Aula - Transições de fase (slide)

$$\frac{dm}{dt} = (a_c - a)\, m - b\, m^3$$

$$m \frac{dm}{dt} = (a_c - a)\, m^2 - b\, m^4$$

①

$$\frac{1}{2} \frac{dm^2}{dt} = (a_c - a)\, m^2 - b\, m^4$$

$$x = m^2$$

$$\frac{dx}{dt} = \underbrace{2(a_c - a)}_{\alpha}\, x - \underbrace{2b}_{\beta}\, x^2$$

$$\frac{dx}{\alpha x - \beta x^2} = 2\, dt$$

$$\frac{dx}{x(\alpha - \beta x)} = 2\, dt$$

$$\frac{1}{x(\alpha - \beta x)} = \frac{A}{x} + \frac{D}{\alpha - \beta x} \Leftrightarrow \frac{A(\alpha - \beta x) + Dx}{x(\alpha - \beta x)}$$

$$A\alpha = 1 \Leftrightarrow A = \frac{1}{\alpha}$$

$$-\beta A + D = 0$$

$$D = +\beta A = +\frac{\beta}{\alpha}.$$

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$$\frac{1}{x(\alpha-\beta x)} = \frac{1}{\alpha x} + \frac{\beta}{\alpha(\alpha-\beta x)}$$

$$\frac{dx}{x} + \frac{\beta\, dx}{\alpha-\beta x} = 2\alpha\, dt$$

$$\frac{dx}{x} + \frac{dx}{\frac{\alpha}{\beta}-x} = 2\alpha\, dt$$

$$\frac{dx}{x} - \frac{dx}{x-\frac{\alpha}{\beta}} = 2\alpha\, dt$$

$$\ln\frac{x(t)}{x_0} - \ln\frac{x(t)-\frac{\alpha}{\beta}}{x_0-\alpha/\beta}$$

$$\ln \frac{x(t)}{x_0}\cdot\frac{x_0-\alpha/\beta}{x-\alpha/\beta} = \ln\frac{1-\alpha/\beta x_0}{1-\alpha/\beta x(t)}$$

$$e^{2\alpha t} = \frac{\overbrace{1-\frac{\alpha}{\beta x_0}}^{\to A}}{1-\frac{\alpha}{\beta x(t)}}$$

$$1-\frac{\alpha}{\beta x(t)} = A e^{-2\alpha t}$$

$$\frac{\alpha}{\beta x(t)} = 1-Ae^{-2\alpha t} \iff x(t) = \frac{\alpha}{\beta\left[1-Ae^{-2\alpha t}\right]}$$

$$m^2(t) = \frac{(a_c - a)}{b\left[1 - A\, e^{-\lambda(a_c - a)t}\right]}$$

$a_c < a \Rightarrow m^2(t) \longrightarrow 0$ qdo $t \to \infty$

$a_c > a \Rightarrow m^2 \longrightarrow \dfrac{a_c - a}{b}$

Conversely, the first-order phase transition can be studied through logistic equation

$$\frac{dm}{dt} = (a_b - a) - b\,m^3 + c\,m^5 \, , \quad (\text{for systems with Symmetry } Z_2).$$

$\uparrow$ control parameter

where $c > 0$ in order to ensure finite values of m.

Although the time behavior of $m(t)$ toward the steady state is more complicated than the previous case, it is possible to establish some general portraits:

<u>Steady state solutions</u>

$m = 0$ and

$(a_b - a) - b m^2 + c m^4 = 0$, where

$$m_*^2 = \frac{b \pm \sqrt{b^2 - 4(a_b - a)c}}{2c}$$

for $b^2 > 4(a_b - a)c \Rightarrow$ we have two solutions for m_*^2.

At $a_f = a_b - \dfrac{b^2}{4c}$, the order parameter jump from 0 to $\pm \dfrac{b}{2c}$.

Another way to see above features consists of evaluating the maximum of $a = a(m)$.

By inverting above relation we have

$$a = a_b + c y^2 - b y \qquad (y = m^2)$$

$$\left.\frac{\partial a}{\partial y}\right|_{a=a_f} = 0 \iff 2cy - b = 0$$

$$y^* = \frac{b}{2c}$$

$$a_f = a_b + c\left(\frac{b}{2c}\right)^2 - b\left(\frac{b}{2c}\right)$$

$$= a_b - \frac{b^2}{4c}.$$

For $a > a_f \Rightarrow m(t) \longrightarrow 0$, irrespectively the initial condition

On the other hand, for $m(t) << 1$ the logistic equation becomes

$$\frac{dm}{dt} \simeq (a_b - a)m \quad \text{and} \quad m(t) \sim e^{(a_b - a)t}$$

for $a_b - a < 0 \rightarrow m(t)$ vanishes for $t \rightarrow \infty$

$a_b - a > 0 \rightarrow m(t)$ increases for $t \rightarrow \infty$ and reach a finite value

Hence, there are three important regions:

$a < a_b \rightarrow m(t) \longrightarrow m_0(a)$

$a_b < a < a_f \longrightarrow m(t) \longrightarrow m^s(f)$ if $m(t) > m^*$

and $m(t) \longrightarrow 0$ if $m(t) < m^*$

This region ~~to~~ corresponds to a bistable/ hysteretic branch and it is a hallmark of a discontinuous phase transition

for $a > a_f \rightarrow m(t) \rightarrow 0$ and

$m(t) \sim e^{(a_b - a)t}$ for $m(t) << 1$

In order to describe/ reproduce above features by means of microscopic systems/ dynamics we resort to the master equation

$$\frac{d}{dt} P(\sigma, t) = \sum_{\sigma' \neq \sigma} \{ W(\sigma|\sigma') P(\sigma', t) - W(\sigma'|\sigma) P(\sigma, t) \}$$

Where $W(\sigma|\sigma') \rightarrow$ transition rate from $\sigma' \rightarrow \sigma$

$W(\sigma'|\sigma) \rightarrow$ transition rate from $\sigma \rightarrow \sigma'$,

and $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_i, \ldots \sigma_N)$ denotes a microscopic configuration of a system with N sites. For systems with Z_2 symmetry, one has 2^N microscopic configurations.

From now on, we shall consider/ focus on our attention in system dynamics in which the next configuration σ' differs from σ only for a spin of a given site. In other words

$$\sigma' \equiv (\sigma_1, \sigma_2, \ldots, -\sigma_i, \ldots, \sigma_N).$$

This simplifies things and we can rewrite the transition rate $w(\sigma/\sigma')$ and $w(\sigma'/\sigma)$ in the following way

$$w(\sigma'|\sigma) = \sum_{i=1}^{N} \delta(\sigma_1', \sigma_1)\,\delta(\sigma_2', \sigma_2) \ldots \delta(\sigma_i', -\sigma_i) .$$
$$\ldots \delta(\sigma_N', \sigma_N)\, w_i(\sigma)$$

where $\delta(\sigma_i', \sigma_i)$ denotes the Kronecker delta and $w_i(\sigma)$ is the transition rate of the ... of the i-th spin change from σ_i to $-\sigma_i$. By inserting above expression in the master equation the term

$$\sum_{\sigma' \neq \sigma} w(\sigma'|\sigma)\, P(\sigma,t) \rightarrow \sum_{i=1}^{N} w_i(\sigma)\, P_i(\sigma,t)$$

Analogously

$$w(\sigma|\sigma') = \sum_{i=1}^{N} \delta(\sigma_1, \sigma_1')\,\delta(\sigma_2, \sigma_2') \ldots, \delta(-\sigma_i, +\sigma_i') .$$
$$\ldots \delta(\sigma_N', \sigma_N)\, w_i(\sigma')$$

and
$$\sum_{\sigma' \neq \sigma} w(\sigma|\sigma')\, P(\sigma', t) \longrightarrow \sum_{i=1}^{N} w_i(\sigma^i)\, P(\sigma^i, t)$$

where

$$\sigma^i = (\sigma_1, \sigma_2, \ldots, -\sigma_i, \ldots, \sigma_N)$$

Hence

$$\frac{dP(\sigma)}{dt} = \sum_{i=1}^{N} \{ w_i(\sigma^i)\, P(\sigma^i, t) - w_i(\sigma)\, P(\sigma, t) \} .$$

The time evolution of a given average $f(\sigma)$ of a state function, $\langle f(\sigma)\rangle = \sum_{\sigma} f(\sigma) P(\sigma,t)$

is given by

$$\frac{d}{dt}\langle f(\sigma)\rangle = \sum_{\sigma} f(\sigma) \frac{dP(\sigma,t)}{dt}$$ or

$$\frac{d}{dt}\langle f(\sigma)\rangle = \sum_{\sigma} f(\sigma) \sum_{i=1}^{N} \{\underbrace{W_i(\sigma^i) P(\sigma^i,t)}_{1} - \underbrace{W_i(\sigma) P(\sigma,t)}_{2}\}$$

The term 2 is just

$$\sum_{i=1}^{N} \sum_{\sigma} f(\sigma) W_i(\sigma) P(\sigma,t) \longrightarrow \sum_{i=1}^{N} \langle f(\sigma) W_i(\sigma)\rangle.$$

For the term (1) we can perform the transformation $\sigma^i \to \sigma$ and

$$f(\sigma) \to f(\sigma^i)$$

$$W_i(\sigma^i) \to W_i(\sigma)$$

$$P(\sigma^i,t) \to P(\sigma,t).$$

We note that $\sum_{\sigma} = \sum_{\sigma^i}$ (summation of all configurations)

and hence

$$\sum_{i=1}^{N} \sum_{\sigma} f(\sigma) W_i(\sigma^i) P(\sigma^i,t) = \sum_{i=1}^{N} \langle f(\sigma^i) W_i(\sigma)\rangle.$$

Therefore

$$\frac{d}{dt}\langle f(\sigma)\rangle = \sum_{i=1}^{N} \langle \{ f(\sigma^i) - f(\sigma) \} W_i(\sigma) \rangle .$$

In particular the average $m = \langle \sigma_j \rangle$ has the following time evolution

$$\frac{d}{dt}\langle \sigma_j \rangle = \sum_{i=1}^{N} \langle \{ (\sigma_j)^i - \sigma_j \} W_i(\sigma) \rangle .$$

$$(\sigma_j)^i = -\sigma_j \quad \text{if} \quad i = j$$

and $\quad (\sigma_j)^i = \sigma_j \quad \text{if} \quad i \neq j .$

Hence

$$\frac{d}{dt}\langle \sigma_j \rangle = -2 \langle \sigma_j W_j(\sigma) \rangle .$$

In the case of majority vote model

$$W_j(\sigma) = \frac{1}{2}\left\{ 1 - (1-2f)\sigma_j S\left(\sum_{\delta} \sigma_{j+\delta}\right) \right\}$$ one has the following logistic equation

$$\frac{d}{dt}\langle \sigma_j \rangle = -\left\{ \left\langle \sigma_j \left(1 - (1-2f)\sigma_j S\left(\sum_{\delta} \sigma_{j+\delta}\right)\right) \right\} \right\rangle$$

$$= -\langle \sigma_j \rangle + (1-2f)\langle \sigma_j^2 S\left(\sum_{\delta} \sigma_{j+\delta}\right) \rangle$$

since $\sigma_j^2 = 1$, one has $\frac{d}{dt} m = -m + (1-2f)\langle S\left(\sum_{\delta} \sigma_{j+\delta}\right)\rangle .$

We need to evaluate $\langle S(\sum_\delta \sigma_{i+\delta})\rangle$

I well evaluate for $K=4$ and $k >> 1$, illustrating the regime of low and large connectivities.

Starting with $K=4$, $\langle S(\sum_\delta \sigma_{i+\delta})\rangle$ can be splitted in two parts:

$$\langle S(\sum_\delta \sigma_{i+\delta})\rangle = \underbrace{S_+(\sum_\delta \sigma_{i+\delta})} - \underline{S_-}(\sum_\delta \sigma_{i+\delta})$$

signal function is positive and majority of neighboring spins are positive

majority of (neighboring) spins are negative

In the case of one-site MFT, we neglect all correlations between nearest neighbor spins and a given joint probability

$$P(\sigma_1, \sigma_2, \ldots, \sigma_N) \approx P(\sigma_1) P(\sigma_2) \ldots P(\sigma_N).$$

Hence

$$S_+(\sum_\delta \sigma_{i+\delta}) \approx \sum_{n=\lceil \frac{k}{2} \rceil}^{K} C_n^K \, P_+^n \, P_-^{k-n}$$

$$S_-(\sum_\delta \sigma_{i+\delta}) \approx \sum_{n=\lceil \frac{k}{2} \rceil}^{k} C_n^K \, P_-^n \, P_+^{k-n}$$

since $P_+ + P_- = 1$ and $m = P_+ - P_-$

$$P_+ = \frac{1+m}{2}$$

$$P_- = \frac{1-m}{2}$$

$K=4$ (rede quadrada) 7

$$\sum_{n=3}^{4} C_n^K \, P_+^{\,n} \, P_-^{\,K-n} - \sum_{n=3}^{4} C_n^K \, P_-^{\,n} \, P_+^{\,K-n}$$

$$= 4\left(\frac{1+m}{2}\right)^3\left(\frac{1-m}{2}\right) + \left(\frac{1+m}{2}\right)^4 - 4\left(\frac{1-m}{2}\right)^3\left(\frac{1+m}{2}\right) - \left(\frac{1-m}{2}\right)^4$$

$$= \frac{1}{16}\left[4(1+m)^2(1-m^2) + (1+m)^4 - (1-m)^4 - 4(1-m)^2(1-m^2)\right]$$

$$= \frac{1}{16}\left[4(1-m^2)\underbrace{\left[(1+m)^2-(1-m)^2\right]}_{4m} + \underbrace{(1+m)^4-(1-m)^4}_{8(m+m^3)}\right]$$

$$= \frac{1}{16}\left[16m(1-m^2) + 8(m+m^3)\right]$$

$$= \frac{1}{16}\left[24m - 8m^3\right] = \frac{3m}{2} - \frac{m^3}{2} = \frac{(3m-m^3)}{2}$$

$$\frac{d}{dt}m = -m + \frac{(1-2f)}{2}(3m-m^3)$$

$$\frac{dm}{dt} = \left[-2 + \frac{3(1-2f)}{2}\right]m - \frac{1}{2}(1-2f)m^3$$

$$\boxed{\frac{dm}{dt} = (1-6f)m - (1-2f)m^3} \quad (4)$$

above procedure is analogous to that used by rewriting the signal function in terms of products of spins.

For $K=4$ $S(\sum_\delta \sigma_{j+\delta})$ can be rewritten as

$$S(\sum_\delta \sigma_{j+\delta}) = \frac{3}{8}(\sigma_1+\sigma_2+\sigma_3+\sigma_4) + \\ -\frac{1}{8}(\sigma_1\sigma_2\sigma_3+\sigma_1\sigma_2\sigma_4+\sigma_1\sigma_3\sigma_4+\sigma_2\sigma_3\sigma_4).$$

and one obtains the same equation to (*) in the previous page.

For $K=6,8,\dots$ and so on $S(\sigma)$ has to consider terms of like $\sigma_1\sigma_3\sigma_4\sigma_5$, $\sigma_1\sigma_3\sigma_4\sigma_5\sigma_6, \dots$ and so on.

Entropy production

Since the above mean-field description hides the irreversible character which we are interested, we shall derive a phenomenological general expression for the entropy production taking into account