# 随机伊辛模型的亚稳态性

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# 提纲

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亚稳态是统计物理中用来描述某种特定现象的术语.

在特定温度压力条件下, 结晶过程需要等待很长的时间, 等待所谓critical droplet的出现. 在critical droplet出现之前, 整个系统看上去更像是液态; 而在critical droplet出现之后, 晶体很快形成.

从势能角度来看, 系统在势能局部极小处停留一个不确定的时间, 然后通过critical droplet很快滑到势能最低点.

# 背景

亚稳态是指触发器无法在某个规定时间段内达到一个可确认的状态。当一个触发器进入亚稳态引时，既无法预测该单元的输出电平，也无法预测何时输出才能稳定在某个正确的电平上。在这个稳定期间，触发器输出一些中间级电平，或者可能处于振荡状态，并且这种无用的输出电平可以沿信号通道上的各个触发器级联式传播下去。
百度百科(http://baike.baidu.com/view/931945.htm)

“亚稳态”是天文学专有名词。
互动百科(http://www.hudong.com/wiki/亚稳态)

在一个具有N个能级的系统中，受激原子通过自发辐射或无辐射跃迁回到较低的受激态或基态，原子在受激态有一平均的逗留时间，一般约10纳秒这个数量级(10的-9次方)。但也有一些能级较低的受激态，原子逗留的时间比较长，约为毫秒数量级(10的-3次方,相差10的5次方)，这种状态称为亚稳态

奇迹百科(http://www.qiji.cn/baike/Detailed/19522.html)

在经典概念中，亚稳态相应于一个局部的自由能极小值，它最终会通过一个活化过程弛豫到稳定的平衡态，一个整体上的自由能极小值。这一过程不同于非稳态的无位垒弛豫，后者是自发进行的。作为一个亚稳态，它的寿命应长于测量的时间尺度。这在实际上取决于实验设备和测量者的耐性。在亚稳态的经典概念中假设体系都是足够大的，因此不须考虑相尺寸或其它动力学效应对体系的影响。一般来说，与小分子相比，高分子进入亚稳态要容易得多。具有多重微结构层次的聚合物体系可因小的相尺寸、组成、外场或其它因素而呈现亚稳态。本文将着重于亚稳态的概念和具有两个有序结构时聚合物相转变过程中亚稳态观测，....

亚稳态的相尺寸对部分结晶聚合物结构与形态的影响，《高分子通报》1999年03期

北京国际数学研究中心: Nucleation and Rare Events, 26 - 28 Sep 2011
This workshop will focus on recent developments in mathematical theory and computational methods in nucleation and rare events with applications in materials science, biophysics and chemistry as well as complex fluids. Participants are a combination of pure and applied mathematicians and theoretical and computational material scientists, biophysicists and/or chemists.

Phase transitions are common occurrences observed in nature and many engineering techniques exploit certain types of phase transition. A phase transition is the transformation of a thermodynamic system from one phase or state of matter to another. Phase transitions often (but not always) take place between phases with different symmetry.

Generally, we may speak of one phase in a phase transition as being more symmetrical than the other. The transition from the more symmetrical phase to the less symmetrical one is a symmetry-breaking process. When symmetry is broken, one needs to introduce one or more extra variables (order parameter) to describe the state of the system. The order parameter may take the form of a complex number, a vector, or even a tensor, the magnitude of which goes to zero at the phase transition. The study in phase transitions involves a combination of modeling, simulation, mathematical analysis and physical predictions.

Phase transition has now become an important field in the interdisciplinary researches. This approach has been widely applied in the research of applied mathematics, physics, chemistry, biology, and material science. The purpose of the program is to bring together people from these different disciplines, to contribute their recent researches, exchange the ideas and discuss further topics.

# 背景

神经网络中遍历性的消失

模拟退火方法

基因网络调控

ICM speakers
1998 R. Schonmann, Metastability and the Ising model.

2002 G Ben Arous, Aging and Spin-glass Dynamics

2006 A. Bovior, Metastability: a potential theoretic approach

(54) R.H.Schonmann, S.B.Shlosman: Wulff droplets and the metastable relaxation of kinetic Ising models. Communications in Mathematical Physics 194 389-462 (1998).

[4] The metastable behavior of the two dimensional Ising model, (with M.P. Qian and J.F. Feng), Proceedings of the International Conference on Dirichlet Forms and Stochastic Processes, 1995, Editors, Z.M. Ma, M.Rockner, & J.A. Yan, W de Gruyter, New York, 73-86.
[5] The metastability of exponentially perturbed Markov chains, (with M.P. Qian and J.F. Feng) Science in China, Series A, Vol.39 (1996), 7-28.
[7] The consensus times of the majority vote process on a torus, J. Stat. Physics, Vol.86, No.3/4, (1997), 779-802.
[8] The metastable behavior of the three dimensional Ising model, I (with M.P. Qian and J.F. Feng) Science in China, Series A, Vol.40, No.8,(1997) 832-842.
[9] The metastable behavior of the three dimensional Ising model, II, (with M.P. Qian and J.F. Feng) Science in China, Series A, vol.40, No.11,(1997) 1129-1135.
[10] The loop erased exit path and the metastability of the biased majority vote process, (with O. Catoni and J. Xie), Stochastic Processes and Their Applications, Vol.86, No.2, (2000) pp231-261.

环面$\Lambda = \{1, 2 \cdots, N\} \times \{1, 2 \cdots, N\}$, 也可以是其他有限图.
状态空间$S = \{-1, +1\}^{\Lambda}$.
$\eta = \{\eta(x), x \in S\} \in S$称为组态, 组态$\eta$具有势能Hamilton量

$$H(\eta) = -\sum_{x \sim y} \eta(x)\eta(y) - h \sum_{x \in S} \eta(x).$$

同号势能低. 如果**外磁场强度**$h > 0$而且比较小, $\underline{+1}$势能最低, $\underline{-1}$其次.
$V(\eta) = e^{-\beta H(\eta)}$, 其中$\beta$为**温度倒数**, 经过归一化, 其概率测度称为Gibbs测度.

以Gibbs测度为不变分布的马氏过程统称为随机伊辛模型.
最常见的是所谓Glauber形式(Glauber Dynamics).
$\xi \longrightarrow \xi^x$的转移速率为

$$e^{-\beta[H(\xi^x)-H(\xi)]}.$$

或者离散时间

$$p(\xi,\xi^x)=\frac{1}{N^2}\frac{e^{-\beta[H(\xi^x)-H(\xi)]}}{1+e^{-\beta[H(\xi^x)-H(\xi)]}}.$$

**Theorem**

设$\sigma(\xi) = \inf\{n, X_n = \xi\}, \quad 1/h << N.$ 令$L = [2/h] + 1$

$$\lim_{\beta\to\infty} \frac{\log E_{\underline{-1}}\sigma(\underline{+1})}{\beta} = 4L - h(L^2 - L + 1) = \Gamma_2; \tag{1}$$

$$\lim_{\beta\to\infty} \frac{\log E_{\underline{+1}}\sigma(\underline{-1})}{\beta} = \Gamma_2 + hN^2. \tag{2}$$

$$\lim_{\beta\to\infty} P_{\underline{-1}}(|\frac{\log \sigma(\underline{+1})}{\beta} - \Gamma_2| < \epsilon) = 1; \tag{3}$$

$$\lim_{\beta\to\infty} P_{\underline{+1}}(|\frac{\log \sigma(\underline{-1})}{\beta} - \Gamma_2 - hN^2| < \epsilon) = 1. \tag{4}$$

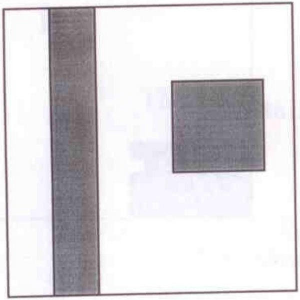
如果$\lim_{\beta\to\infty} P_\xi(\sigma(\underline{-1}) < \sigma(\underline{+1})) = 1$，则称$\xi$为次临界的(subcritical)，如果极限为0则称$\xi$为超临界的(supercritical).

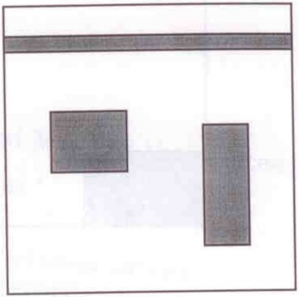
如何判断? $\xi$ 与$\{x \in \Lambda; \xi(x) = 1\}$一一对应，定义

$$\mathcal{R} = \{\xi, \xi\text{由分离的矩形组成}\}.$$

对于$\xi \in \mathcal{R}$定义

$$L(\xi) = \begin{cases} L_2 & \text{if } \xi \text{ contains a rectangle } k \times N, k \geq 2; \\ \max\{l_1 \wedge l_2, & l_1 \times l_2 \text{ is a rectangle of } \xi\}. \end{cases}$$





**Theorem**

假定$\xi \in \mathcal{R}, \xi \neq \underline{+1}, \underline{-1}, \epsilon > 0.$

(1) *If* $L(\xi) < L_2$, *then* $\xi$ *is subcritical, and*

$$\lim_{\beta \to \infty} \frac{\log E_\xi \sigma(\underline{-1})}{\beta} = (L(\xi) - 1)h;$$

$$\lim_{\beta \to \infty} P_\xi(|\frac{\log \sigma(\underline{-1})}{\beta} - (L(\xi) - 1)h| < \epsilon) = 1.$$

(2) *If* $L(\xi) > L_2$, *then* $\xi$ *is supercritical, and*

$$\lim_{\beta \to \infty} \frac{\log E_\xi \sigma(\underline{+1})}{\beta} = 2 - h.$$

$$\lim_{\beta \to \infty} P_\xi(|\frac{\log \sigma(\underline{+1})}{\beta} - (2 - h)| < \epsilon) = 1;$$

# 结论

初态$\xi \in \mathcal{R}$, 所谓的shrink and growth.
$\xi \longrightarrow \xi^{(-)}$, 小的矩形消失, 短边渐次消减, 短于$L_2$的边都将消失;

$$\lim_{\beta\to\infty} P_\xi(|\frac{\log\sigma(\xi^{(-)})}{\beta} - (I(\xi)-1)h| < \epsilon) = 1.$$

$$I(\xi) = \begin{cases} 1 & \text{if } \xi \text{ contains no subcritical rectangle;} \\ \max\{l_1 \wedge l_2, & l_1 \times l_2 \text{ is a subcritical rectangle of } \xi\}. \end{cases}$$

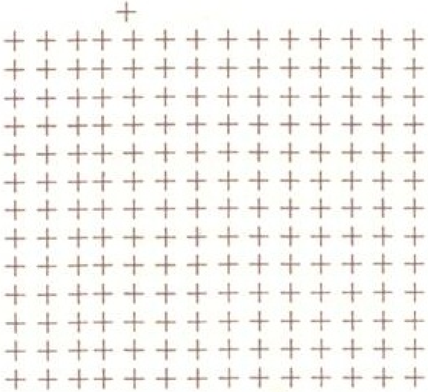
$\xi^{(-)} \longrightarrow \underline{+1}$, 然后再长成(大)矩形,
(1) 若$\xi^{(-)} \neq \underline{-1}$, 大矩形变成更大矩形

$$\lim_{\beta\to\infty} P_{\xi^{(-)}}(|\frac{\log\sigma(\underline{+1})}{\beta} - (2-h)| < \epsilon) = 1.$$

(2) 若$\xi^{(-)} = \underline{-1}$, 问题归结为如何从$\underline{-1}$演化为$\underline{+1}$

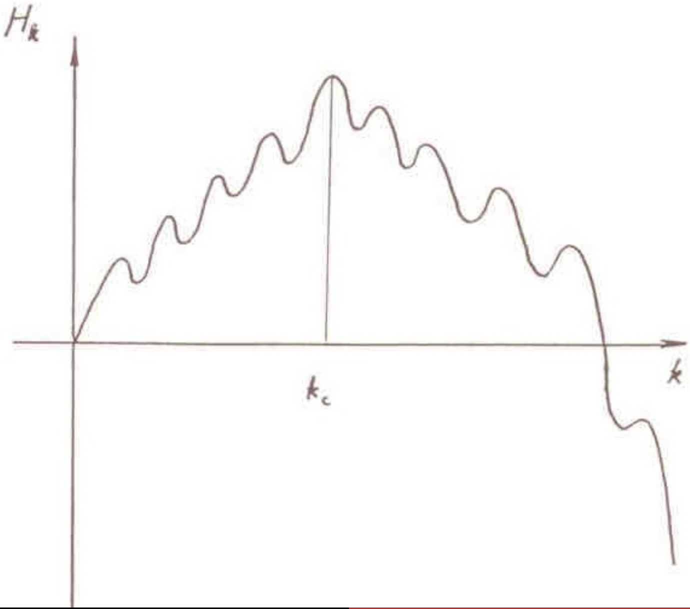
$$\lim_{\beta\to\infty} P_{\xi^{(-)}}(|\frac{\log\sigma(\underline{+1})}{\beta} - \Gamma_2| < \epsilon) = 1.$$

从消减变为增长,中间有一分水岭,

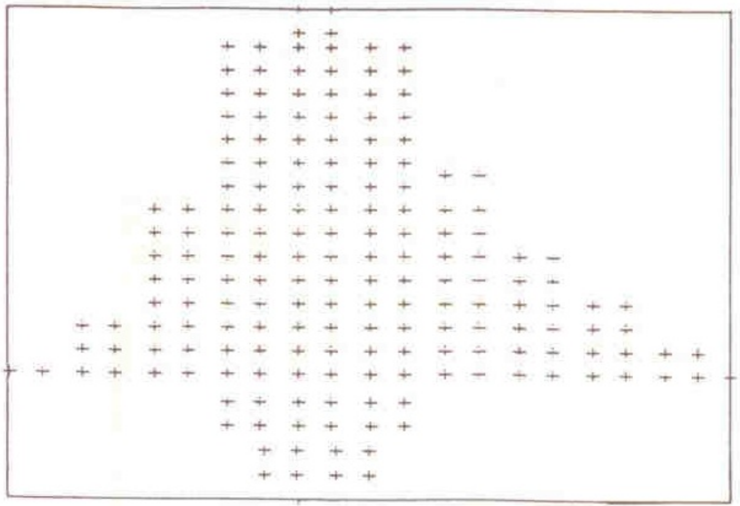


(a) A critical point

# 结论



如果是一般初态$\xi \notin \mathcal{R}$，一些不规则的+1分支先行扩展，变成规则的矩形($\mathcal{R}$)，以后的演化如前所述.



# 推广

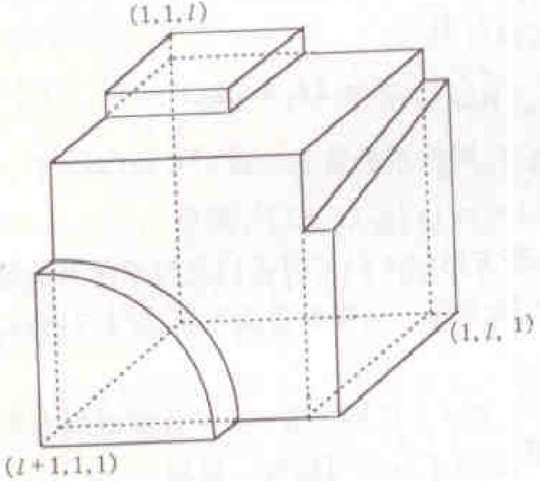



图 1　简单组态

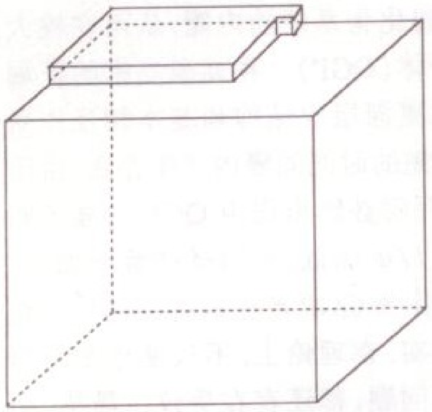
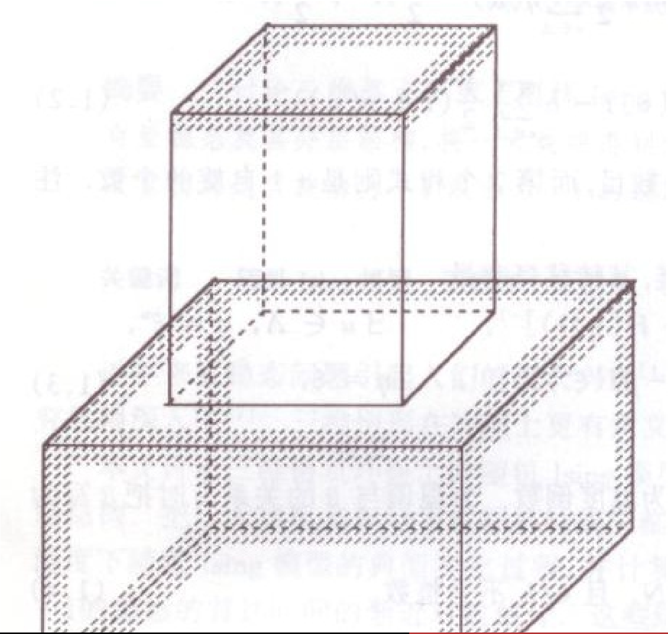


图 3　临界组态

# 推广



# 推广

基本假设: 有限状态空间$S$上一族马氏链, 转移概率$\mathbf{P}^\beta$满足

$$(1)\lim_{\beta\to\infty} p^\beta(\xi,\eta)=p^\infty(\xi,\eta);$$

$$(2)\lim_{\beta\to\infty}\frac{-\log p^\beta(\xi,\eta)}{\beta}\ \text{存在并记为}\ C(\xi,\eta)$$

$$(3) C(\xi,\eta)>0 \quad if \quad p^\infty(\xi,\eta)=0.$$

$\mathbf{P}^\infty$是可约的, $A_1, A_2, \cdots, A_n$是其常返类, 称为**吸引子**, 再定义

$$B_i=\{\xi;\quad P_\xi^\infty(\sigma(A_i)<\infty)>0\},$$

称为相应的**吸引域**, 其中$\sigma(K)=\inf\{n, X_n\in K\}$.

令$\tau(K) = \inf\{n, X_n \notin K\}$.

**Theorem**

假设初值$\xi \in A_i \subset B_i$. 则

$$\lim_{\beta\to\infty} \frac{1}{\beta} \log E_\xi^\beta \tau(B_i) = T(B_i);$$

$$\lim_{\beta\to\infty} \frac{-1}{\beta} \log P_\xi^\beta (X_{\tau(B_i)} = \eta) = -T(B_i) + T_{\xi\eta}(B_i);$$

$$\lim_{\beta\to\infty} P_\xi^\beta (X_{\tau(B_i)} \in \{\eta \notin B_i,\ T_{\xi\eta}(B_i) = T(B_i)\}) = 1.$$

$T(B_i) = \min\{\sum_{k=0}^{l} C(\xi_k\xi_{k+1}), \quad \xi_0, \xi_1, \cdots, \xi_l$从$A_i$到$B_i^c\}$.
其中$\xi_0, \xi_1, \cdots, \xi_{l-1} \in B_i, \xi_l \notin B_i$
$T_{\xi\eta}(B_i) = \min\{\sum_{k=0}^{l} C(\xi_k\xi_{k+1}), \quad \xi_0, \xi_1, \cdots, \xi_l$从$A_i$到$B_i^c\}$
其中$\xi_0 = \xi,\ \xi_l = \eta$.

# 推广

**Theorem**

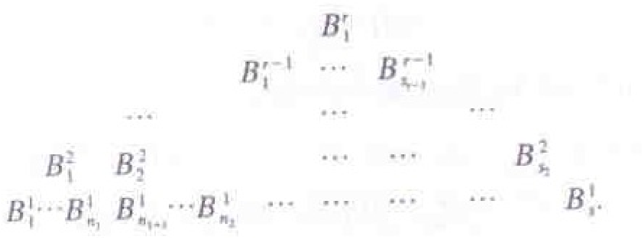
假设初值$\xi \in B_i \setminus \cup_{j \neq i} B_j$. 设$\delta > 0$, 则$\tau(B_i)/E_\xi^\beta \tau(B_i)$收敛于指数分布, 参数为1.

$$\lim_{\beta \to \infty} P_\xi^\beta (e^{(T(B_i)-\delta)\beta} < \tau(B_i) < e^{(T(B_i)+\delta)\beta}) = 1.$$

# 推广

分层结构，逐级定义高阶吸引子和高阶吸引域.

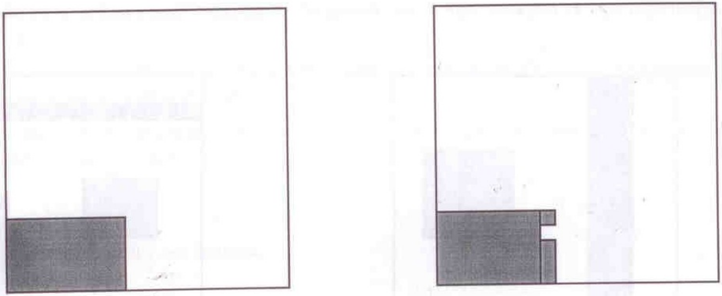
在合适的时间尺度，我们看见马氏链在吸引子$A_1, A_2, \cdots, A_n$之间转移，根据它们彼此间到达的时间长短可以进一步划分等价类，成为高一级的吸引子，再定义高一级的吸引域.



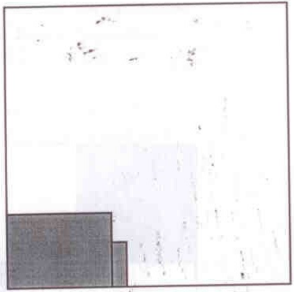
可逆性便于势能计算,但整套理论并不需要可逆性,
majority-voter model on a torus

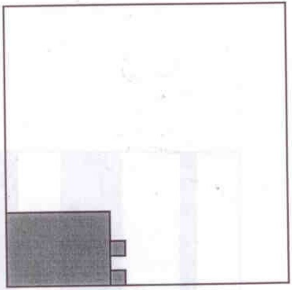
$$p(\xi,\xi^x)=\begin{cases}1-\delta & \text{if } \xi(x) \text{ disagrees with majority of its neigbors}\\ \delta & \text{if } \xi(x) \text{ agrees with majority of its neigbors}\end{cases}$$

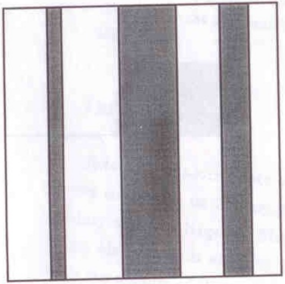
层数较少,可以计算,还可以非对称.

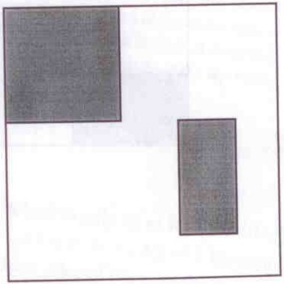


# 应用









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