinite range

Consider now the infinite-range Ising model, where every neighbour talks to each other. We then take the coupling to be uniformly $\frac{J}{N}$ between all spins, so:

$$H = -\frac{J}{2N}\sum_{i,j} s_i s_j - B\sum_i s_i \tag{2.22}$$

Defining the magnetization as:

$$m = \sum_i \frac{s_i}{N} \implies mN = \sum_i s_i \tag{2.23}$$

we can write the Hamiltonian purely in terms of m:

$$H = -\frac{J}{2N}\left(\sum_i s_i\right)^2 - h\sum_i s_i = -\frac{J}{2N}(Nm)^2 - BNm \tag{2.24}$$

so:

$$\frac{E}{N} = -\frac{1}{2}Jm^2 - Bm \tag{2.25}$$

This is exactly the $\frac{E}{N}$ we had before!

So while we did an approximation in the Ising case for the energy of a configuration by replacing every spin with its mean in the mean-field approximation, here the approximation is exact. This is one example where the two coincide (and it is intuitive that it would - if the system is all-to-all with equal coupling then the average literally is equivalent to the microscopic spin degrees of freedom) but its worth noting that this is not always the case - example to be given towards the end of the talk. Have to be careful with intuition!

2.4 Critical Exponents

Scaling of quantities at phase transitions:

$$c = \frac{\mathrm{d}E}{\mathrm{d}T} \sim c_\pm |T - T_c|^{-\alpha} \tag{2.26}$$

(at $B = 0$, as $T \to T_c$):

$$m \sim (T_c - T)^\beta \tag{2.27}$$

$$\chi = \left.\frac{\partial m}{\partial B}\right|_{B=0} \sim |T - T_c|^{-\gamma} \tag{2.28}$$

(at fixed T, take $B \to 0$)

$$m \sim B^{1/\delta} \tag{2.29}$$

Also, we can look at correlation function:

$$\langle \phi(\mathbf{x})\phi(\mathbf{y}) \rangle = \begin{cases} \frac{1}{r^{d-2+\eta}} & r \ll \eta \\ e^{-r/\eta} & r \gg \eta \end{cases} \tag{2.30}$$

where:

$$\xi \sim |T - T_c|^\nu \tag{2.31}$$

MFT predicts (universality!):

$$\alpha = 0, \beta = \frac{1}{2}, \gamma = 1, \delta = 3, \eta = 0, \nu = \frac{1}{2} \tag{2.32}$$

The ones for correlation functions being computed by doing the path integral at quadratic order (wherein it is solvable/Gaussian), i.e. only consider quadratic order contributions to the free energy.

2.5 Critical Dimensions

Saw how $q \to \infty$ seems to make MFT exact. When else is it useful? Usual considerations are in terms of spatial dimensions of the system:

- d_c^{upper} is the dimension where the transition changes to mean-field like (e.g. $d_c^{\text{upper}} = 4$ for $\phi - 4$ theory). To see this, we want fluctuations/correlations to be small, i.e. $\left\langle \phi^2 \right\rangle \gg \langle \phi \rangle$, so:

$$R = \frac{\int_0^\xi d^d x \left\langle \phi(\mathbf{x})\phi(0) \right\rangle}{\int_0^\xi d^d x m_0^2} \sim \frac{1}{m_0^2 \xi^d} \int_0^\xi dr \frac{r^{d-1}}{r^{d-2}} \sim \frac{\xi^{2-d}}{m_0^2} \tag{2.33}$$

  with MFT exponents:

$$m_0 \sim |T - T_c|^{1/2}, \xi \sim |T - T_c|^{-1/2} \tag{2.34}$$

  so:

$$R \sim |T - T_c|^{\frac{d-4}{2}} \tag{2.35}$$

  which is small only for $d > 4$, setting the upper critical dimension. Notably for the Ising model the $d = 2, 3$ critical exponents disagree with MFT.

- d_c^{lower} is the dimension below which there is no phase transition (e.g. all 1D systems have $d_c^{\text{lower}} \geq 1$ due to entropic arguments (domain walls of energy ϵ that does not scale with L, entropy $\Delta S = -\epsilon/T$, L/a positions for domain wall so $\Delta S = k_B \log(L/a)$. So if $T > 0$ and L large, the entropy gain dominates), all 2D systems with continuous order parameters have $d_c^{\text{lower}} \geq 2$ due to Mermin-Wagner (If we had SSB, then we would have massless Goldstone Bosons/fluctuations which are strong enough to destroy the SSB))

3 Review: Large-size critical behavior of infinitely coordinated systems

(Botet and Jullien, Phys. Rev. B 28, 3955 (1983))

Consider $q = N$ infinitely coordinated systems. Usually we think about the limit where $N \to \infty$, but here they argue for (and then check analytically/numerically) a scaling argument for the scaling of thermodynamic quantities with system size N.

3.1 Scaling Argument

Consider correlation length:

$$\xi \sim |T - T_c|^{-\nu} \tag{3.1}$$

and a thermodynamic quantity which is singular at the transition:

$$A \sim |T - T_c|^a \tag{3.2}$$

Scaling hypothesis:

$$A \sim |T - T_c|^a F_a(L/\xi) \tag{3.3}$$

where $F_a(x \to \infty) = \text{const}$ in the thermodynamic limit, and $F_a(x \to 0) \sim x^{\omega_a} = -a/\nu$ for A to be analytic at $T = T_c$ for L finite, so:

$$A \; T \overset{\sim}{=} T_c \; L^{\omega_a} \sim L^{-a/\nu} \tag{3.4}$$

This hypothesis is valid for $d < d_c^{\text{upper}}$. However - L, d lose their meaning in systems with infinite coordination. We replace ξ with N_c/a coherence number, which we suppose diverges:

$$N_c \; N \overset{\sim}{=} \infty \; |T - T_c|^{-\nu^*} \tag{3.5}$$

In the short-range case N_c is the sites in volume ξ^d, here it is just a tool. Thermodynamic quantities scale as:

$$A \; N \overset{\sim}{=} \infty \; |T - T_c|^{a_{\text{MF}}} \tag{3.6}$$

so we modify scaling hypothesis:

$$A \sim |T - T_c|^{a_{\text{MF}}} F_a^*(N/N_c) \tag{3.7}$$

with $F_a^*(x \to \infty) = \text{const.}$ and $F_a^*(x \to 0) = x^{\omega_a}, \omega_a = -a_{\text{MF}}/\nu^*$. So then at $T = T_c$:

$$A_{T=T_c} \sim N^{\omega_a} \sim N^{-a_{\text{MF}}/\nu^*} \tag{3.8}$$

They then argue ν^* via comparing with a system at $d = d_c$ and $L = N^{1/d_c}$. For $L \to \infty$, this short range system has MF behaviour. If we assume (a) that the scaling argument applies at the critical dimension and (b) the infinite and finitely coordinated system has the same scaling exponents, then $N_c \sim \xi^{d_c}$ and so:

$$\nu^* = \nu_{\text{MF}} d_c \tag{3.9}$$

Note: Scaling is not quite correct at $d = d_c$ (logarithmic corrections due to corrections), could argue that the fluctuations dissapear in the infinite range limit (and they check this in the examples). So:

$$A \; T \overset{\sim}{=} T_c \; N^{\omega_a} = N^{-\frac{a_{\text{MF}}}{\nu_{\text{MF}} d_c}} \tag{3.10}$$

3.2 Analytical ($d_c^{\text{upper}} = 4$) Examples

- For infinite range classical Ising model compute m analytically (taking the energy we wrote down earlier as a starting point), finding that:

$$m^2 \sim \frac{|T_c - T|}{T_c} \left(\frac{N}{N_c}\right)^{-1/2} \times \frac{\int \dots \left(\frac{N}{N_c}\right)^{-1/2}}{\int \dots \left(\frac{N}{N_c}\right)^{-1/2}} \tag{3.11}$$

  which is precisely the scaling form of $F_\alpha(x)$ and $\alpha_{\text{MF}} = \frac{1}{2}$. N_c has an exponent $\nu^* = 2$, consistent with $\nu^* = \nu_{\text{MF}} d_c^{\text{upper}}$ with $\nu_{\text{MF}} = 1/2$ and $d_c^{\text{upper}} = 4$ for short-range Ising.

- Infinite range Heisenberg model:

$$H = -\frac{J}{N} \sum_{i \neq j} \mathbf{S}_i \cdot \mathbf{S}_j \tag{3.12}$$

  Same analysis (Z only differs by terms of $\mathcal{O}(\frac{1}{N})$ and only driven by thermal (not quantum) fluctuations so $d_c^{\text{upper}} = 4$ is the same).

- Spherical Model:

$$H = -\frac{J}{N} \left(\sum_i \sigma_i\right)^2 \tag{3.13}$$

  with:

$$\sum_i \sigma_i^2 = \frac{N}{4} \tag{3.14}$$

  again, similar conclusions ($d_c^{\text{upper}} = 4$, this model has many of the same features phase-wise as infinite range Ising).

3.3 Mixed Numerical/Analytical Example: Anisotropic XY model in transverse field

$$H = -\frac{1}{NS}\sum_{i<j}(X_i X_j + \gamma Y_i Y_j) - \Gamma \sum_i Z_i \tag{3.15}$$

d-dimensional quantum model has same critical behaviour in temperature as classical Ising in $d+1$, with gap Δ is the inverse of the coherence length in the classical example, so:

$$\Delta \sim L^{-1} \tag{3.16}$$

and $d_c = 3$. Believed that for $\gamma = 1$/isotorpic case that this equivalence does not hold, and $z = 2$ - classical model in $d+2$ dimensions? So $d_c = 2$.

They calculate the magnetization/gap analytically with MF analysis and numerically otherwise.

$$m^2 = \frac{1}{NS}\langle 0| \left(\sum_i X_i\right)^2 |0\rangle \tag{3.17}$$

$$m^2 = \frac{1}{NS}\langle 0| \left(\sum_i X_i\right)^2 + \left(\sum_i Y_i\right)^2 |0\rangle \tag{3.18}$$

3.4 Mean-Field Analysis ($N = \infty$)

For mean-field, they rewrite:

$$H = -\frac{1}{2Ns}\left(J_x^2 + \gamma J_y^2 - K_x - \gamma K_y\right) - \Gamma J_z \tag{3.19}$$

with:

$$J_x = \sum_i X_i, \quad K_i = \sum_i X_i^2 \tag{3.20}$$

Wherein we can neglect the K terms as $N = \infty$:

$$H = -\frac{1}{2J}(J_x^2 + \gamma J_y^2) - \Gamma J_z \tag{3.21}$$

Consider to be one spin of size NS, treat classically and minimize:

$$E(\theta,\phi) = -\frac{J}{2}(\sin^2\theta\cos^2\phi + \gamma\sin^2\theta\sin^2\phi) - \Gamma J\cos\theta \tag{3.22}$$

and calculate $m = J_x/J = \sin\theta\cos\phi$, yielding:

$$m_\infty = (1-\Gamma^2)^{1/2} \quad \Gamma < 1 \tag{3.23}$$

$$m_\infty = 0 \quad \Gamma > 1 \tag{3.24}$$

and the isotropic case gives the same result. Δ can be obtained the gap with the frequency of the motion of the large spin. Replacing J_z by its mean field value, we find:

$$\Delta_\infty = 0 \quad \Gamma \leq 1 \tag{3.25}$$

$$\Delta_\infty = [(\Gamma-1)(\Gamma-\gamma)]^{1/2} \quad \Gamma \geq 1 \tag{3.26}$$

so:

$$\Delta_\infty \sim (\Gamma - \Gamma_c)^{s_{\mathrm{MF}}} \tag{3.27}$$

with $s_{\mathrm{mf}} = 1/2$ for $\gamma \neq 1$, $s_{\mathrm{mf}} = 1$ for $\gamma = 1$.

3.5 Numerics

Spin-1/2 makes the K_α terms simple constants (as just identities) so we can use the "Mean-field limit" for finite N. Studied in large N criticality ($N \sim 150$), since H only connects $|j,m\rangle$ states with $|j,m\pm 2\rangle$ states, diagonalization of $(N/2)\times(N/2)$ matrices. Numerically they find:

$$\Delta \sim \exp(-aN), \quad m - m_\infty \sim N^{-1} \quad \Gamma < 1 \tag{3.28}$$

$$\Delta \sim N^{-1/3}, m \sim N^{-1/3} \quad \Gamma = 1 \tag{3.29}$$

$$\Delta - \Delta_\infty \sim N^{-1}, \quad m \sim N^{-1/2} \quad \Gamma > 1 \tag{3.30}$$

They then check against the found critical exponents against the general scaling relations and find them to be in agreemnet numerically. They also check $S=1$ and find agreement, $S=3/2$ less clear due to system size limitations. Remark - these numerical results are confirmed analytically 20 years later by Dusuel/Vidal, in next section.

3.6 $\gamma = 1$ Analytics

For the $\gamma = 1$ case, the Hamiltonian is diagonal in the j,m basis adn they can write down the eigenvalues, magnetization, gap immediately. They then find magnetizations $\Delta = N^{-1}$ and $m = m_\infty + O(1/N)$ with MF recovered with $N \to \infty$. Scaling forms are consistent if $\nu_{\text{MF}} = 1/2$ like Ising is assumed and $d_c = 2$.

They also provide a numerical analysis of a quantum model with Yang-Lee edge singularity, i.e. TFIM with complex/imaginary field:

$$H = -\frac{J_x^2}{2J} - \Gamma J_z - ihJ_x \tag{3.31}$$

3.7 Takeaways

Simple argument for scaling! Has been checked for $O(n=1), O(n=\infty)$ classical models with $d_c = 4$ and numerically in quantum models (XY models). Could be applied to complicated models to derive critical dimension via scaling arguments. Interpretations of numerical results in parameters regions where infinite coordination physics is expected, e.g. if studying systems with r^{-p} interactions which behave like infinite coordination, or systems with high q...

4 Analytical Arguments for Scaling (Dusuel and Vidal PRL 93, 237204 (2004))

Analytical Arguments for the Scaling Behaviour as postulated by Botet/Jullien (e.g $\Delta \sim N^{-1/3}$) is confirmed by a combination of $O(1/N)$ expansion (Holstein-Primakoff), continuous unitary transformation + scaling argument. LMG in spin operators is given by:

$$H = -\frac{J}{N}\sum_{i<j}(X_iX_j + Y_iY_j) - h\sum_i Z_i = -\frac{J}{N}(1+\gamma)(S^2 - S_z^2 - N/2) - 2hS_z - \frac{J}{2N}(1-\gamma)(S_+^2 + S_-^2) \tag{4.1}$$

Analyze this via Holstein-Primakoff into bosonic operators:

$$S_Z = S - a^\dagger a = N/2 - a^\dagger a \tag{4.2}$$

$$S_+ = S_-^\dagger = (2S - a^\dagger a)^{1/2} a = N^{1/2}(1 - a^\dagger a/N)^{1/2} a \tag{4.3}$$

and then expand Taylor expand the square roots (as you may have done in a condensed matter class to solve the ferromagnetic Heisenberg model), obtaining an expansion in $\frac{1}{N}$:

$$H = H_0 + H_2^+ + H_2^- \tag{4.4}$$

$$H_0 = \sum_{\alpha,\delta\in\mathbb{N}} \frac{h_{0,\alpha}^{(\delta)} A_\alpha}{N^{\alpha+\delta-1}} \tag{4.5}$$

$$H_2^+ = \sum_{\alpha,\delta\in\mathbb{N}} \frac{h_{2,\alpha}^{(\delta)} (a^\dagger)^2 A_\alpha}{N^{\alpha+\delta}} \tag{4.6}$$

$$A_\alpha = (a^\dagger)^\alpha a^\alpha \tag{4.7}$$

They combine this with a continuous unitary technique to diagonalize order by order in $O(\frac{1}{N})$, letting l be a scaling parameter and:

$$H(l) = U^\dagger(l) H U(l) \tag{4.8}$$

wherein we have the flow equation:

$$\partial_l H(l) = [\eta(l), H(l)], \quad \eta(l) = -U^\dagger(l)\partial_l U(l) \tag{4.9}$$

such that $H(l=\infty)$ is diagonal (original proposal for anti-Herm generator $\eta(l)$ is $\eta(l) = [H_d(l), H_{\text{od}}(l)]$ (diagonal/off diagonal parts) but they use $\eta(l) = H^+2(l) - H_2^-(l)$), Expectation values of eigenstates of H for operators Ω can be evaluated by solving $\partial_l \Omega(l) = [\eta(l), \Omega(l)]$ and they use this to confirm $\Delta(N) \sim N^{-1/3}$, as well as the scaling of the ground state energy, magnetization, two-point functions.

$$E_0(N) \sim -1 - \frac{1-\gamma}{2n} + \frac{a_e}{N^{4/3}} \tag{4.10}$$

$$\frac{2\langle S_z \rangle}{N} \sim 1 + \frac{1}{N} + \frac{a_z}{N^{2/3}} \tag{4.11}$$

$$\frac{4\left\langle S_x^2 \right\rangle}{N^2} \sim \frac{a_{xx}}{N^{2/3}} \tag{4.12}$$

$$\frac{4\left\langle S_y^2 \right\rangle}{N^2} \sim \frac{a_{yy}}{N^{4/3}} \tag{4.13}$$

$$\frac{4\langle S_z \rangle}{N^2} \sim 1 + \frac{2}{N} + \frac{a_{zz}}{N^{2/3}} \tag{4.14}$$

5 Adiabatic Dynamics (Caneva, Fazio, and Santoro, J. Phys.: Conf. Ser. 143 012004 (2009))

Caneva, Fazio, and Santoro, J. Phys.: Conf. Ser. 143 012004 (2009)

5.1 Model and review

Look at LMG model, but study its dynamics at the phase transition (mean-field like, but adiabatic dynamics are interesting):

We study (spin-1/2):

$$H = -\frac{2}{N}\sum_{i<j}(X_iX_j + \gamma Y_iY_j) - \Gamma\sum_i Z_i \tag{5.1}$$

Rewrite using $S_x = \sum_i X_i$ (and so on):

$$H = -\frac{1}{N}[S_x^2 + \gamma S_y^2] - \Gamma S_z \tag{5.2}$$

commutes with S^2, does not couple different parity states as $[H, S^2] = [H, \pi_i Z_i] = 0$. For $\gamma = 1$ it is also that $[H, S_z] = 0$.

Second order Qphase transition at $\gamma_c = 1$ characterized by mean field.

$$m_\infty = (1-\Gamma^2)^{1/2} \quad \Gamma < 1 \tag{5.3}$$

$$m_\infty = 0 \quad \Gamma > 1 \tag{5.4}$$

and the isotropic case gives the same result. Δ can be obtained the gap with the frequency of the motion of the large spin. Replacing J_z by its mean field value, we find:

$$\Delta_\infty = 0 \quad \Gamma \leq 1 \tag{5.5}$$

$$\Delta_\infty = [(\Gamma-1)(\Gamma-\gamma)]^{1/2} \quad \Gamma \geq 1 \tag{5.6}$$

Gap scaling:

$$\Delta_N - \Delta_\infty \sim N^{-1/3} \quad \gamma \neq 1 \tag{5.7}$$

$$\Delta_N - \Delta_\infty \sim N^{-1} \quad \gamma = 1 \tag{5.8}$$

Scaling behaviour for identification of dynamic regimes. Note that teh relevant gap is not the equilibrium gap between the ground/first excited state, but scaling is identical.

5.2 Adiabatic Dynamics

$\Gamma \gg 1$ at $t_{\text{in}} = -\infty$ to $\Gamma = 0$ at $t = 0$:

$$\Gamma(t) = -t/\tau \tag{5.9}$$

for $t \in (t_{\text{in}}, \tau]$.

Simulation is simplified by this fact; GS for $\Gamma \gg 1$ is fully up polarized, so belongs to $S = N/2$. Since S is a constant of motion, we can restrict to this subpace, and look at $|N/2, S_z\rangle$ basis for $S_z = -N/2, \ldots N/2$, wherein the Shrodinger evolution:

$$|\psi(t)\rangle = \sum_{j=1}^{N/2+1} u_{2j-1}(t)|N/2, -N/2 - 2 + 2j\rangle \tag{5.10}$$

amounts to:

$$i\,\frac{\mathrm{d}u_{2j-1}}{\mathrm{d}t} = \sum_k A_{j,k}u_{2k-1}(t) \tag{5.11}$$

Odd amplitudes drop out due to parity conservation, so only need to consider $(N/2+1)\times(N/2+1)$ symmetric matrix A to simulate.

Adiabaticity can be quantified via residual energy (depends on τ - slower the time, smaller the residual energy):

$$E_{\text{res}} = E_{\text{fin}} - E_{\text{gs}} = \langle\psi(t_{\text{fin}})|H(t_{\text{fin}})|\psi(t_{\text{fin}})\rangle - E_{\text{gs}} \tag{5.12}$$

or via incomplete magnetization:

$$m_{\text{inc}} = m_{\text{gs}} - m(t) \tag{5.13}$$

with:

$$m^2 = \frac{4}{N^2}\langle\psi|S_x^2 + S_y^2|\psi\rangle \tag{5.14}$$

For $\gamma = 0$, both are related and only depend on the average value of S_x^2.

5.3 Numerics

$N = 1024$ spins, $\tau \sim 10^3 - 10^4$. The adiabaticity (as quantified by E_{res} and m_{inc}) is roughly independent of γ as long as $\gamma \neq 1$ where the system acquires XY-symmetry, so we take $\gamma = 0$.

Three different regimes - fast quenches involve all instantaneous levels (i.e. strongly not adiabatic), with E_{res} close to maximal and not N-dependent. For larger τ, second intermediate regime with $E_{\text{res}} \sim \tau^{-3/2}$. Further larger values of τ gives $E_{\text{res}} \sim \tau^{-2}$.

Probability of exciting system into first excited state is given by Landau-Zener formula (probability of exciting a system through an avoided level crossing where $\Delta E = \alpha t$ and a gap of 2Δ at $t = 0$. i.e.:

$$H(t) = \begin{pmatrix} \frac{\alpha t}{2} & H_{12} \\ H_{12}^* & -\frac{\alpha t}{2} \end{pmatrix} \tag{5.15}$$

):

$$P_{LZ} \approx e^{-\alpha\Delta^2\tau} \tag{5.16}$$

The Δ that appears here is not the gap between the GS/first excited state, but between the GS and the second excited state.

The maximum system size for a defect free quench can be estimated as:

$$\frac{1}{N_{\text{free}}} \sim \left(\frac{|\ln P_{\text{ex}}|}{\alpha}\right)^{3/2} \frac{1}{\tau^{3/2}} \tag{5.17}$$

The residual energy per site is then (TODO - what??)

$$\frac{E_{\text{res}}}{N} \sim \frac{1}{N^2}\frac{N}{N_{\text{free}}}N \sim \frac{\text{const.}}{\tau^{3/2}} \tag{5.18}$$

What about the last regime where $\frac{E_{\text{res}}}{N} \sim \tau^{-2}$? This is the usual error in adiabatic evolution (usual?? - Ok, I've now looked at `https://www.prl.res.in/~library/gpdf/e-books/Springer_e-books/Quantum%20Annealing%20and%20Other%20Optimization%20Methods%202005.pdf` Simulated Quantum Annealing by Real-time evolution 4.3.2 and it basically appears to be (a) fairly universal behaviour numerically and (b) Derivable analytically, though their proof is not very physically intuitive/quick), Can we see this via:

$$H_{\text{pert}} = \begin{pmatrix} 0 & H_{12} \\ H_{12}^* & 0 \end{pmatrix} \tag{5.19}$$

where $\frac{|H_{12}|}{\hbar} = \frac{\Delta}{2} = \omega_{12}$ is the rabi frequency, duration of the adiabatic change is $\frac{|H_{12}|}{\alpha} = \tau$ so we want $\omega_{12}\tau \sim \tau^2 \gg 1$ i.e. $1 \gg \frac{1}{\tau^2}$ for adiabaticity?), but they also try to give a physical explanation via Landau-Zener.

They also explain this via Landau-Zener, but requires some modification. The two-level LZ theory applies to fast enough quenches, but deviations arise for larger τ. This is because there is more than one avoided crossing. The timescale for jumping is probability of asymptotic jump with the slope at the crossing point:

$$\Gamma_{\text{jump}} \sim \frac{P(\infty)}{P'(\Gamma_{\text{cross}})} \tag{5.20}$$

and $\Gamma_{\text{jump}} \sim \exp(\tau)$ for $\tau \gg 1$, so consecutive transitions are not independent.

They thus consider a three level system, where instead of a final time of $tf = \infty$ they have a finite evolution at $\Gamma_f = t_f/\tau = 2$, with Hamiltonian:

$$H = \begin{pmatrix} -\Delta_1\Gamma & \Omega_1 & 0 \\ \Omega_1 & \Delta_1\Gamma & \Omega_2 \\ 0 & \Omega_2 & \Delta_3\Gamma + a_3 \end{pmatrix} = \begin{pmatrix} -\Delta_1 t/\tau & \Omega_1 & 0 \\ \Omega_1 & \Delta_1 t/\tau & \Omega_2 \\ 0 & \Omega_2 & \Delta_3 t/\tau + a_3 \end{pmatrix} \tag{5.21}$$

modifing the LZ transition probability for t_f finite:

$$P_{\text{ex}}(\tau) \sim \underbrace{P_{\text{LZ}}(\tau)}_{e^{-\pi\Omega_1^2\tau/\Delta_1}} + (1-2P_{\text{LZ}})\frac{1}{16\Gamma_1^4\frac{\tau^2}{\Delta_1^2}(1+\frac{\Delta_1^2}{\Omega_1^2}\Gamma_f^2)^3} \sim \frac{1}{\tau^2} \tag{5.22}$$

Where $t_f \to \infty$ recovers the usual probability (How?).

For intermediate τ the third

Δ_3 controls the slope of the crossing, a_3 controls the position of the crossing. For moderate slope and far crossings, P_{ex} is unaffected (reduces to the 2-level case), for τ large/highly adiabatic, both the slope and location modifies the effective duration of FTLZ/finite-time Landau-Zener, "the transposition of the effect in the LMG model is simply to stop the probability from relaxing towards the asymptotic value when the system has reached the second avoided crossing." - in any case the 3-level analysis seems to reproduce the τ^{-2} behaviour.

5.4 Takeaway

- Adiabatic dynamics has three regimes; τ small for which strongly non-adiabatic (many transitions), τ intermediate (lowest critical dynamically accessible gap dominates the evolution, so 2-level dynamics with $\sim \tau^{-3/2}$), τ large (strongly adiabatic, general feature of adiabatic dynamics, they also explain through multi-level + finite time LZ model).

5.5 Quantum Criticality in Infinite-Range Ising (Curro, Danesh, and Singh, Phys. Rev. B 110, 075112 (2024))

(Curro, Danesh, and Singh, Phys. Rev. B 110, 075112 (2024)) They study the infinite-range quantum TFIM and show devitations from MFT! So can't necessarily trust the averaging intuition.

Infinite-range quantum Ising model:

$$H = -\frac{J}{2N}\left(\sum_i Z_i\right)^2 - B\sum_i X_i \tag{5.23}$$

with $J = 1$. Mean-field theory approach to replace with:

$$H_{\text{mf}} = -m_z Z - BX \tag{5.24}$$

and then determine $m_z = \langle Z \rangle$ self-consistently, but the properties of this model differ from the mean-field behaviour. In this paper, they leverage that the Hamiltonian only depends on:

$$S_z = \sum_i Z_i, \quad S_x = \sum_i X_i \tag{5.25}$$

which both commute with the total spin:

$$S^2 = \sum_i S_i^2 = \sum_i (X_i^2 + Y_i^2 + Z_i^2) \tag{5.26}$$

So this is conserved under the dynamics; can fragment into total-spin $s \in [0, 1, \ldots 2s+1]$ sectors, with $\dim \mathcal{H}_s = 2s+1$. We can diagonalize each numerically efficiently (and in the paper they compute spectral properties for thousands of spins).

They study energy gaps Δ_1, Δ_2 between the ground and first/second excited states, differs from MF behavior (though the linear-to-zero transition is predicted). For Δ_2 MF Δ_2 does not go below $2J$, but the quantum simulation shows $\Delta_2 \to 0$ as a cascade of states comes down and becomes zero energy as $N \to \infty$ at QCP. A plot of the gaps confirms that $\Delta \sim N^{-1/3}$ in the thermodynamic limit. MFT overestimates Δ_1/Δ_2 by $J/2J$, using perturbation theory in the large-field limit.

They also use quantum Fischer information to study the quantum criticality, namely the entanglement of the state at the QCP (c.f. mean field theory gives a product state, so no QFI):

$$F_Q(\hat{O}) = 2\sum_{i,j} \frac{(p_i - p_j)^2}{p_i + p_j} |\langle i|\hat{O}|j\rangle|^2 \tag{5.27}$$

Where they take $\hat{O} = S_z$. $f_q = F_Q/N$ diverges at the QCP as $N \to \infty$, with $f_Q \sim T^{-1}$, $f_Q \sim |h - h_c|^{-1/2}$ as $T \to 0, h \to h_c = 1$ consistent with $\gamma - z\nu = 1/2$ with $\gamma = 1/2, z = 1, \nu = 1/2$.

Susceptibilities: Transverse magnetization approximately fits mean field behaviour (though misses enhancement near the critical point as $h \to h_x^{-1}$) and longitudinal magnetization is consistent with MFT.

They also study heat capacity and transverse magneitzation at finite temperature.

They apply this to Thuliam Vanadate materials (where they see rapid spin-spin decoherence in NMR experiments from quantum critical fluctuations - inconsistent with mean field behaviour, but consistent with QCP).