Statistical mechanics of long-range interacting systems: Lecture 2

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Plan

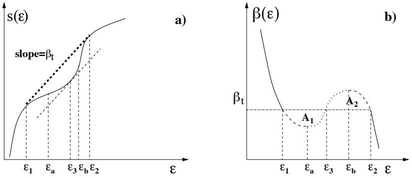
- The Blume-Capel model:phase diagram in the canonical and microcanonical ensembles
- Short and long-range interactions: the Nagel-Kardar model
- Broken ergodicity in the Kardar-Nagel model
- Metastability and instability in presence of long-range interactions
- The min-max method

Tutorial

- Transfer matrix and the Kardar-Nagel model
- Counting the states in the Kardar-Nagel model
- The Creutz algorithm to simulate the microcanonical ensemble.

Ensemble inequivalence

Non concave entropy



- Negative heat capacity $\partial^2 s/\partial\varepsilon^2 = -(c_V T^2)^{-1}$
- Maxwell's equal area condition $\int_{\varepsilon_1}^{\varepsilon_2} d\varepsilon(\beta(\varepsilon) - \beta_t) = 0$, using $\beta = ds/d\varepsilon$, implies that $f(\beta_t, \varepsilon_1) = f(\beta_t, \varepsilon_2)$.

Blume-Capel model

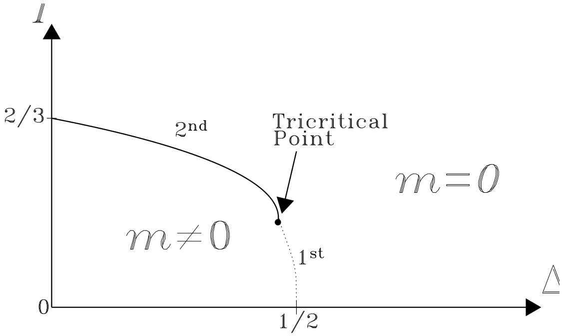
$$H_{BC} = \Delta \sum_i S_i^2 - \frac{J}{2N} \sum_{i,j} S_i S_j \qquad S_i = 0, \pm 1$$

Order parameters

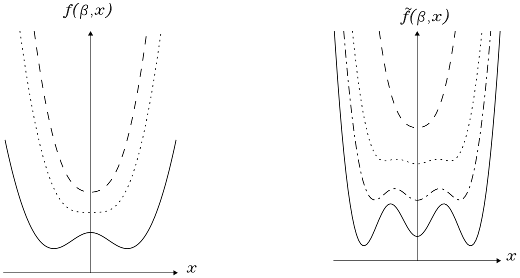
- magnetization $m = (N_+ - N_-)/N$, $N = N_+ + N_- + N_0$.
- quadrupolar moment $q = (N_+ + N_-)/N$

The free energy in the canonical ensemble of this model is known and the phase diagram shows second and first order phase transitions separated by a tricritical point at $\Delta/J = \ln 4/3$, $T/J = 1/3$. The first order transition at zero temperature is easily located by equating the energies of the ferromagnetic and of the paramagnetic phases ($J = 1$): $E_{ferro} = \Delta - 1/2$, $E_{para} = 0$. The second order transition at $\Delta = 0$ is the usual Curie-Weiss transition for a spin one system, obtained by solving the consistency equation $(\exp(\beta m) - \exp(-\beta m))/(\exp(\beta m) + \exp(-\beta m) + 1) = m$.

Phase diagram in the canonical ensemble



Landau free energy: second and first order transitions



Free energy $f(\beta, m)$ vs. m for different values of the inverse temperature $\beta = 1/T$. The left panel shows the case of a *second* order phase transition, for temperature values T =0.8 (dashed line), 0.63 (dotted), 0.4 (solid) and $\Delta = 0.1$. The right panel shows the case of a *first* order phase transition with $\Delta = 0.485$ when $T = 0.5$ (dashed), 0.24 (dotted), 0.21 (dash-dotted), 0.18 (solid).

Solution in the microcanonical ensemble

Typical configuration

$$++++++++--------0000000--------+++++0000+++$$

Given N_+,N_- and N_0, one can exchange any pair in the group of up, down and zero spins without changing the energy.

$$\Omega = \frac{N!}{N_+!N_-!N_0!}$$

In the Stirling approximation, $\ln n! = n \ln n - n$, $S = k_B \ln \Omega$ is

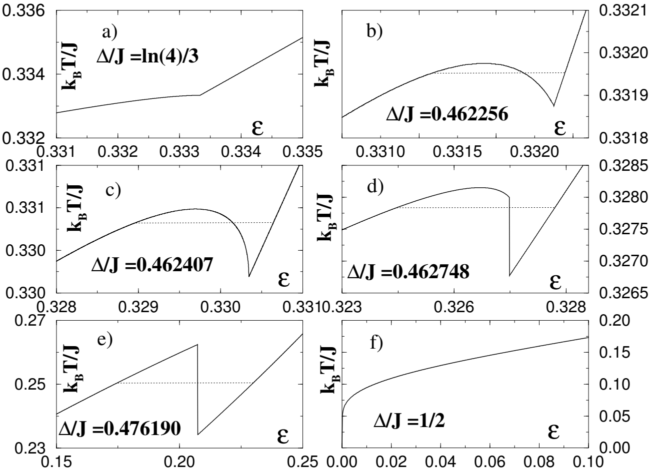
$$S = -k_B N[(1-q)\ln(1-q) + \frac{1}{2}(q+m)\ln(\frac{q+m}{2}) + \frac{1}{2}(q-m)\ln(\frac{q-m}{2})$$

$$\varepsilon = \frac{E}{N} = \Delta(q - Km^2)$$

with $K = J/2\Delta$

Maximize $s = S/N$ with respect to m to get $s(\varepsilon)$. Then $1/T = ds/d\varepsilon$.

Caloric curves



Expansion around the microcanonical tricritical point

Expanding entropy

$$s = k_B(s_0 + Am^2 + Bm^4 + \dots)$$

with $\epsilon = \varepsilon/\Delta$

$$s_0 = -(1-\epsilon)\ln(1-\epsilon) - \epsilon\ln\epsilon + \epsilon\ln 2$$

$$A = -K\ln(\frac{\epsilon}{2(1-\epsilon)}) - \frac{1}{2\epsilon}$$

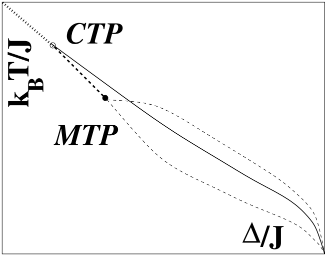
$$B = -\frac{K^2}{2\epsilon(1-\epsilon)} + \frac{K}{2\epsilon^2} - \frac{1}{12\epsilon^3}$$

Continuous transition at $A = 0, B < 0$. Critical line in agreement with canonical

Tricritical point at $A = B = 0$

- Canonical $K_{tr} \approx 1.0820$, $\beta_{tr}\Delta = 1.3995$
- Microcanonical $K_{tr} \approx 1.0813$, $\beta_{tr}\Delta = 1.3998$

Phase diagram in the microcanonical ensemble



- Canonical (CTP) and microcanonical (MTP) tricritical points do not coincide.
- The microcanonical transition line splits in two at the microcanonical tricritical point, giving rise to a temperature jump.
- The region between the two microcanonical lines is accessible only to metastable and unstable states in the microcanonical ensemble (coexistence region)

Classification

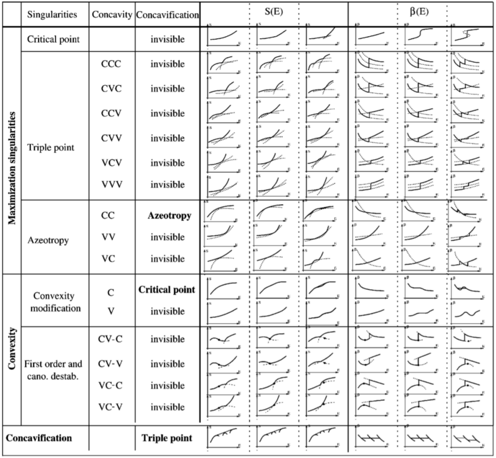


Fig. 3. Codimension 1 singularities. The three curves $S(E)$ and $\beta(E)$ for each singularity correspond to the situation just before the singularity is crossed, right at the singularity, and just after it. See the text for comments; the meaning of the curves is as in Fig. 2, and dotted lines represent metastable or unstable microcanonical branches.

Short and long range interactions: the Nagel-Kardar model

$$H = -\frac{K}{2}\sum_{i=1}^{N}(S_i S_{i+1} - 1) - \frac{J}{2N}\left(\sum_{i=1}^{N} S_i\right)^2 ,$$

Let $U = -(1/2)\sum_i (S_i S_{i+1} - 1)$ be the number of antiferromagnetic bonds in a given configuration characterized by N_+ up spins and N_- down spins, e.g. $N_+ = 12$, $N_- = 8$, $U/2 = 2$

$$+ + + + + + | - - - - - | + + + + | - - - | + +$$

N_+ (N_-) spins are divided into $U/2$ segments, thus counting arguments yield to leading order in N

$$\Omega(N_+, N_-, U) \approx 2 \begin{pmatrix} N_+ \\ U/2 \end{pmatrix} \begin{pmatrix} N_- \\ U/2 \end{pmatrix} .$$

The order N prefactor would count the number of ways of putting U ordered segments on the lattice.

Entropy

Expressing N_+ and N_- in terms of $N = N_+ + N_-$ and the magnetization $M = N_+ - N_-$, and denoting $m = M/N$, $u = U/N$ and the energy per spin $\epsilon = E/N$, one finds that the entropy per spin, $s(\epsilon, m) = \frac{1}{N} \ln \Omega$ is given in the thermodynamic limit by

$$\begin{aligned} s(\epsilon, m) &= \frac{1}{2}(1+m)\ln(1+m) + \frac{1}{2}(1-m)\ln(1-m) \\ &- u\ln u - \frac{1}{2}(1+m-u)\ln(1+m-u) \\ &- \frac{1}{2}(1-m-u)\ln(1-m-u)\ , \end{aligned}$$

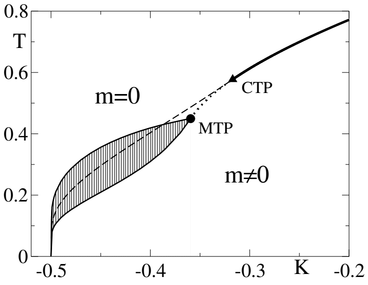
where u satisfies

$$\epsilon = -\frac{J}{2}m^2 + Ku\,.$$

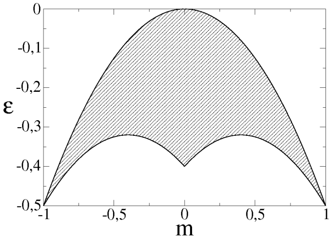
By maximizing $s(\epsilon, m)$ with respect to m one obtains both the spontaneous magnetization $m_s(\epsilon)$ and the entropy $s(\epsilon) \equiv s(\epsilon, m_s(\epsilon))$ of the system for a given energy.

Phase diagram

Microcanonical and canonical (K, T) phase diagram.
$K_{MTP} \simeq -0.359$ ($K_{CTP} = -\ln 3/2\sqrt{3} \simeq -0.317$)
The transition at $T = 0$ is obtained by imposing that the state with alternating down and up spins $+-+-+-\cdots$ has the same energy as the ferromagnetic state $+++++\cdots$



Broken ergodicity

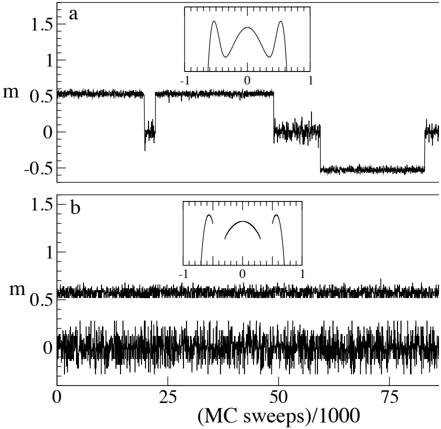


$N_+ > N_-$ (positive magnetization states). Then
$0 < U < 2N_- = N - M$, the right bound corresponding to configurations where all down spins are isolated.
$+++++|-|+++|-|++++|-|+++++$
This in turn implies, in the $N \to \infty$ limit,

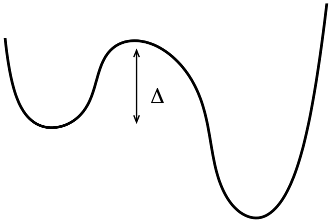
$$0 \leq u = \frac{\varepsilon}{K} + \frac{J}{2K} m^2 \leq 1 - m$$

In the figure $K = -0.4$ and $J = 1$

Numerical results



Metastability



$$\tau \sim e^{N\frac{\Delta f}{k_B T}} \quad \text{canonical} \quad , \quad \tau \sim e^{N\frac{\Delta s}{k_B}} \quad \text{microcanonical}$$

to be compared with $\tau \sim \exp N^{(d-1)/d}$ in d dimensions.
Griffiths, Weng and Langer, 1966; Antoni, SR and Torcini, 2004; Schreiber, Mukamel and SR, 2005

Metastability and instability for the Blume-Capel model

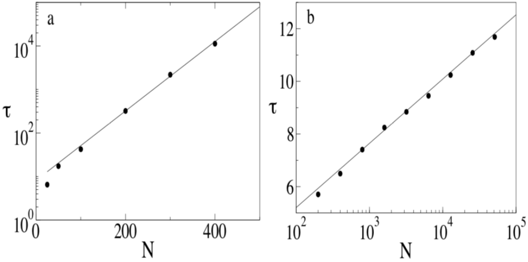


FIG. 9: Life times of states with $m = 0$ where these states are (a) metastable ($K = -0.4,\ \epsilon = -0.318$), and (b) stable ($K = -0.25,\ \epsilon = -0.2$).

Fokker-Planck equation for the magnetization

Magnetization is assumed to evolve diffusively in an overdamped motion where the potential is given by the entropy $s(m)$

$$\frac{\partial P(m,t)}{\partial t} = -\frac{\partial}{\partial m}\left(\frac{\partial s(m)}{\partial m} P(m,t)\right) + D\frac{\partial^2 P(m,t)}{\partial m^2}$$

with $D \sim 1/N$
For an (unstable) quadratic minimum of $s(m) = am^2$ and an initial $m = 0$ state, $P(m,0) = \delta(0)$

$$P(m,t) \sim \exp\left(-\frac{am^2 e^{-at}}{D}\right).$$

In order to reach a value of m of $O(1)$

$$\tau(N) \sim -\ln D \sim \ln N$$

The min-max method

Let us assume that the canonical partition sum can be written in the following form

$$Z(\beta, N) = \int dx \exp(-NU(\beta, x))$$

with U a differentiable function of β and x, a dummy variable. Then $\phi(\beta) = \beta f(\beta) = \inf_x U(\beta, x)$. Let us introduce the Legendre-Fenchel transform of U $s(\varepsilon, x) = \inf_\beta(\beta\varepsilon - U(\beta, x))$. Then, one can prove that

$$s(\varepsilon) = \sup_x(s(\varepsilon, x)) = \sup_x \inf_\beta(\beta\varepsilon - U(\beta, x))$$

Inverting the inf with the sup, one gets the concave envelope of $s(\varepsilon)$

$$s^*(\varepsilon) = \inf_\beta \sup_x(\beta\varepsilon - U(\beta, x))$$

On the other hand the Legendre-Fenchel transform of both s and s^* is ϕ. We use $\sup \inf \leq \inf \sup$.

Long and short-range XY model

$$H = -K \sum_{i=1}^{N} \cos(\theta_{i+1} - \theta_i) + \frac{J}{2N} \sum_{i,j=1}^{N} [1 - \cos(\theta_i - \theta_j)]$$

$$Z \sim \int zdz \prod_{i=1}^{N} d\theta_i \exp\left(-\frac{N\beta}{2} z^2 + \beta z \sum_{i=1}^{N} \cos\theta_i + \beta K \sum_{i=1}^{N} \cos(\theta_{i+1} - \theta_i) \right)$$

The integral over the θ_i can be performed using the transfer operator method

$\mathcal{T}\psi(\theta) = \int d\alpha \exp(\beta z(\cos\theta + \cos\alpha)/2 + \beta K \cos(\theta - \alpha)\psi(\alpha)$.

$$Z = \int zdz \exp\left(-\frac{N\beta}{2} z^2 + N \ln \lambda(\beta z, \beta K) \right)$$

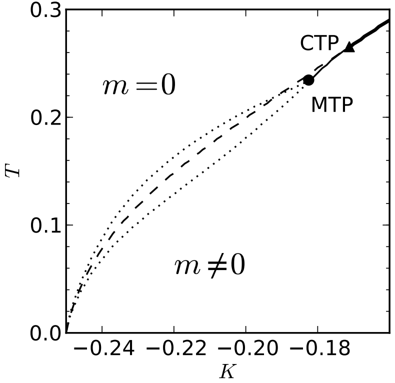
where $\lambda(\beta z, \beta K)$ is the maximal eigenvalue of the transfer operator. Entropy is then obtained using the min-max method.

$$s(\varepsilon) = \sup_z \inf_\beta \left[\beta\varepsilon - \beta \frac{(1+z^2)}{2} + \ln \lambda(\beta z, K\beta) + \frac{1}{2} \ln \frac{2\pi}{\beta} \right]$$

Conclusions of Lecture 2

- Ensemble inequivalence is a generic feature of systems with long-range interactions.
- The phase diagram of the Blume-Capel model shows ensemble inequivalence.
- Ensemble inequivalence is present also for spin models with both nearest-neighbour and mean-field interaction.
- Simulations performed in the microcanonical ensemble (Creutz algorithm) reveal ergodicity breaking and exponentially long transition times when more then one local entropy maximum is present (metastability).
- The min-max method is a useful tool to obtain microcanonical entropy for a specific class of models.

Phase diagram



Tutorial

- Transfer matrix and the Kardar-Nagel model
- Counting the states in the Kardar-Nagel model
- The Creutz algorithm to simulate the microcanonical ensemble.

Transfer matrix for the 1d Ising model and the Nagel-Kardar model

$$H = -J\sum_i \sigma_i \sigma_{i+1} - h\sum_i \sigma_i$$

$$\mathbf{T} = \begin{pmatrix} \exp(\beta(J+h)) & \exp(-\beta J) \\ \exp(-\beta J) & \exp(\beta(J-h)) \end{pmatrix}$$

Eigenvalues

$$\lambda_\pm = \exp(\beta J)\left[\cosh(\beta h) \pm \sqrt{\sinh^2(\beta h) + \exp(-4\beta J)}\right]$$

- Use the maximal eigenvalue to derive the free energy of the Nagel-Kardar model.
- Derive the critical line and the tricritical point in the canonical ensemble
- Use the min-max method to derive the entropy.

Microcanonical Monte Carlo (Creutz algorithm)

Probe microstates with energy $\leq E$. This is implemented by adding an auxiliary variable, the "demon",

$$E_S + E_D = E$$

with $E_D > 0$. Start with $E_S = E$, $E_D = 0$ and attempt a spin flip. Accept the move if the energy decreases and give the excess energy to the demon

$$E_S \to E_S - \Delta E \quad , \quad E_D \to E_D + \Delta E \quad , \quad \Delta E > 0$$

If instead the energy increases, take the needed energy from the demon

$$E_S \to E_S + \Delta E \quad , \quad E_D \to E_D - \Delta E \quad , \quad \Delta E > 0$$

Reject the move if the demon does not have the needed energy. Detailed balance is satisfied and the microcanonical measure is stationary.
One can also prove that

$$p(E_D) \propto \exp(-\beta_\mu E_D) \text{ and } \beta_\mu = 1/ < E_D >$$

$\beta(\epsilon)$ in the Curie-Weiss model in the microcanonical ensemble