

司 錄 哥



从两个箭头谈起

J. -M. Liu (刘俊明)

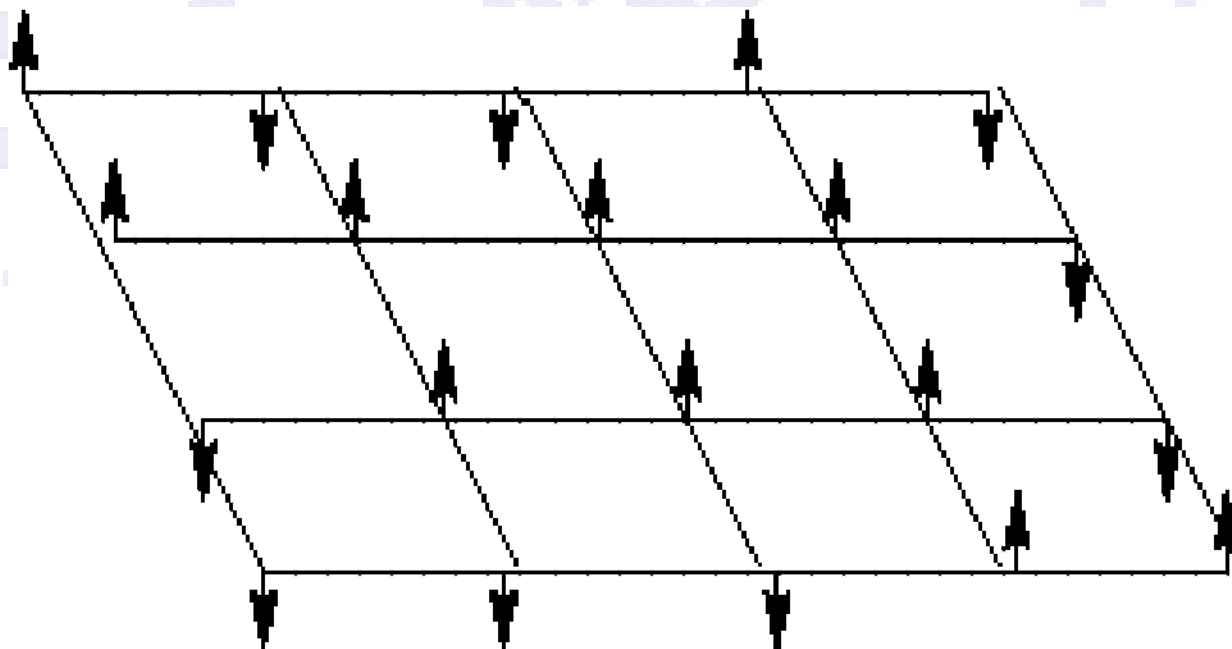
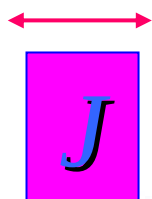
Email: liujm@nju.edu.cn

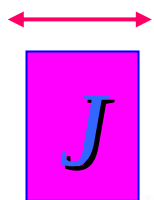
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南京大学物理系
南京微结构国家实验室



按一定空间对称性排列，大小不变
存在交互作用
扩展到一维、二维和三维体系 $\Rightarrow$ 点阵





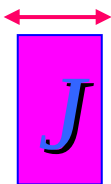
按一定空间对称性排列，大小不变
存在交互作用
扩展到一维、二维和三维体系 $\Rightarrow$ 点阵

$$H_{ij} = -J \cdot S_i \cdot S_j$$

$$H = -\frac{1}{2} J \cdot \sum_{\langle i,j \rangle} S_i \cdot S_j - h \cdot \sum_{\langle i \rangle} S_i, \quad S_i = \pm 1$$

$$H = -\frac{J_{FM}}{2} \cdot \sum_{\langle i,j \rangle} S_i \cdot S_j - \frac{J_{AF}}{2} \cdot \sum_{[i,j]} S_i \cdot S_j - h \cdot \sum_{\langle i \rangle} S_i, \quad S_i = \pm 1$$





系统微观状态 $\{S\}=\{S_1, S_2, S_3, \dots, S_i\}$

配分函数:

$$Z_N = \sum_{\{S\}} \exp(-\beta H(\{S\})), \quad \beta = 1/kT$$

自由能:

$$F = -kT \ln Z_N$$

平均磁矩:

$$M(h, T) = \langle S \rangle = -\frac{1}{N} \frac{\partial F(h, T)}{\partial h}$$

极化率:

$$\chi = \frac{\partial M(h, T)}{\partial h} = -\frac{1}{N} \frac{\partial^2 F(h, T)}{\partial h^2} \geq 0$$

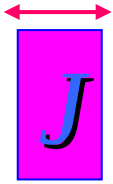
能量:

$$E = F - T \frac{\partial F(h, T)}{\partial T} = -T^2 \frac{\partial F(h, T)/T}{\partial T}$$

比热:

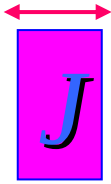
$$C = \frac{\partial E(h, T)}{\partial T}$$





Ernst ISING





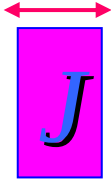
Ising其人

Ernst Ising的简历: May 10, 1900 - May 11, 1998

List of publications

1. E. ISING, *Beitrag zur Theorie des Ferro- und Paramagnetismus*
Dissertation, Mathematisch-Naturwissenschaftliche Fakultät der
Hamburgischen Universität Hamburg, 1924. Unpublished.
2. E. ISING, *Beitrag zur Theorie des Ferromagnetismus*
Zeitschrift fuer Physik 31 (1925) 253-258. (number of citations of this
paper 1975-2001 according ISI citation index: 603).
3. E. ISING, *Goethe as a Physicist*, *American Journal of Physics* 18
(1950) 235-236.

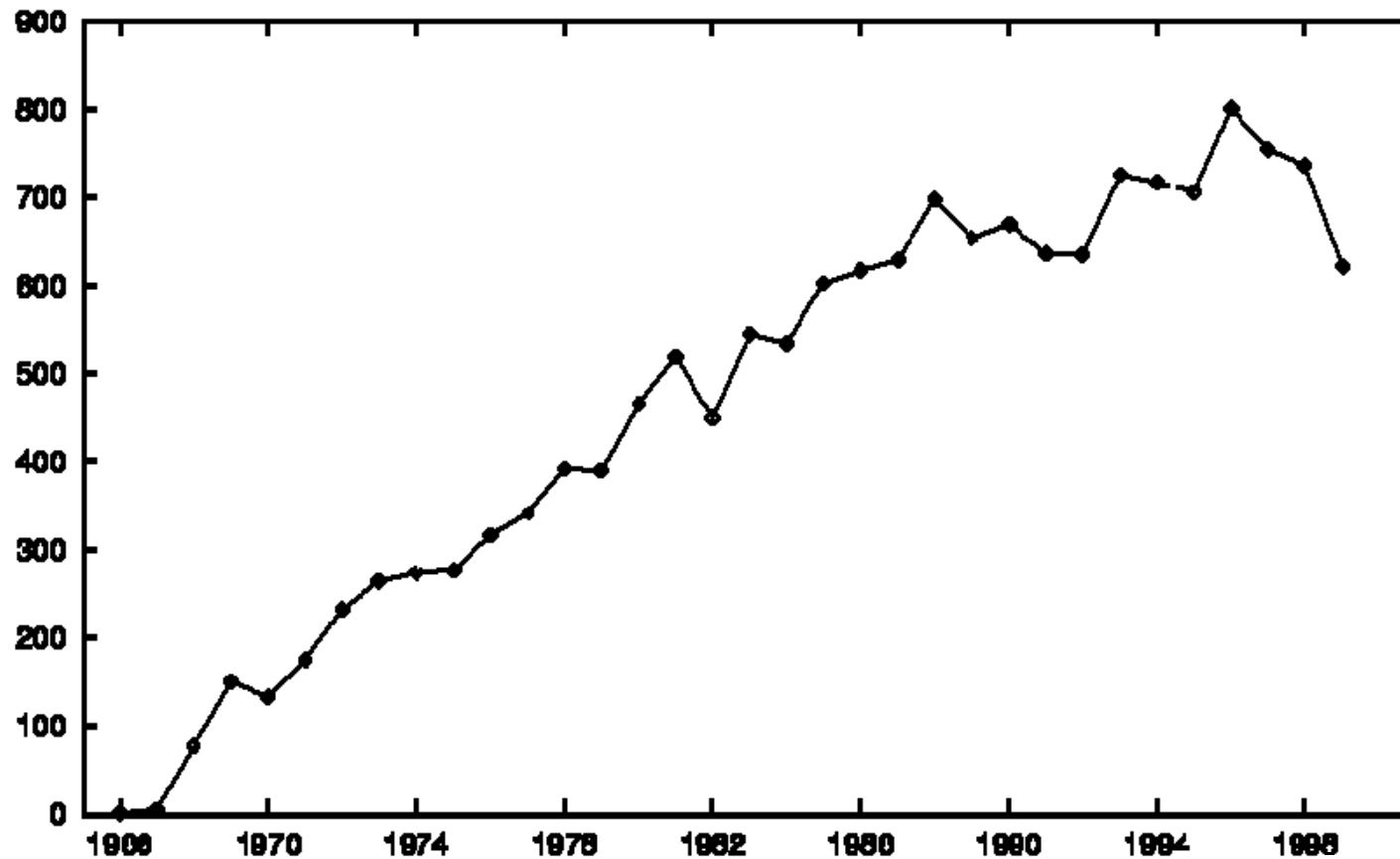




Ising模型

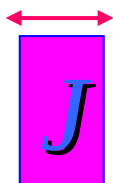
S. G. Brush, History of the Lenz-Ising Model, Rev. Mod. Phys 39
(1962) 883-893

Ising model (number of publications)



成名观





Ising模型应用于相变

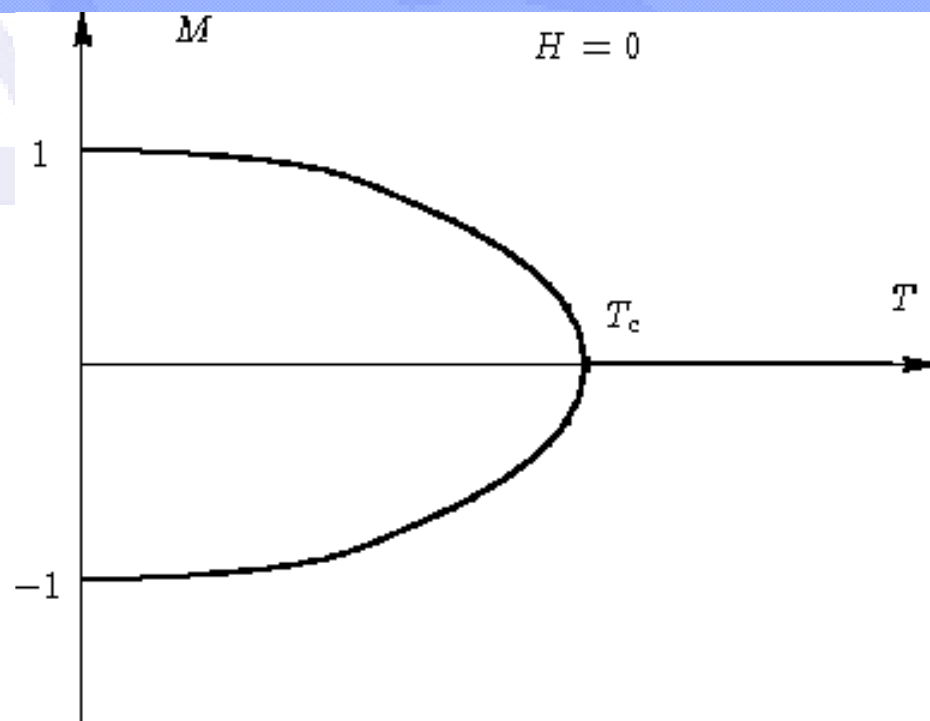
零场、对称情况：

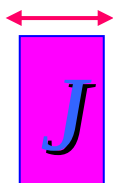
熵希望箭头排列无序，而能量希望箭头排列有序

T 很高时熵赢， $M=0$

T 很低时能量赢， $M=\pm 1$

零场下相变：
存在一个临界点 T_c 。





Ising模型应用于相变

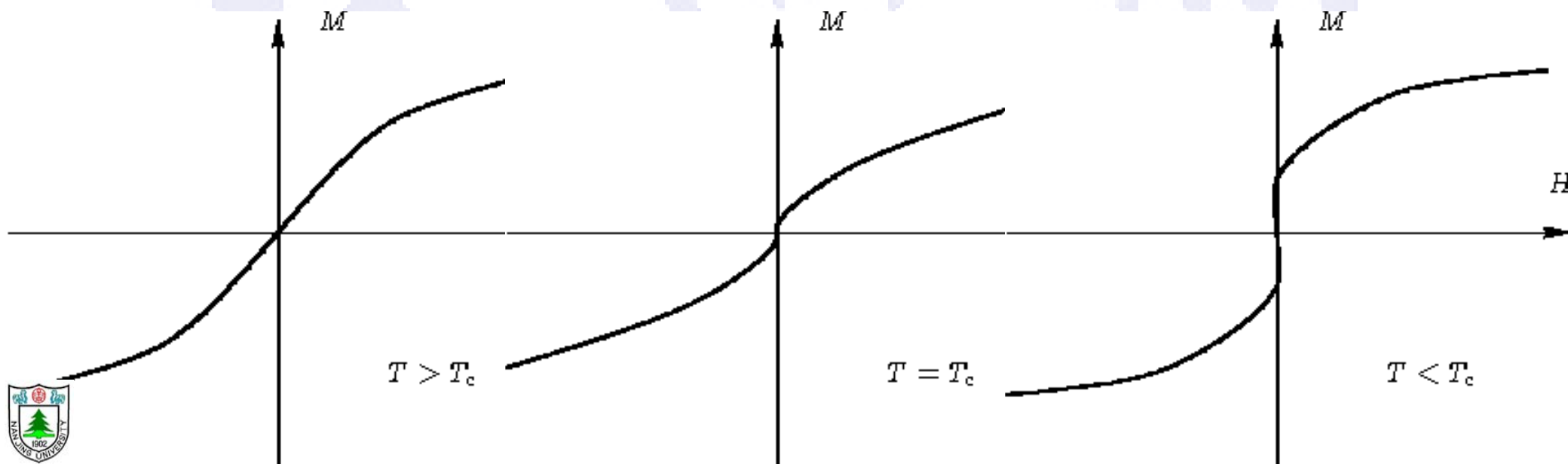
非零场情况:

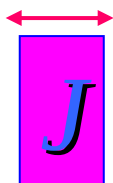
系统“磁矩”就依赖于外场 H 了— $M(H, T)$ 。
那么 $H \Rightarrow 0$ 时发生什么情况?

$T > T_c$

$T = T_c$

$T < T_c$





Ising模型应用于相变

非零场情况:

系统“磁矩”就依赖于外场 H 了— $M(H, T)$ 。
那么 $H \Rightarrow 0$ 时发生什么情况?

$T=T_c$

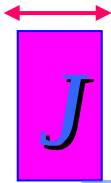
$$\lim_{H \Rightarrow \pm 0} M(H, T) = 0, \quad \lim_{H \Rightarrow \pm 0} \frac{\partial M(H, T)}{\partial H} \Rightarrow \infty, \quad T = T_c$$

所以在临界点处极化率无穷大：一级相变！

$$\langle (\Delta M)^2 \rangle = \frac{\chi \cdot kT}{V}$$

所以在临界点处涨落无穷大



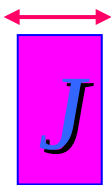


Ising模型的应用：刘俊明的**乐趣**！

我们该如何来扩张Ising模型？

1. 箭头指向空间任意一个方向 (*Potts model*)--useful for compressible multicomponent mixtures。注意到吴法岳教授的工作！
2. 将箭头表示为矢量，交互作用写成： $\sigma_i \cdot \sigma_j$ ，即*Heisenberg model*
3. 引入到空间复杂点阵之间 (fcc, bcc, trigonal, hexagonal...)
4. 引入一些亚点阵，相互嵌套 (*decorated models*)
5. 引入长程关联
6. 让交互作用成为空间的函数：玻璃中的玩具模型
7. 引入动力学(kinetic)和取向(re-orientation)涨落：时间关联行为

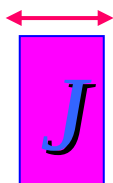




类Ising模型：挑战与机会！

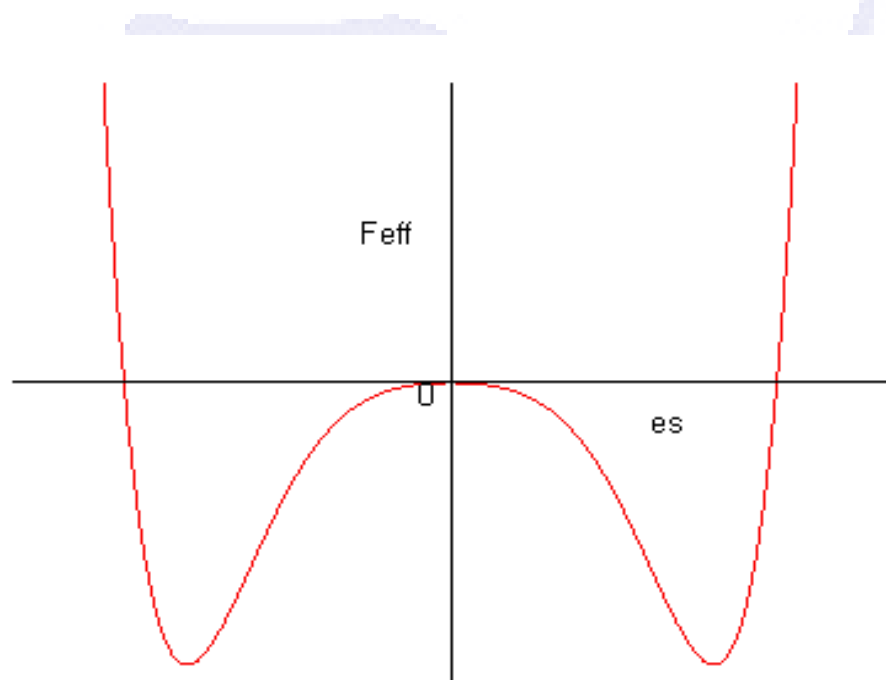
1. Ising模型及其变种原则上进行严格求解十分困难，这仅仅以二维Ising模型的Onsager解就足够说明这一点。
2. 三维Ising模型严格解是不是存在现在问题。
3. 怎么办？两种方法并行不悖！
4. 连续化处理：例如Langevin方程。
5. 蒙特卡罗模拟：最为成功的方法。有关Ising模型每年的论文绝大部分都是蒙特卡罗方法的结果。
6. 蒙特卡罗方法中有Metropolis代数、动力学代数(Kawasaki)、Glauber代数、Wang-Landau代数等等，很多很多！

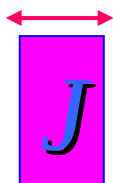




感谢Ising模型：第一类工作一回线动力学

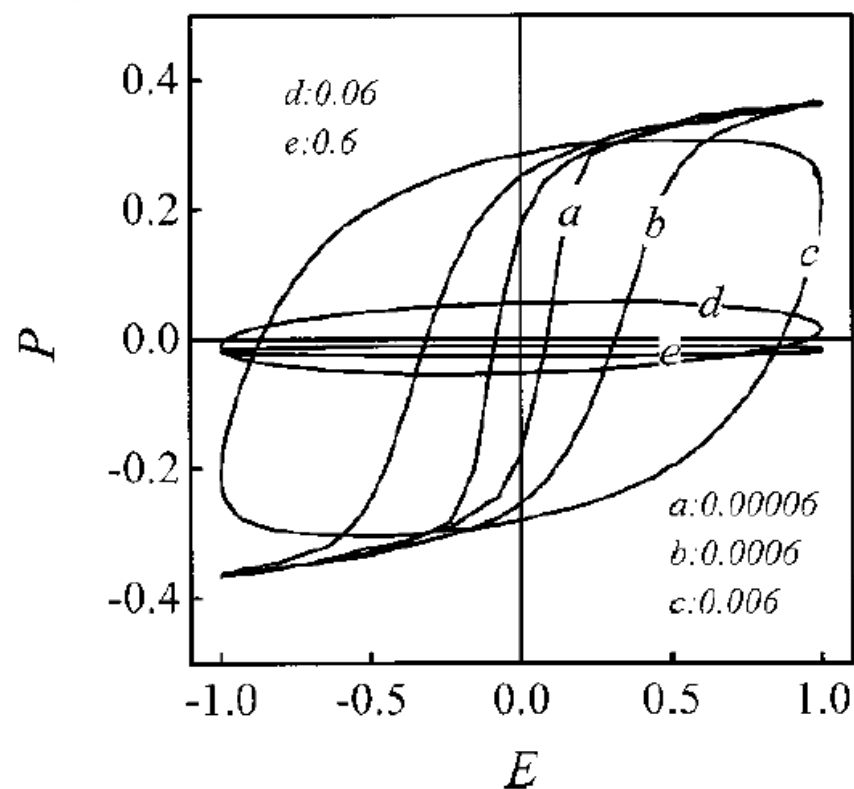
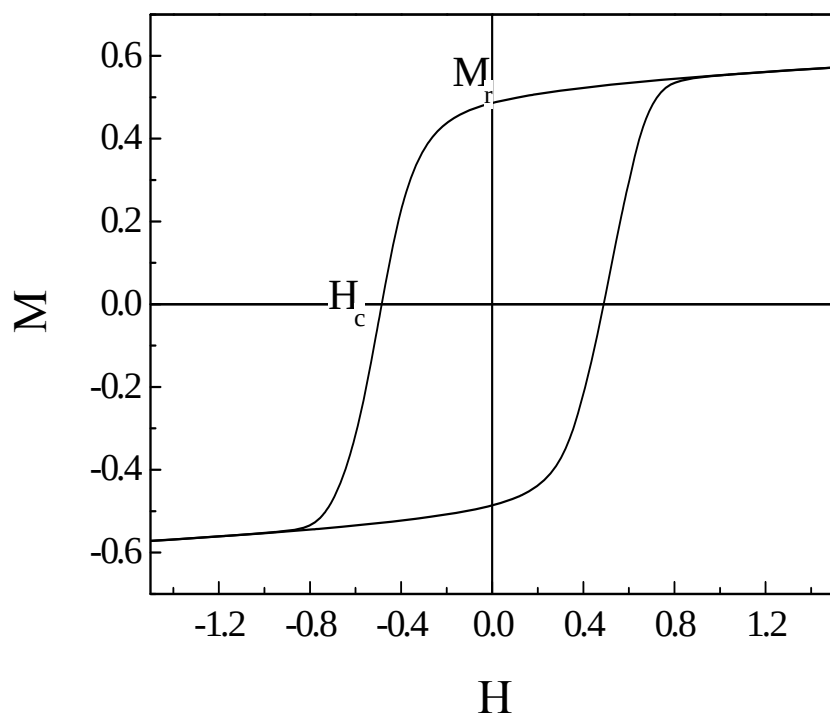
自旋系统或者铁电系统中回线的演示





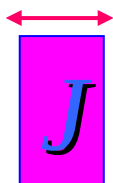
感谢Ising模型：第一类工作一回线动力学

为什么要研究回线动力学问题？



物理：特征时间问题





感谢Ising模型：第一类工作一回线动力学

基本模型： $h=h_0 \cdot \sin(2\pi f \cdot t)$

Heisenberg model

$$H = - \sum_{\langle i, j \rangle} \vec{S}_i \vec{S}_j - h \sum_i \vec{S}_i$$

Potts model

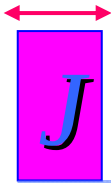
$$H = - \sum_{\langle i, j \rangle} S_i^n S_j^n - h \sum_i S_i^n$$

Ising model

$$H = - \sum_{\langle i, j \rangle} S_i S_j - h \sum_i S_i$$

where $S_i, S_j = +1, -1$

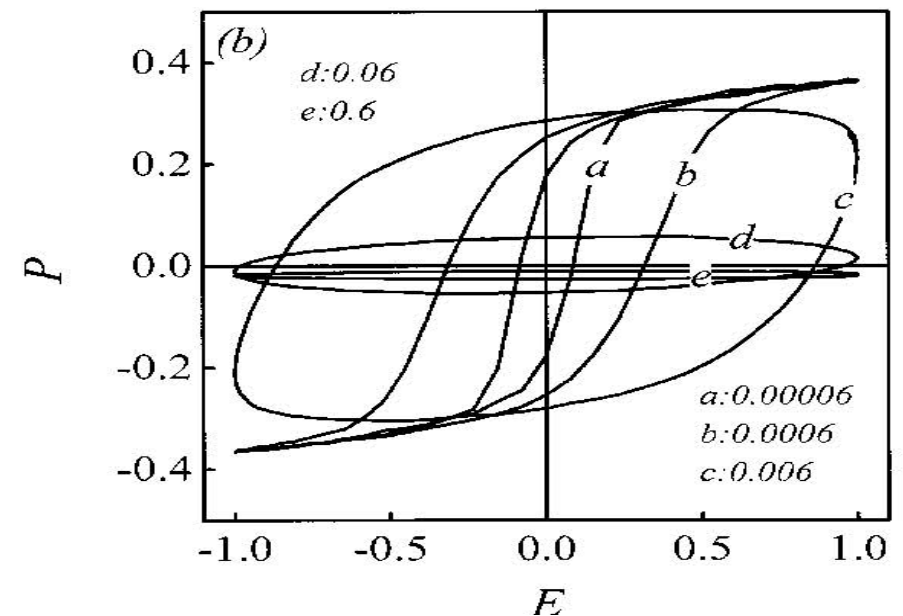
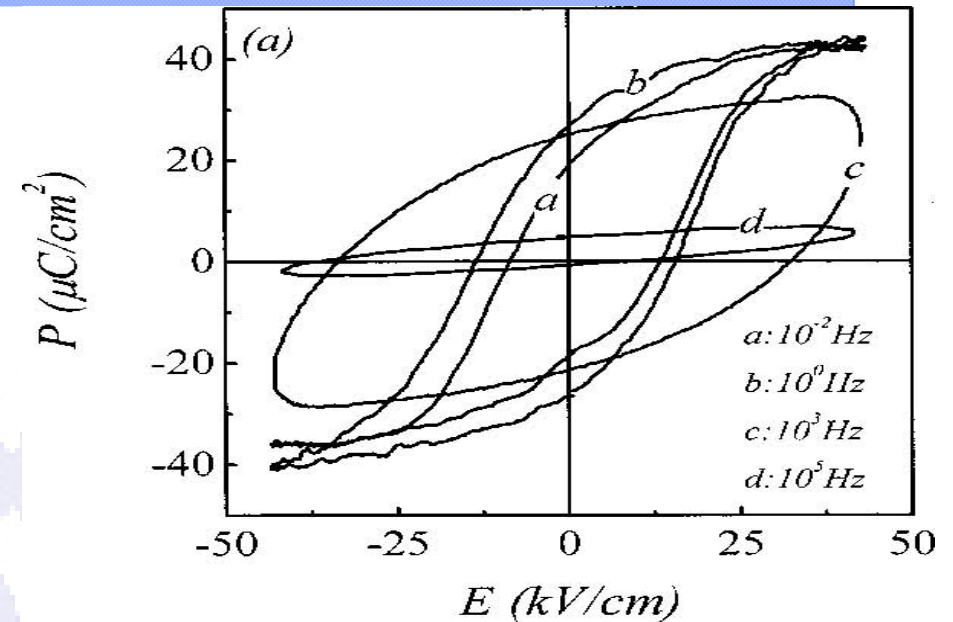


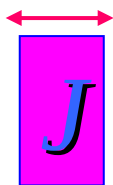


感谢Ising模型：第一类工作—回线动力学

基本模型： $h=h_0 \cdot \sin(2\pi f \cdot t)$

- Hysteresis loops at different f measured for PZT thin films
- simulated for the model lattice
- under fixed field amplitude E_0 . The inserted numbers show the values of f .

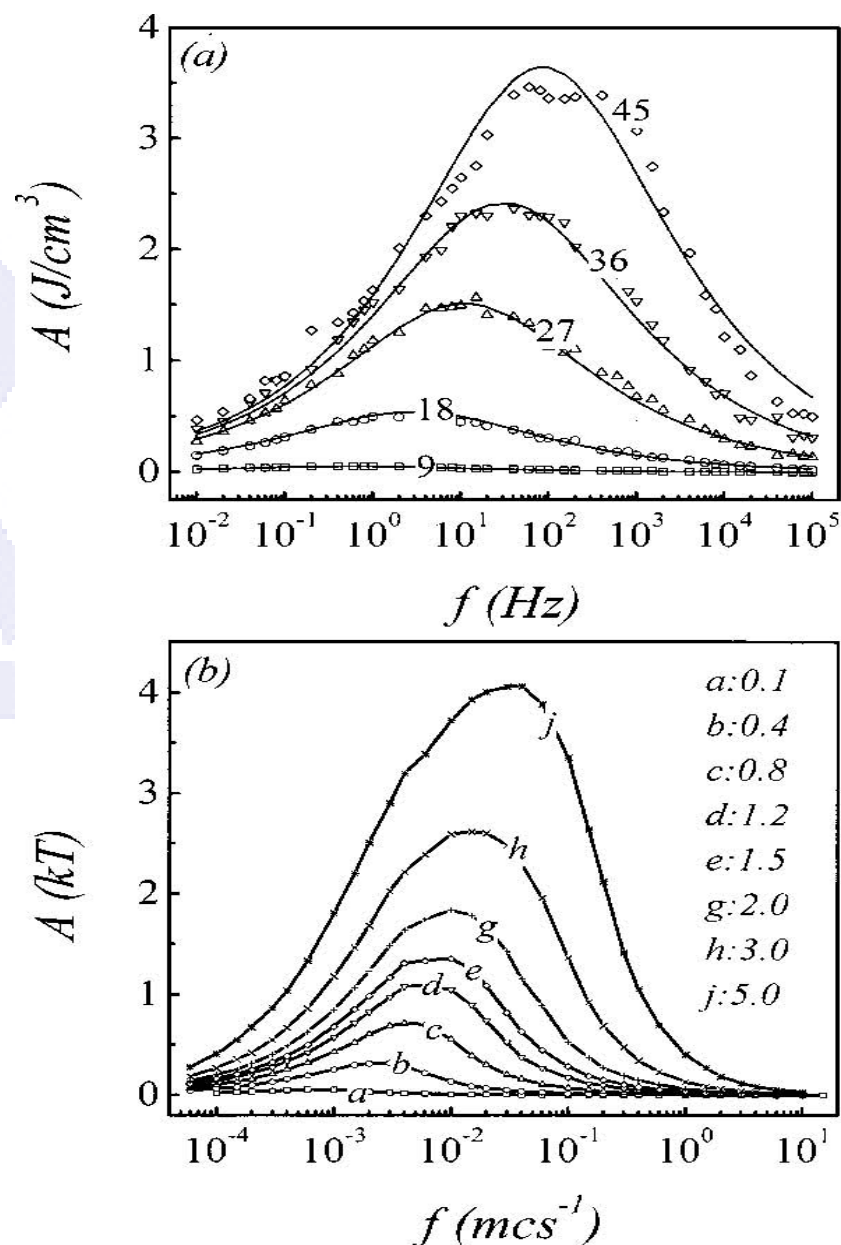


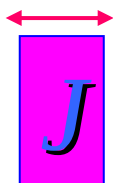


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感谢Ising模型：第一

基本模型： $h=h_0 \cdot \sin(2\pi f \cdot t)$

$$W(\eta) = \tau_1^d \cdot A(f, E_0)$$

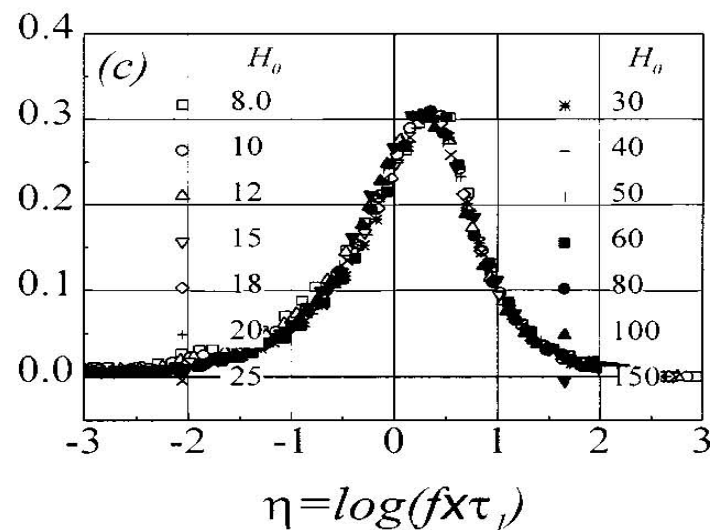
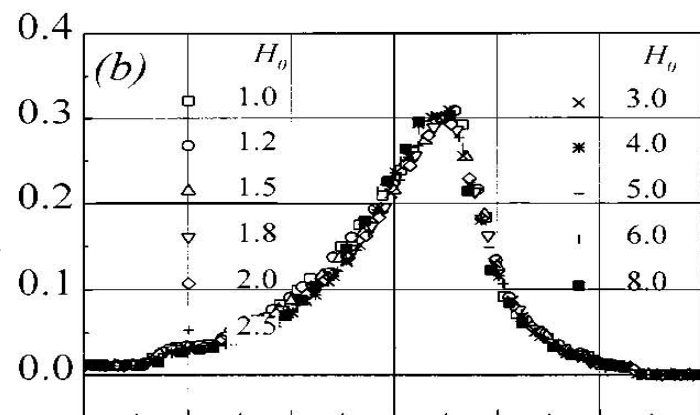
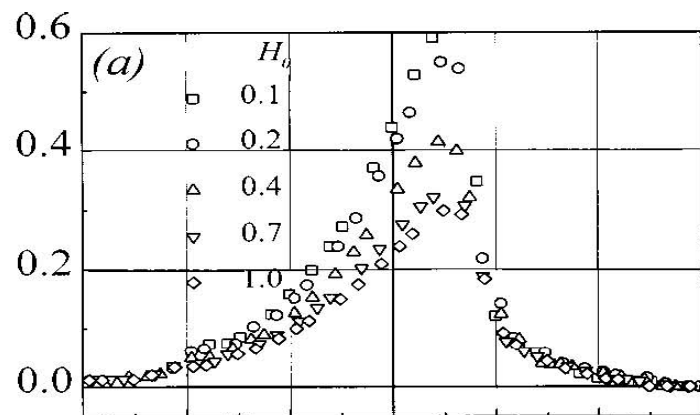
$$W(\eta) = f_1^{-d} \cdot A(f, E_0)$$

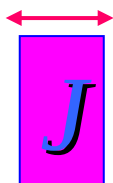
$$d \equiv 1$$

$W(\eta) \times 10^{-3}$

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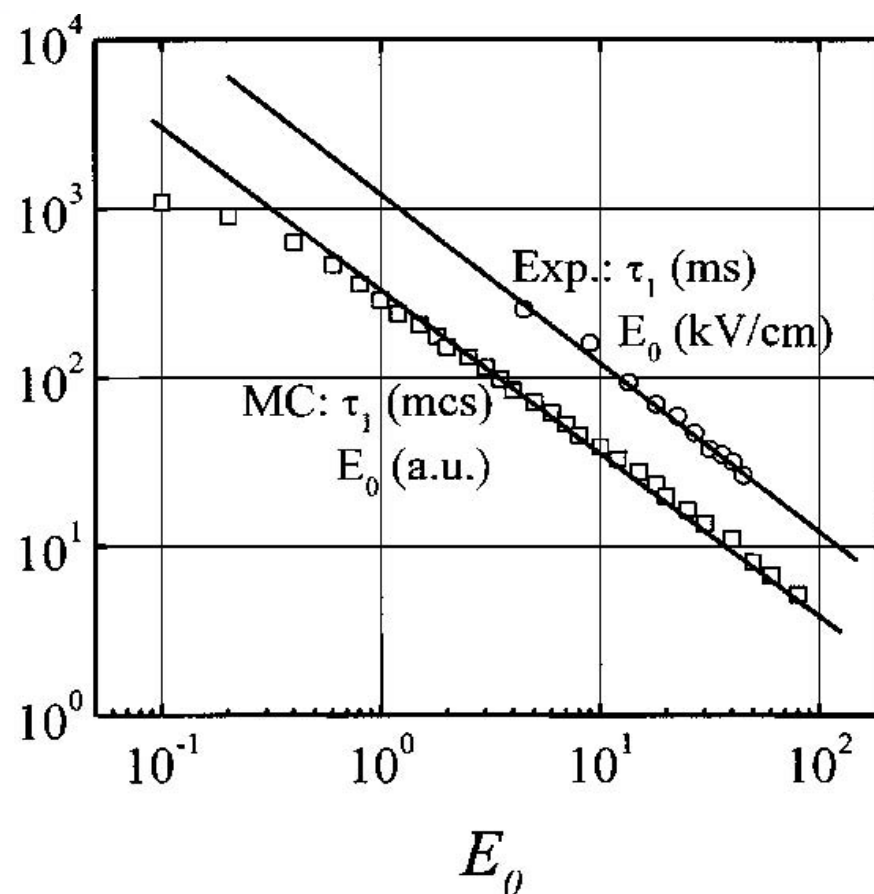
感谢Ising模型：第一类工作—回线动力学

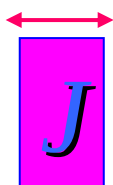
基本模型： $h=h_0 \cdot \sin(2\pi f \cdot t)$

$$d \equiv 1$$

$$\tau_1 \propto h_0^{-d}$$

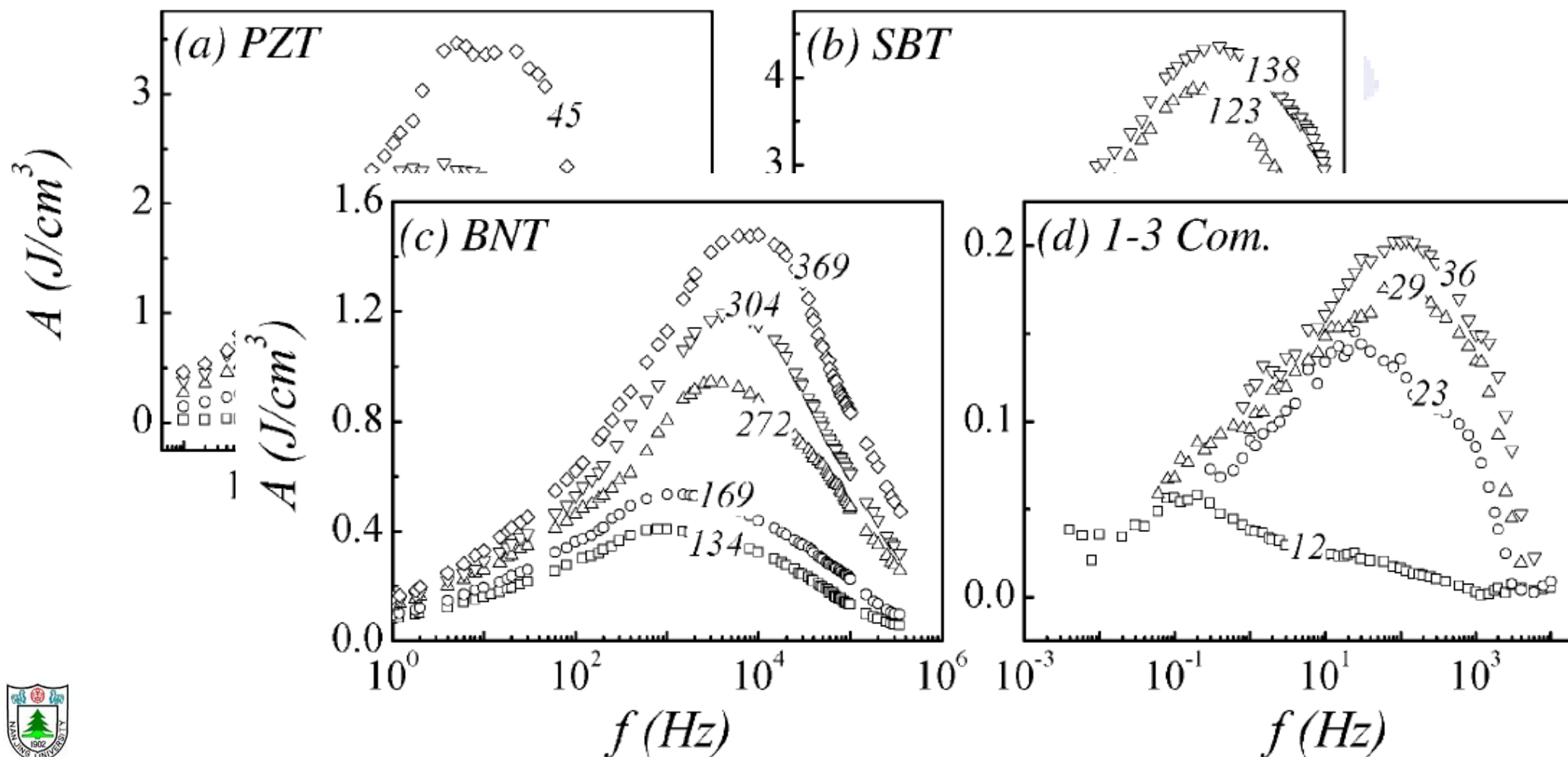
$$\tau_1(E_0)$$

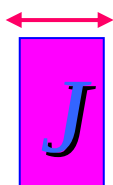




感谢Ising模型：第一类工作—回线动力学

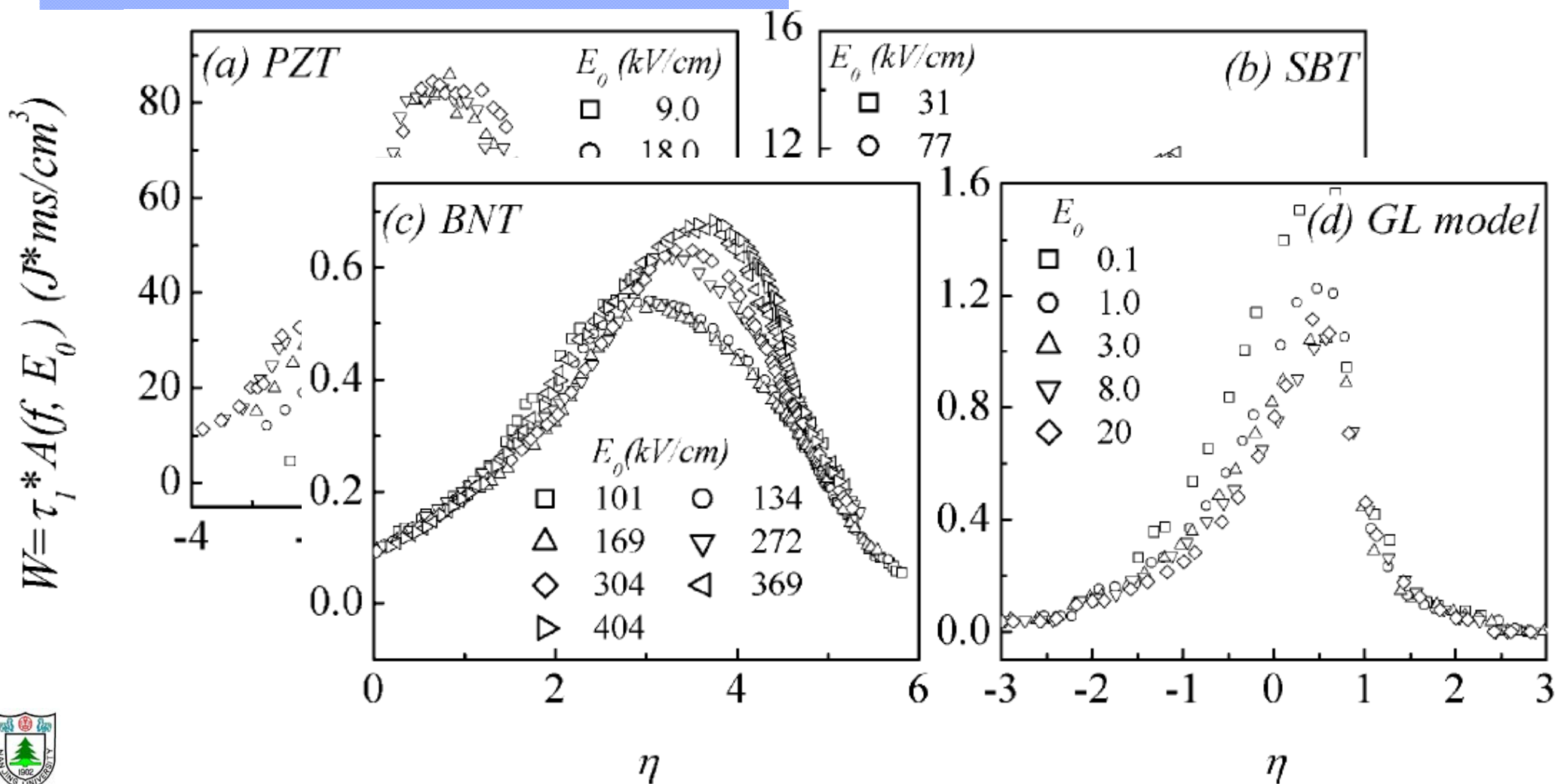
实验验证：铁电薄膜

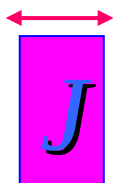




感谢Ising模型：第一类工作—回线动力学

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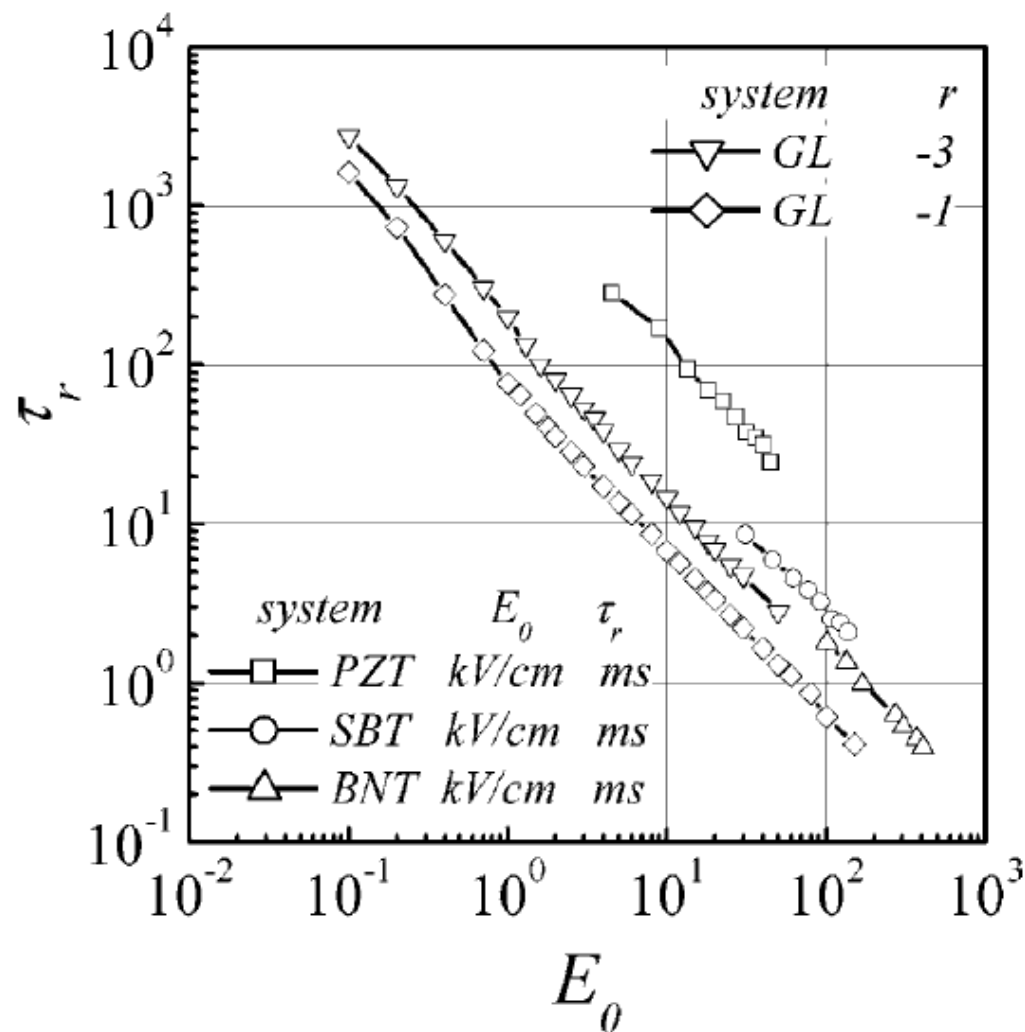


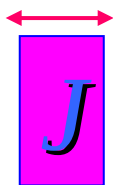
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实验验证：铁电薄膜

$$d \equiv 1$$

$$\tau_1 \propto E_0^{-d}$$

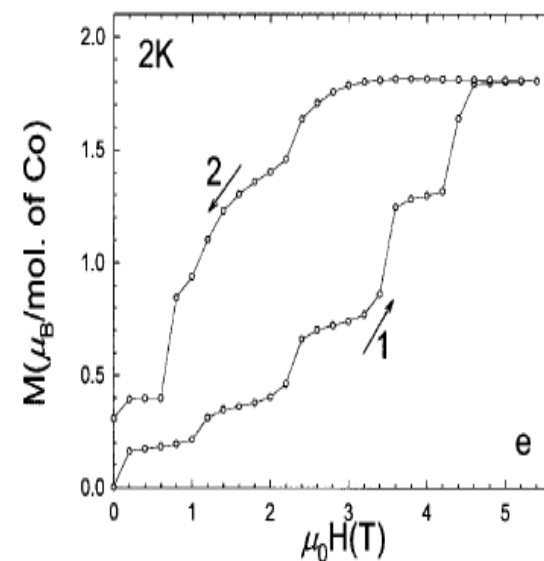
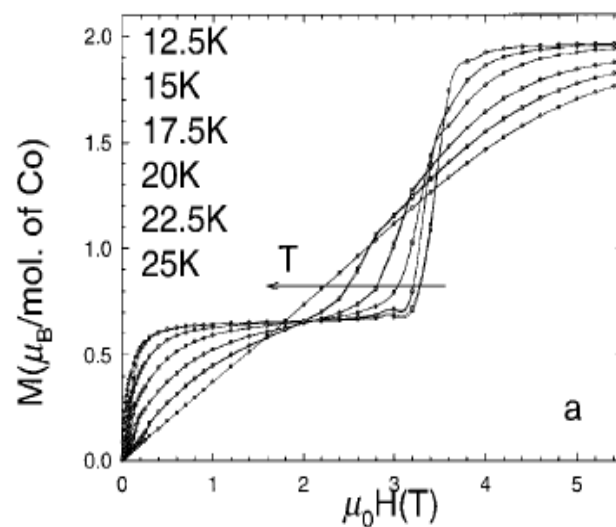
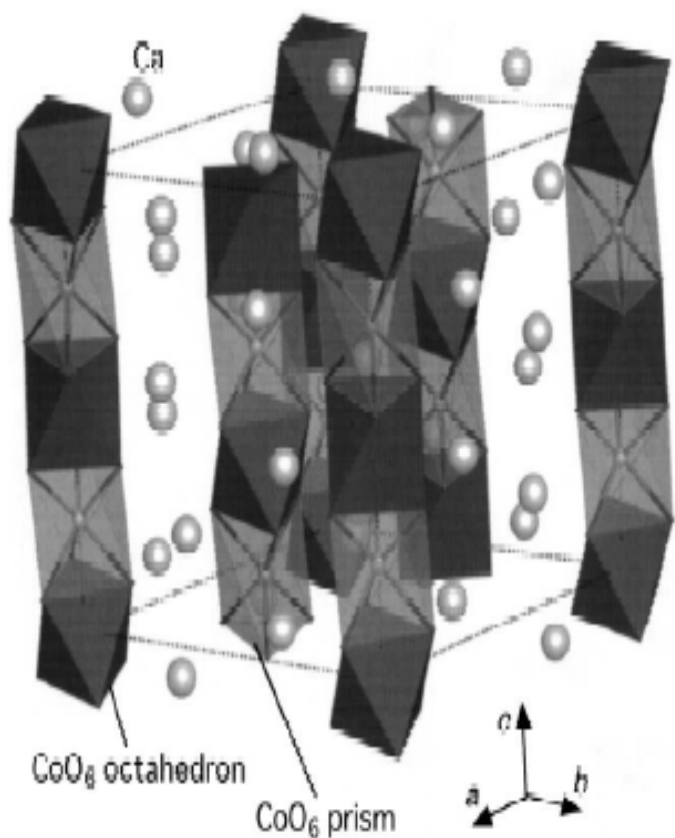


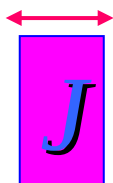


感谢Ising模型：第二类工作—自旋玻璃体系

自旋玻璃中的失措与台阶行为：

- $\text{Ca}_3\text{Co}_2\text{O}_6$ 的晶体结构与自旋结构。
- 自旋失措行为

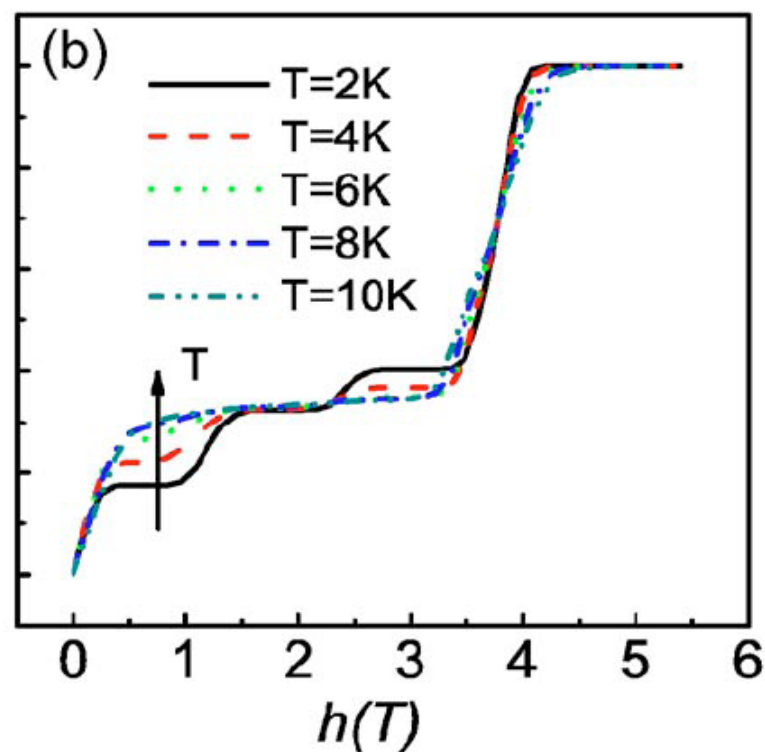
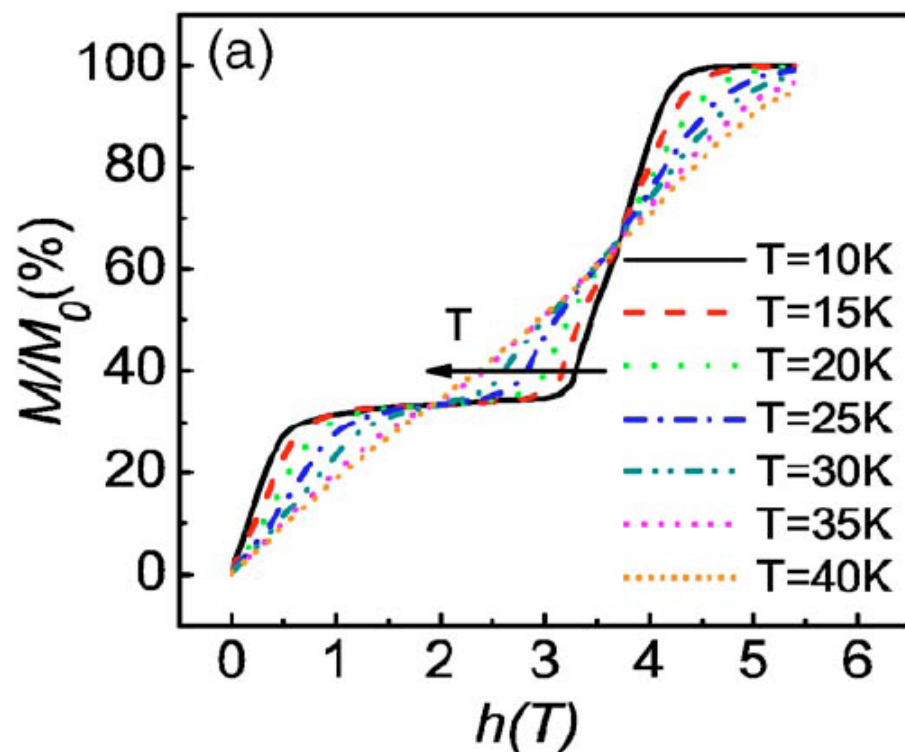


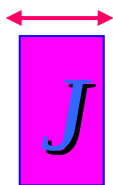


感谢Ising模型：第二类工作—自旋玻璃体系

二维三角点阵中的自旋失措：

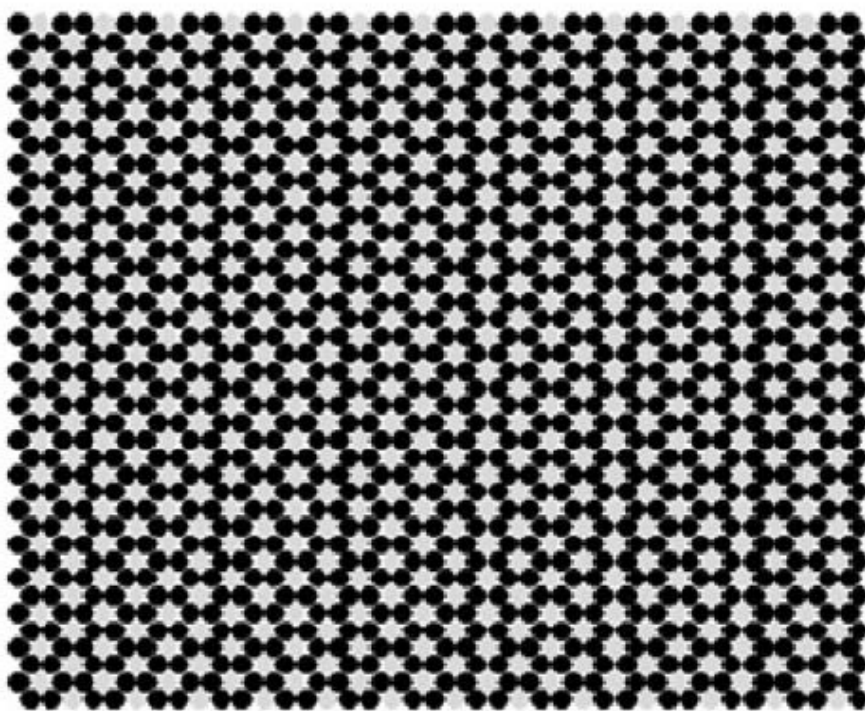
$$H = - \sum_{[m,n]} (J + J\Delta_{m,n}) S_m^e S_n^e - h\mu_B g \sum_m S_m^e$$





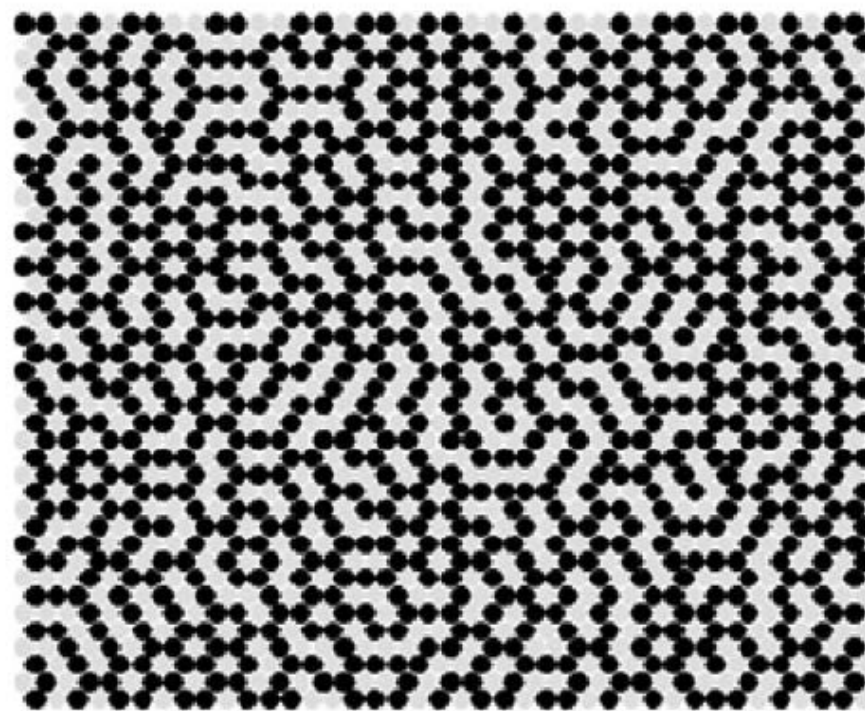
感谢Ising模型：第二类工作—自旋玻璃体系

二维三角点阵中的自旋失措：



(a)

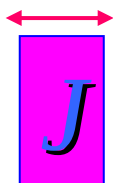
$T=10 \text{ K}, h=1.8 \text{ T}$



(b)

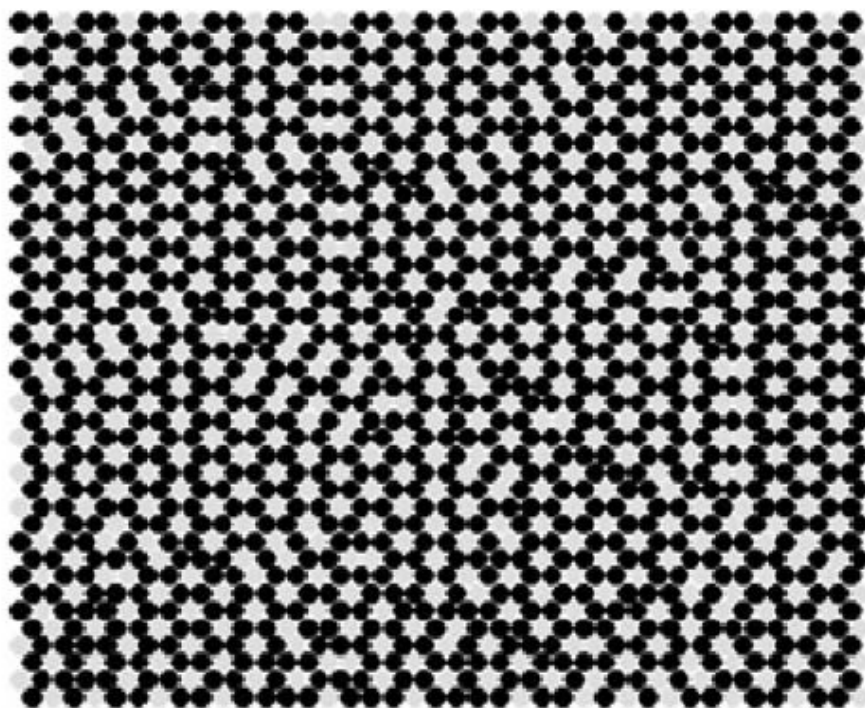
$T=2 \text{ K}, h=0.6 \text{ T}$





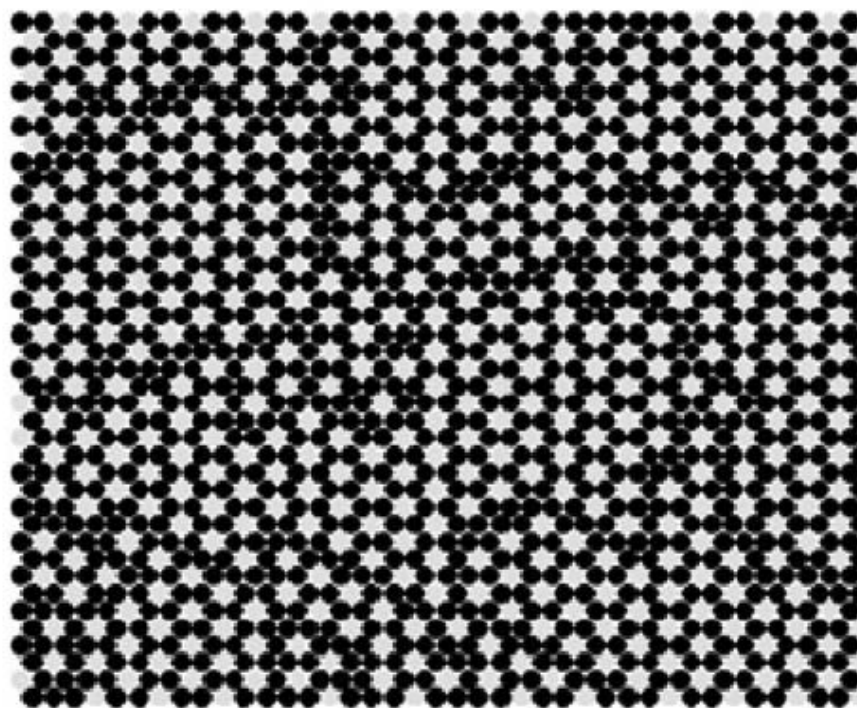
感谢Ising模型：第二类工作—自旋玻璃体系

二维三角点阵中的自旋失措：



(c)

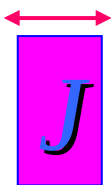
$T=2 \text{ K}, h=1.8 \text{ T}$



(d)

$T=2 \text{ K}, h=3.0 \text{ T}$



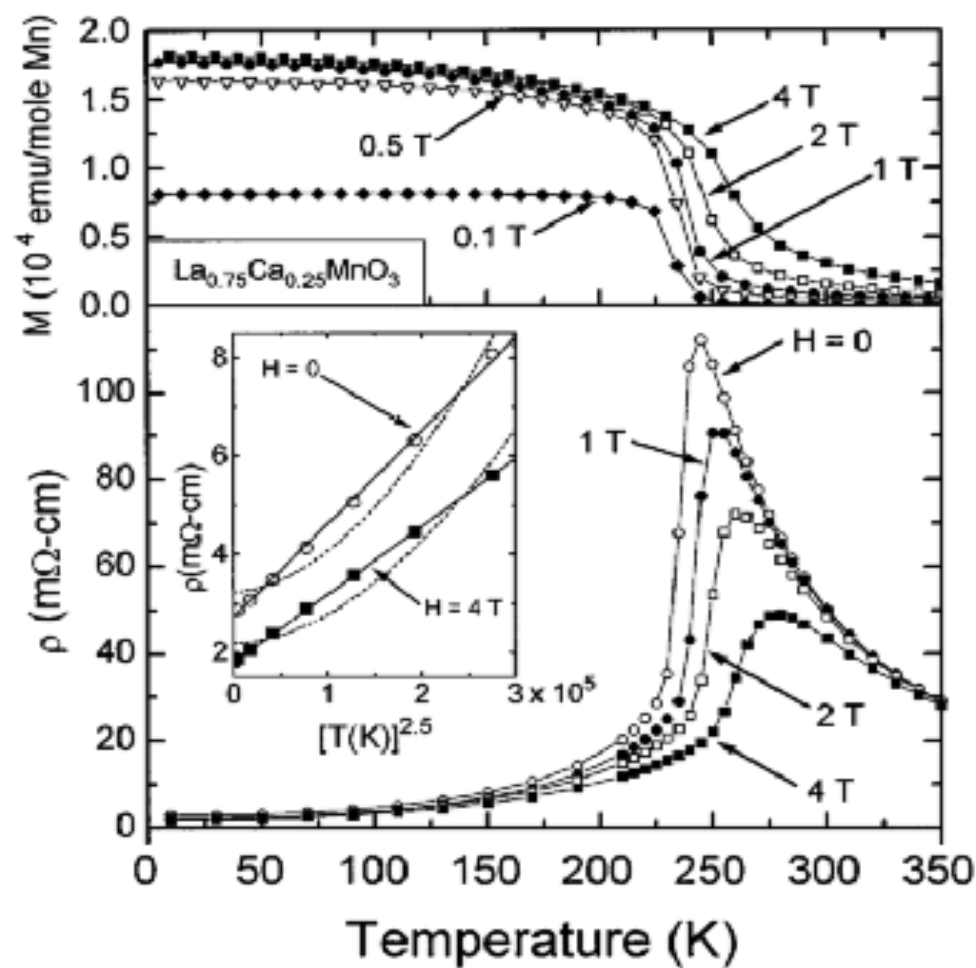


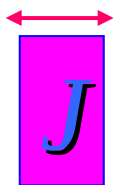
感谢Ising模型：第三类工作—庞磁电阻

什么是庞磁电阻？Ising模型、自旋玻璃、电阻网络等等

锰氧化物中的庞磁电阻

1. 自旋、电荷、轨道、声子四维空间的相互作用
2. 凝聚态物理最漂亮也最复杂的体系！





双交换作用

$$- \sum_{ia\gamma\gamma'\sigma\downarrow} t_{\gamma\gamma'}^a d_{i\gamma\sigma}^\dagger d_{i+a\gamma'\sigma\downarrow}$$

Hund法则

$$- J_H \sum_i \mathbf{s}_i \cdot \mathbf{S}_i$$

Jahn-Teller效应

$$E_{JT} \sum_i [2(q_{1i}n_i + q_{2i}\tau_{xi} + q_{3i}\tau_{zi}) + \beta q_{1i}^2 + q_{2i}^2 + q_{3i}^2]$$

锰氧化物

库仑排斥

$$U' \sum_i n_{ia} n_{ib} + V \sum_{\langle i,j \rangle} n_i n_j$$

超交换作用

$$J_{AF} \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



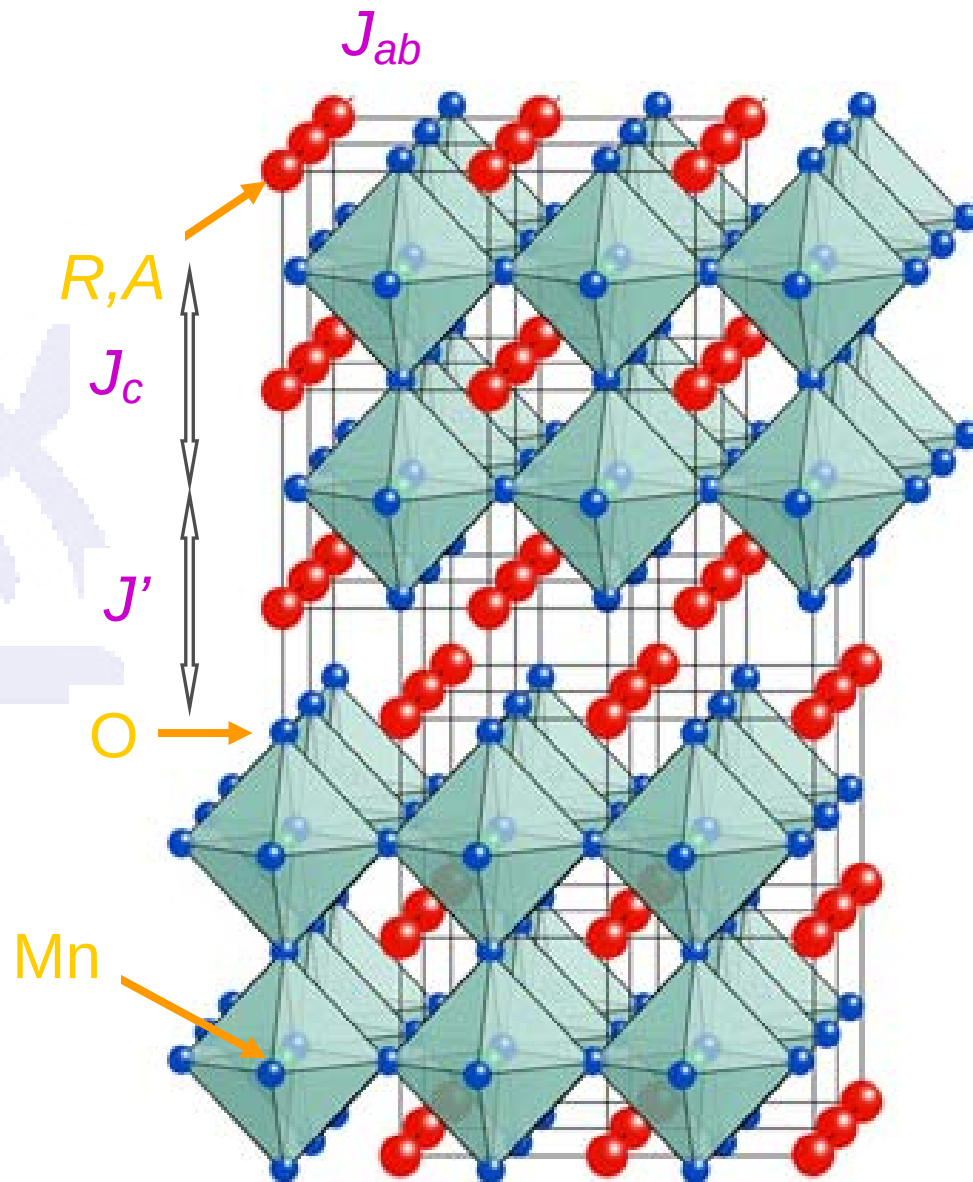
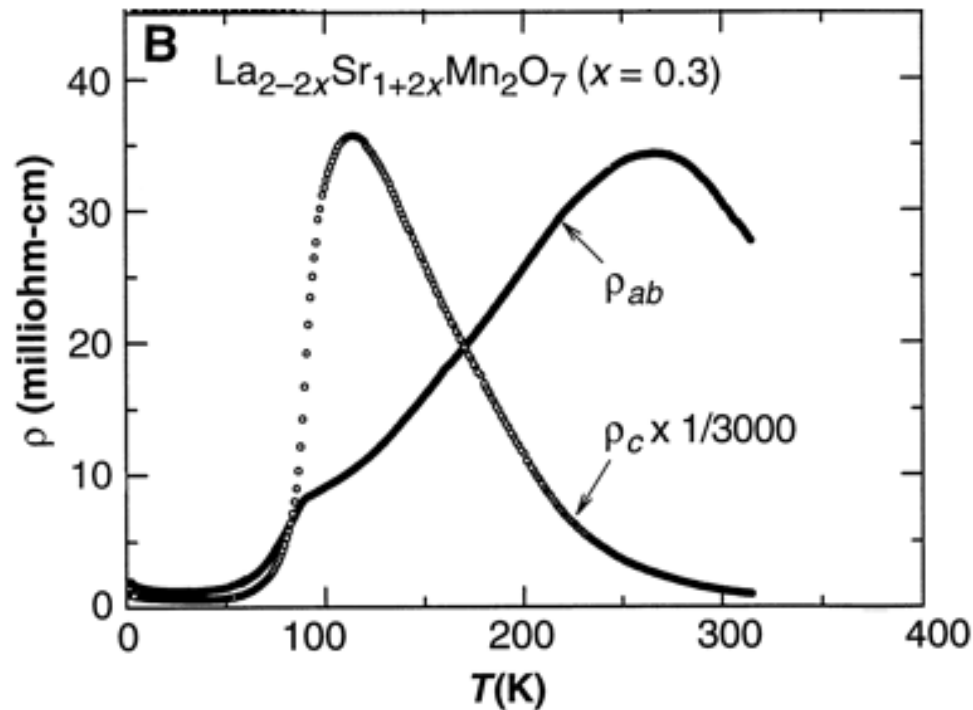
感谢Ising模型：第三类工作—庞磁电阻

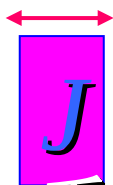
J

层状锰氧化物



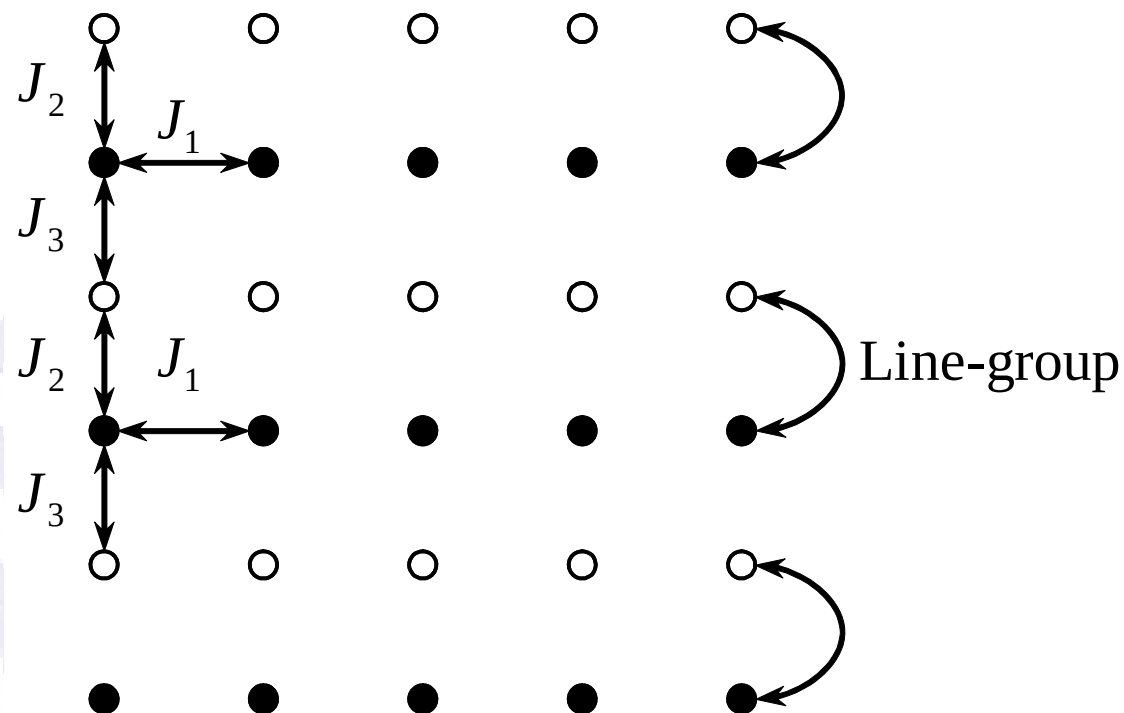
$$|J_{ab}| > |J_c| > |J'| > 0$$





感谢Ising模型：第三类工作—庞磁电阻

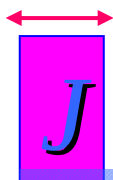
看看Ising模型如何运用？



$$H_{1i} = \sum_j [-J_1(S_{i,j-1} + S_{i,j+1})S_{i,j} - J_2S_{i+1,j}S_{i,j} - J_3S_{i-1,j}S_{i,j}]$$

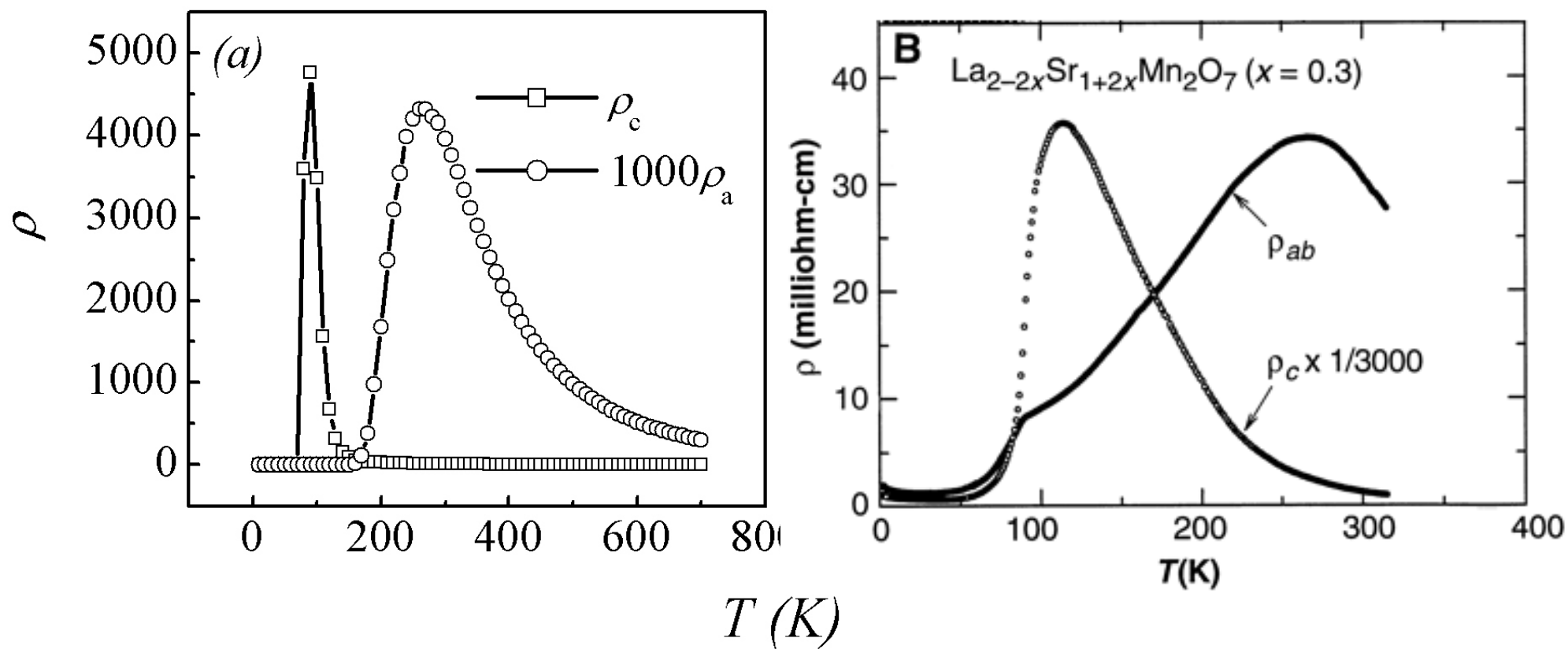
$$H_{2i} = \sum_j [-J_1(S_{i,j-1} + S_{i,j+1})S_{i,j} - J_2S_{i-1,j}S_{i,j} - J_3S_{i+1,j}S_{i,j}]$$

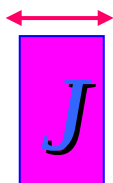




感谢Ising模型：第三类工作—庞磁电阻

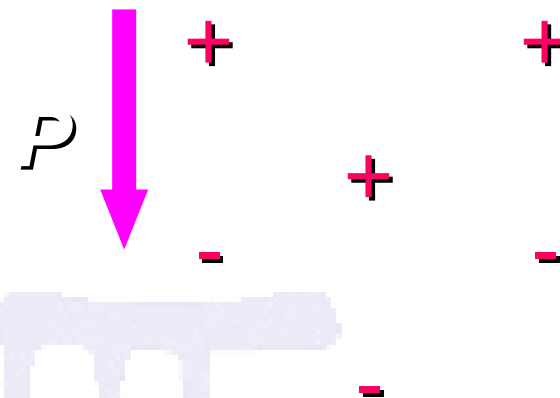
模拟结果：





感谢Ising模型：第四类工作—铁电畴长大

把Ising模型推广到实际铁电体：



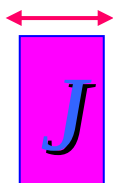
$$F = F_{ld} + F_{gr} + F_{di} + \dots$$

$$F_{ld}(\vec{P}) = A_1(P_x^2 + P_y^2) + A_{11}(P_x^4 + P_y^4) + A_{12}P_x^2P_y^2 + A_{111}(P_x^6 + P_y^6)$$

$$A_1 = \alpha(T - T_c), \quad \alpha > 0$$

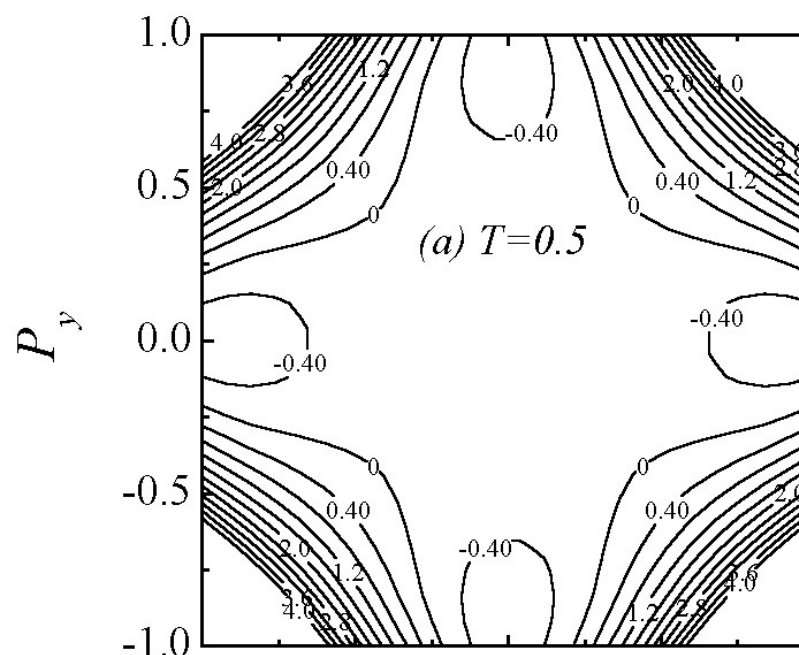
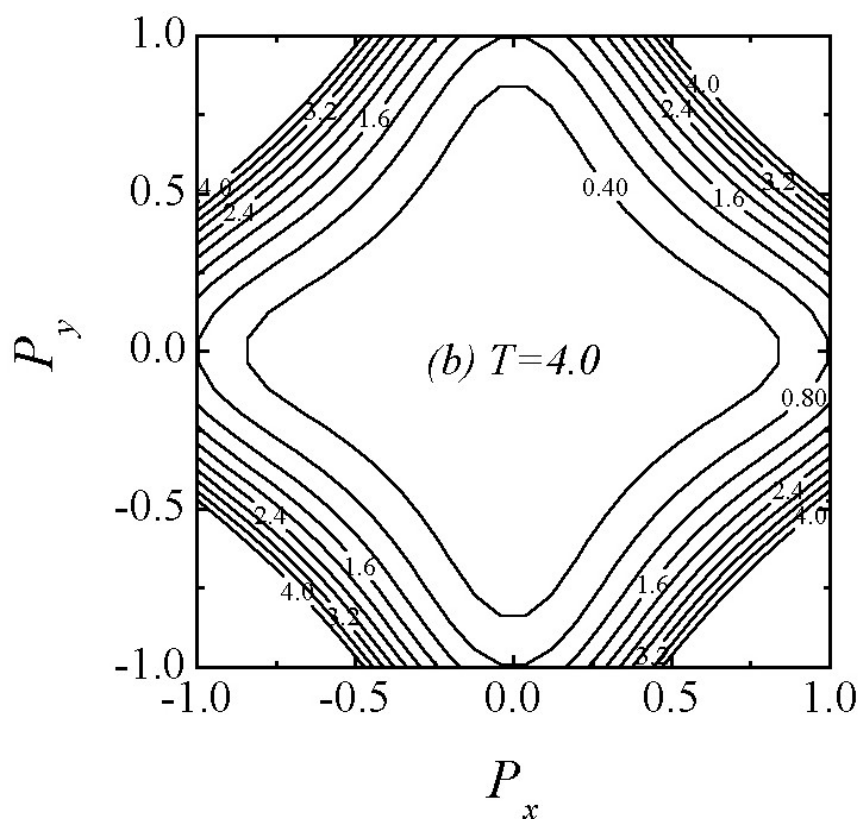
$$F_{gr}(P_{i,j}) = \frac{1}{2} \left[G_{11}(P_{x,x}^2 + P_{y,y}^2) + G_{12}P_{x,x}P_{y,y} + G_{44}(P_{x,y} + P_{y,x})^2 + G'_{44}(P_{x,y} - P_{y,x})^2 \right]$$

$$F_{di}(P_i) = \frac{1}{8\pi\epsilon_0\chi} \sum_{<j>} \left[\frac{P(r_i)P(r_j)}{|r_i - r_j|^3} - \frac{3[P(r_i)(r_i - r_j)][P(r_j)(r_i - r_j)]}{|r_i - r_j|^5} \right]$$

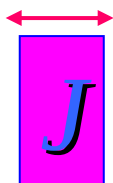


感谢Ising模型：第四类工作—铁电畴长大

每一能量项的作用：朗道项

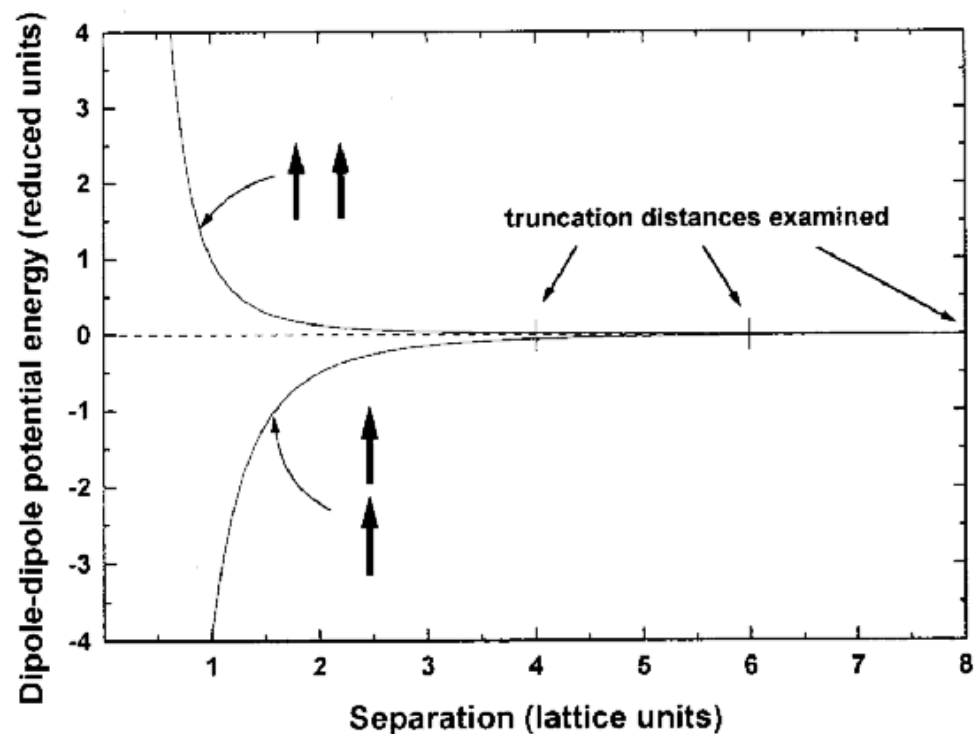
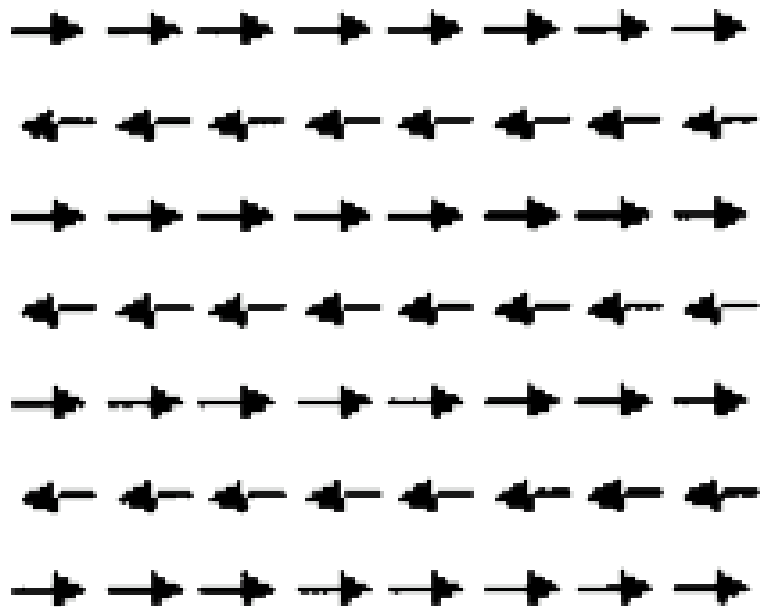


$$F_{ld}(\vec{P}) = A_1(P_x^2 + P_y^2) + A_{11}(P_x^4 + P_y^4) + A_{12}P_x^2P_y^2 + A_{111}(P_x^6 + P_y^6)$$

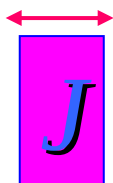


感谢Ising模型：第四类工作—铁电畴长大

每一能量项的作用：电极化能

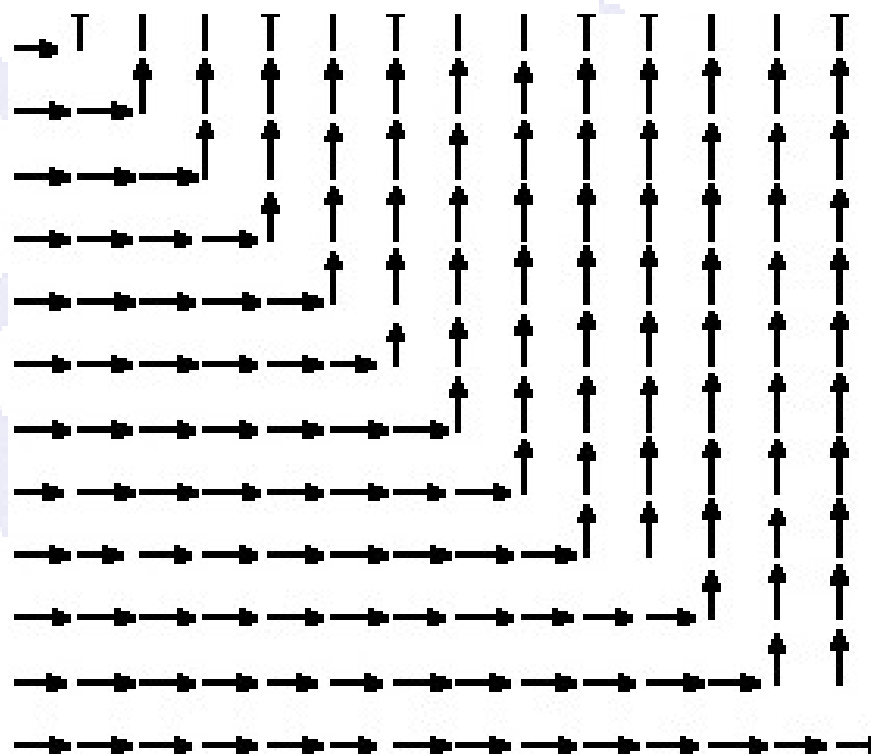


$$F_{di}(P_i) = \frac{1}{8\pi\epsilon_0\chi} \sum_{\langle j \rangle} \left[\frac{P(r_i)P(r_j)}{|r_i - r_j|^3} - \frac{3[P(r_i)(r_i - r_j)][P(r_j)(r_i - r_j)]}{|r_i - r_j|^5} \right]$$

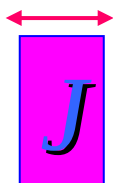


感谢Ising模型：第四类工作—铁电畴长大

每一能量项的作用：畴界能

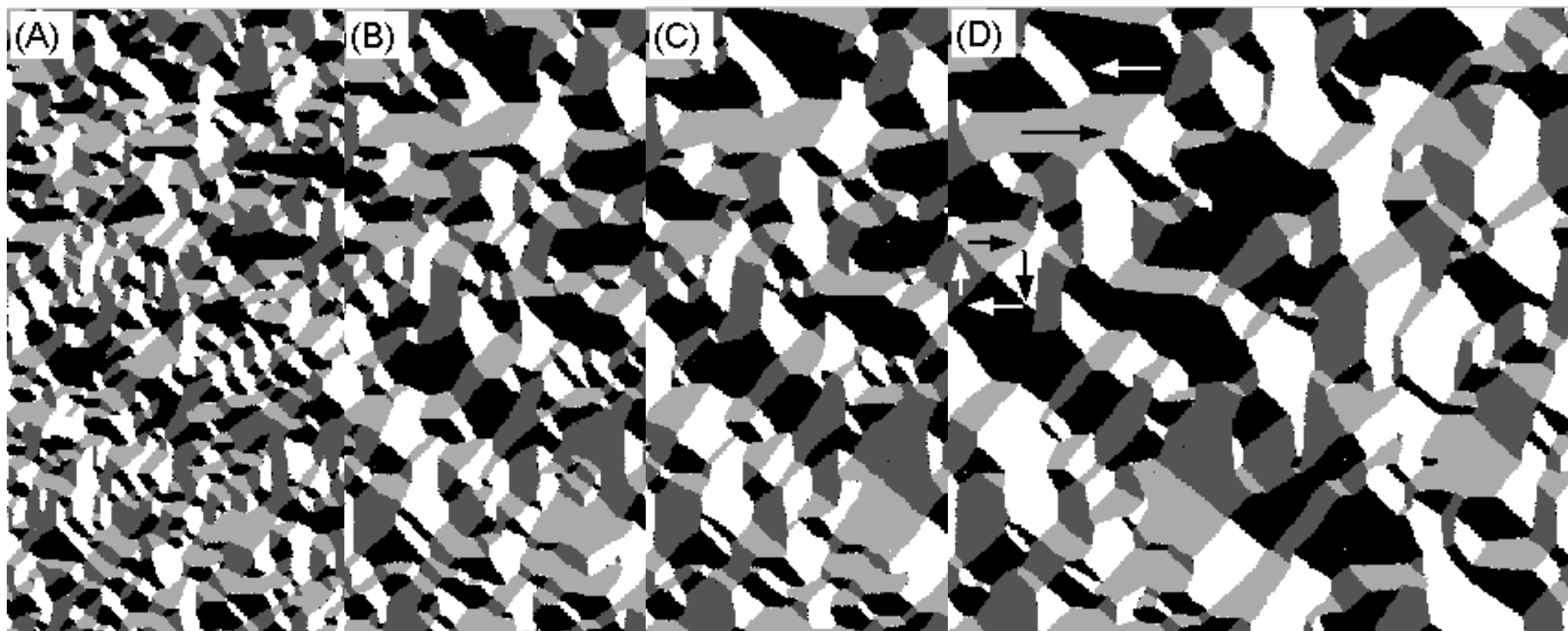


$$F_{gr}(P_{i,j}) = \frac{1}{2} \left[G_{11}(P_{x,x}^2 + P_{y,y}^2) + G_{12}P_{x,x}P_{y,y} + G_{44}(P_{x,y} + P_{y,x})^2 + G'_{44}(P_{x,y} - P_{y,x})^2 \right]$$



感谢Ising模型：第四类工作—铁电畴长大

举例：看看铁电畴演化 $T/T_c=0.5$



Publications on Ising model

PRB 58, 633 (1998)

PRB 65, 014416 (2002)

PRB 69, 094414 (2004)

PRB 70, 132403 (2004)

PRB 73, 212415 (2006)

PRB 75, 064415 (2007)

PRB 60, 7113 (1999)

PRB 66, 054416 (2002)

PRB 70, 132101 (2004)

PRB 73, 014107 (2006)

PRB 74, 134421 (2006)

APL 79, 236 (2001)

APL 86, 022501 (2005)

APL 90, 062905 (2007)

APL 81, 4014 (2002)

APL 89, 092909 (2006)



Thank you for your attention !

