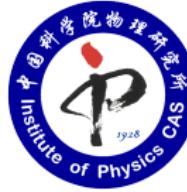


# 蒙特卡洛方法及其在磁性模型中的应用

郑睿

导师 刘邦贵研究员



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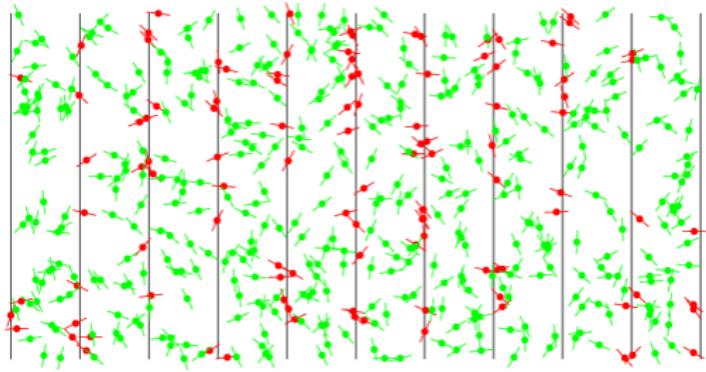
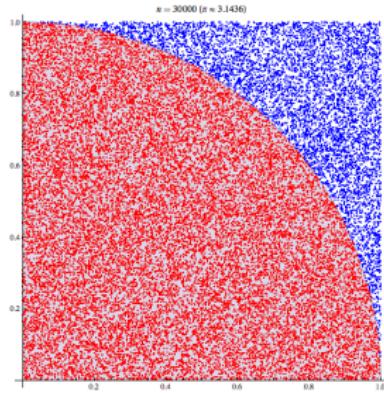
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# 数学起源

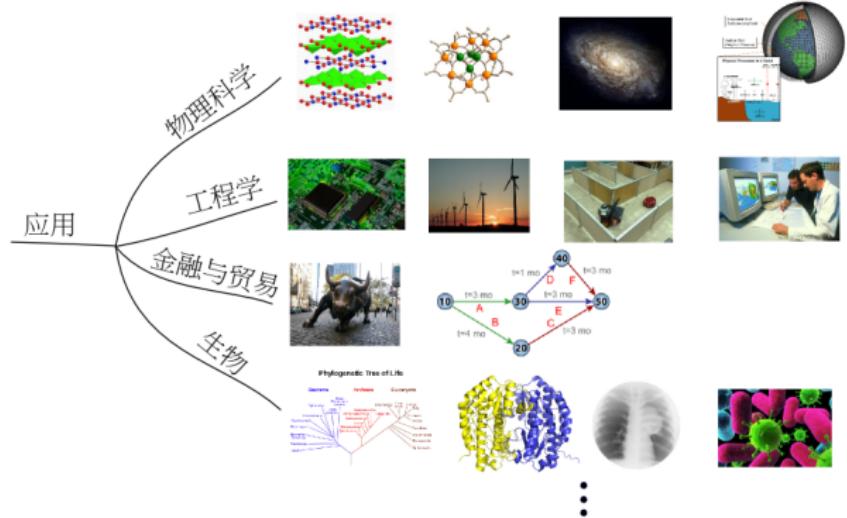
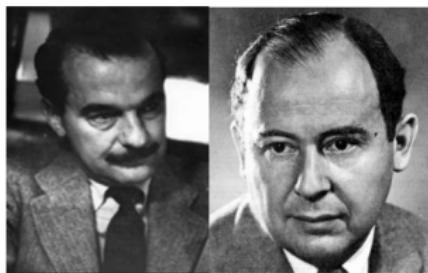
17世纪，Bernoulli提出大数定理：当试验次数足够多时，事件发生的频率无穷接近于该事件发生的概率。

$$\lim_{n \rightarrow \infty} P\left\{ \left| \frac{n_x}{n} - p \right| < \epsilon \right\} = 1$$



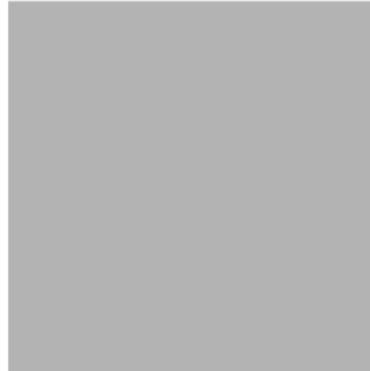
# 正式提出与发展应用

1930s Enrico Fermi, 1940s John von Neumann, Stanislaw Ulam  
和Nicholas Metropolis处理中子散射实验数据时，提出了蒙特卡洛方法。



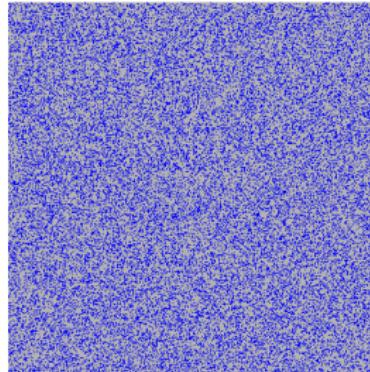
# 基本框架

- 定义一个问题所要求的输入范围(如态空间);
- 在此范围内根据某个概率分布(如玻尔兹曼分布)随机产生输入;
- 对输入进行某种运算(如计算物理量);
- 统计结果(如得到物理量平均值以及误差).



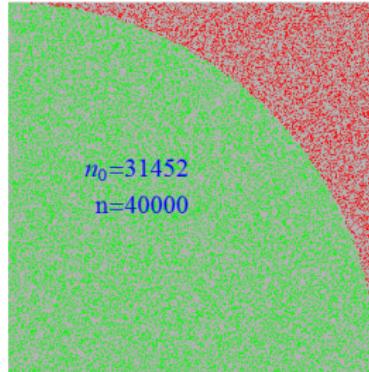
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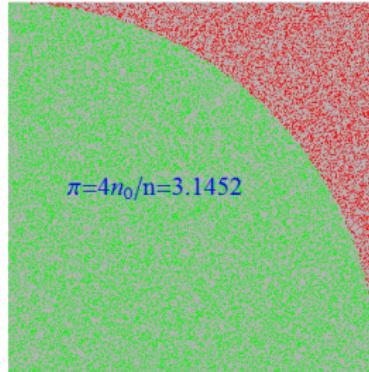
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# 基本框架

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- 统计结果(如得到物理量平均值以及误差).



# 参考文献



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*A Guide to Monte Carlo Simulations in Statistical Physics (2nd ed.).*

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M.E.J. Newman and G.T. Barkema

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## ① 简介

## ② 经典蒙特卡洛方法

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## ⑥ 价键基矢投影算法

# 理论基础

- 简单性抽样

$$y = \frac{1}{b-a} \int_a^b f(x) dx \quad y_{est} = \frac{1}{N} \sum_i f(x_i)$$

- 重要性抽样

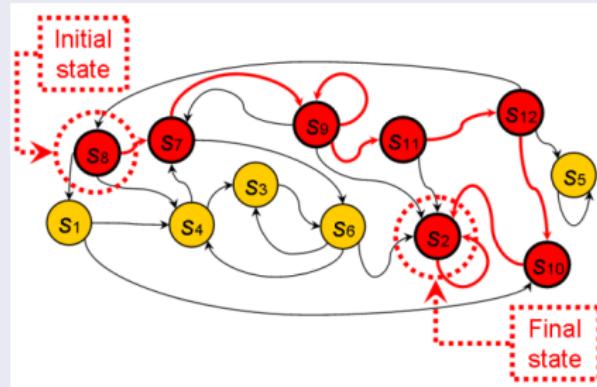
$$y = \frac{1}{b-a} \int_a^b \frac{f(x)}{p(x)} p(x) dx \quad p(x) = \frac{f'(x)}{\int_a^b f'(x) dx}$$

$$y_{est} = \frac{1}{b-a} \frac{1}{N} \sum_i O(x_i) \quad O(x) = \frac{f(x)}{p(x)}$$

$$\langle O(x) \rangle = \int_{x \in X} O(x) p(x) dx \quad \bar{O}_{est} = \frac{1}{N} \sum_i O(x_i)$$

# 重要性抽样实现方式

## Markov链与细致平衡方程

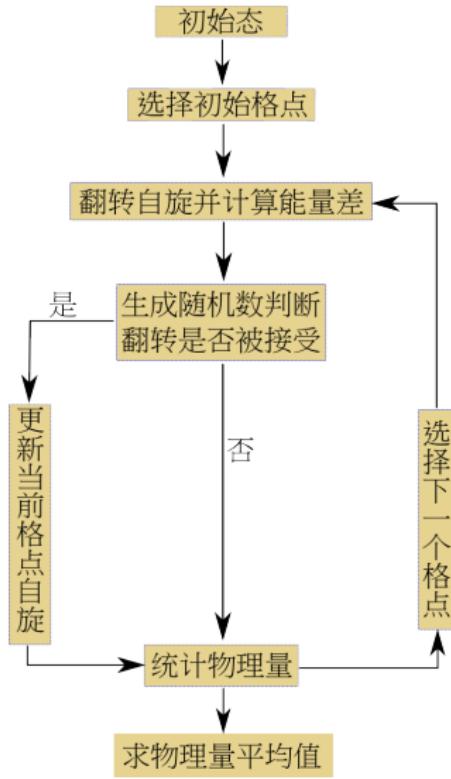


$$p(x_i)W(x_i \rightarrow x_j) = p(x_j)W(x_j \rightarrow x_i)$$

$$W(x_i \rightarrow x_j) = \begin{cases} \frac{1}{\tau_0} \exp(-\frac{\delta H}{k_B T}) & \delta H > 0 \\ \frac{1}{\tau_0} & otherwise \end{cases}$$

$$W(x_i \rightarrow x_j) = \frac{1}{2\tau_0} [1 - \tanh(\frac{\delta H}{2k_B T})]$$

# 局域Metropolis翻转方式



# 动态关联与临界减速

Markov链统计误差:

$$\langle(\delta O)^2\rangle = \frac{1}{N}[\langle O^2 \rangle - \langle O \rangle^2](1 + 2\frac{\tau_O}{\delta t})$$

$\delta t \ll \tau_O$ 时

$$\langle(\delta O)^2\rangle = 2\frac{\tau_O}{\tau_{obs}}[\langle O^2 \rangle - \langle O \rangle^2]$$

相变点附近

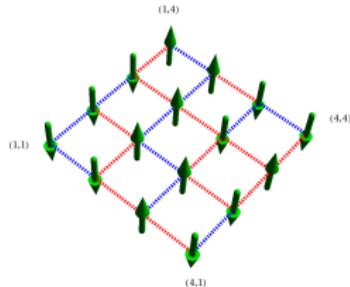
$$\tau \propto \xi^z \propto |1 - T/T_c|^{-\nu z}$$

Table: Ising模型不同算法所对应的动力学指数 $z$ 比较

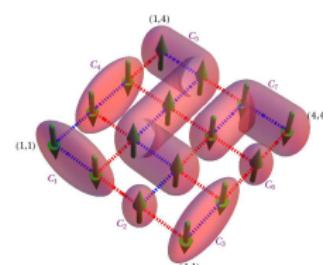
dimension d	Metropolis	Wolff	Swendsen Wang
2	$2.167 \pm 0.001$	$0.25 \pm 0.01$	$0.25 \pm 0.01$
3	$2.02 \pm 0.02$	$0.33 \pm 0.01$	$0.54 \pm 0.02$
4	-	$0.25 \pm 0.01$	$0.86 \pm 0.02$

# Swendsen-Wang 算法

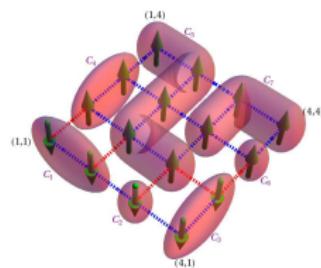
自旋相反不成键，自旋相同以概率 $p = 1 - \exp(-2\beta J)$ 成键



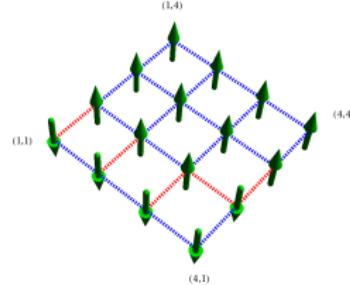
(a) 当前态 $|S\rangle$



(b) 长完团簇 $|(S, C)\rangle$



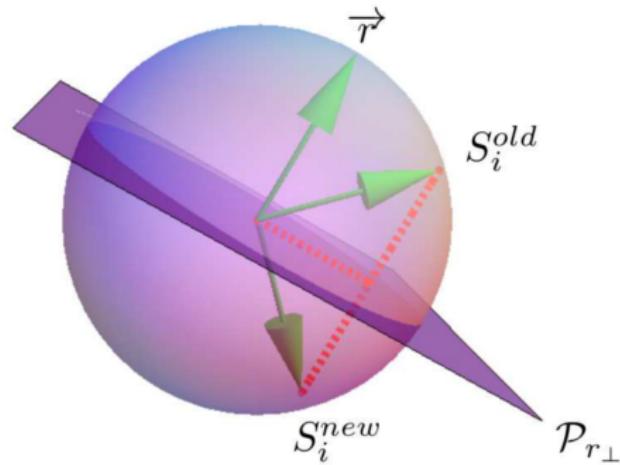
(c) 翻转团簇 $|(S', C)\rangle$



(d) 新态 $|S'\rangle$

# Wolff算法

对经典Heisenberg模型，定义一种广义自旋翻转操作：

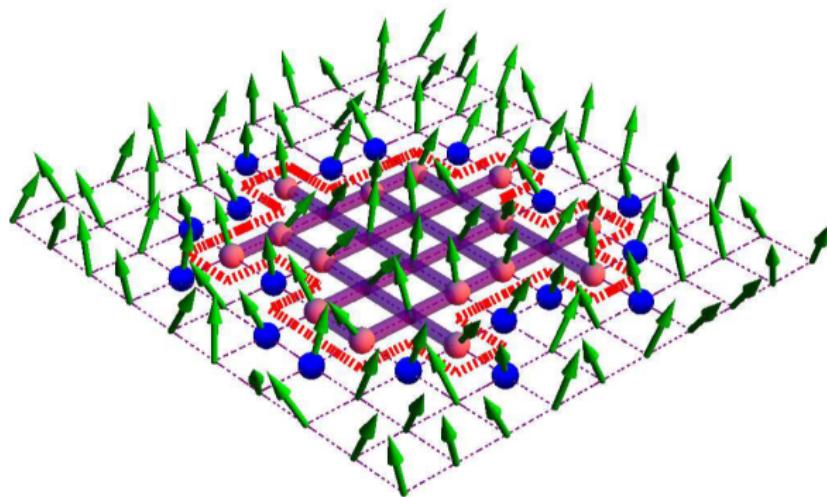


$$S_i^{old} \rightarrow S_i^{new} = R(\vec{r}') S_i^{old} = S_i^{old} - 2(S_i^{old} \cdot \vec{r}') \vec{r}'$$

# Wolff算法

成键概率:

$$p(S_i^{new}, S_j) = 1 - \exp\{\min[0, \beta J S_i^{new} \cdot [1 - R(\vec{r})] S_j]\}$$



# 物理量统计方式

## 自旋表象

$$C = \frac{1}{N} \frac{\partial \langle H \rangle}{\partial T} = \frac{1}{Nk_B T^2} (\langle H^2 \rangle - \langle H \rangle^2)$$

$$\chi = \frac{1}{N} \lim_{H \rightarrow 0} \frac{\partial \langle m \rangle}{\partial H} = \frac{N}{k_B T} (\langle M^2 \rangle - \langle M \rangle^2)$$

## 团簇表象(improved estimator)

- 多团簇Swendsen-Wang算法

$$\langle M^2 \rangle = \frac{1}{N^2} \sum_{i,j} \langle \sigma_i \sigma_j \rangle = \frac{1}{N^2} \sum_c \langle V_c^2 \rangle$$

- 单团簇Wolff算法

$$\langle V_c \rangle = \left\langle \frac{V_c}{N} V_c \right\rangle = \frac{1}{N} \langle V_c^2 \rangle$$

$$\langle M^2 \rangle = \langle V_c \rangle / N$$

# 临界性质

## 临界关系

$$M \propto t^\beta \quad \chi \propto t^{-\gamma} \quad C \propto t^{-\alpha} \quad \xi \propto t^{-\nu}$$

## 有限尺度效应

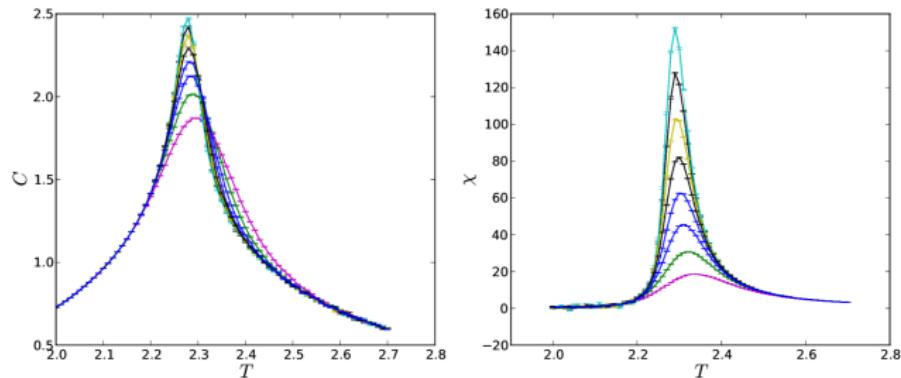


Figure: 二维Ising模型的比热 $c_v$ 与磁化率 $\chi$ (尺寸 $L$ 从30到100)

# 有限尺寸标度分析

## 标度关系

定义磁四极矩(binder cumulant)

$$U_4 = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}$$

在临界点附近

$$M_L(t) = L^{-\beta/\nu} G_M(tL^{1/\nu})$$

$$\chi_L(t) = L^{\gamma/\nu} G_\chi(tL^{1/\nu})$$

$$C_L(t) = L^{\alpha/\nu} G_C(tL^{1/\nu})$$

$$\xi_L(t) = LG_\xi(tL^{1/\nu})$$

$$U_{4L}(t) = G_{U_4}(tL^{1/\nu})$$

# 有限尺寸标度分析

## 确定相变点

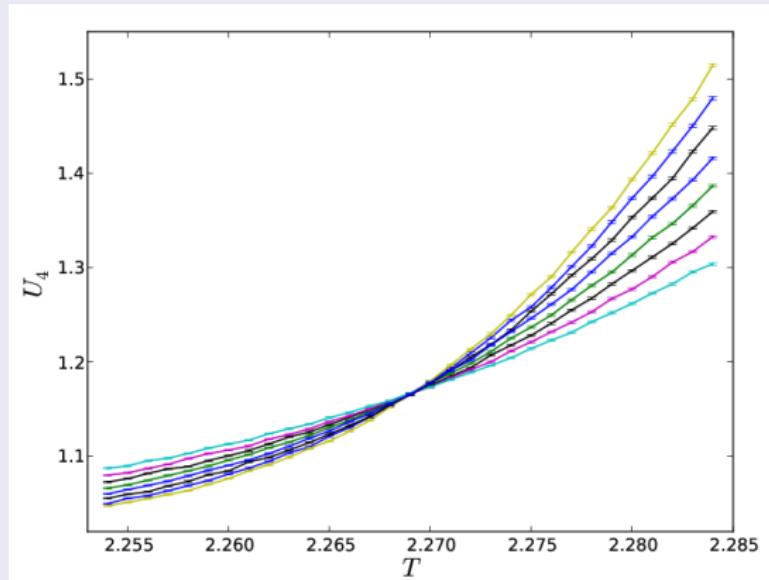


Figure: 利用磁四极矩得到二维Ising模型相变点(尺寸 $L$ 从70到140)

# 有限尺寸标度分析

## 确定临界指数

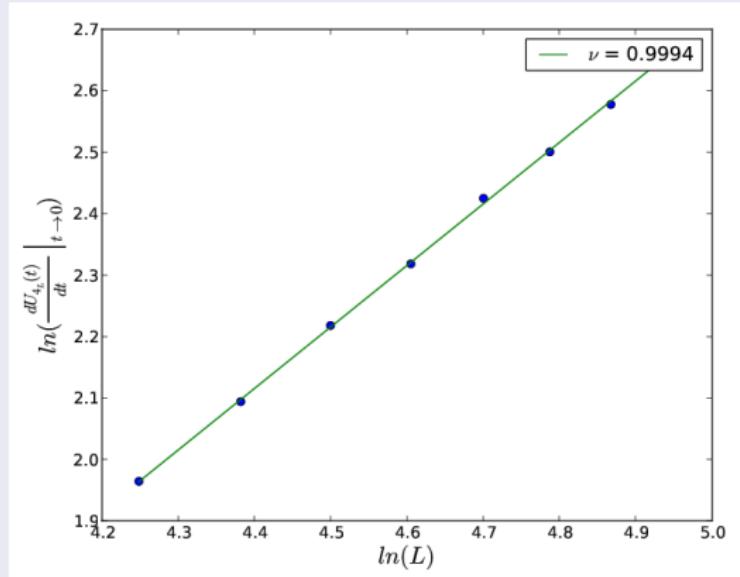


Figure: 利用相变点处磁四极矩对L的导数得到 $\nu$

# 有限尺寸标度分析

## 确定临界指数

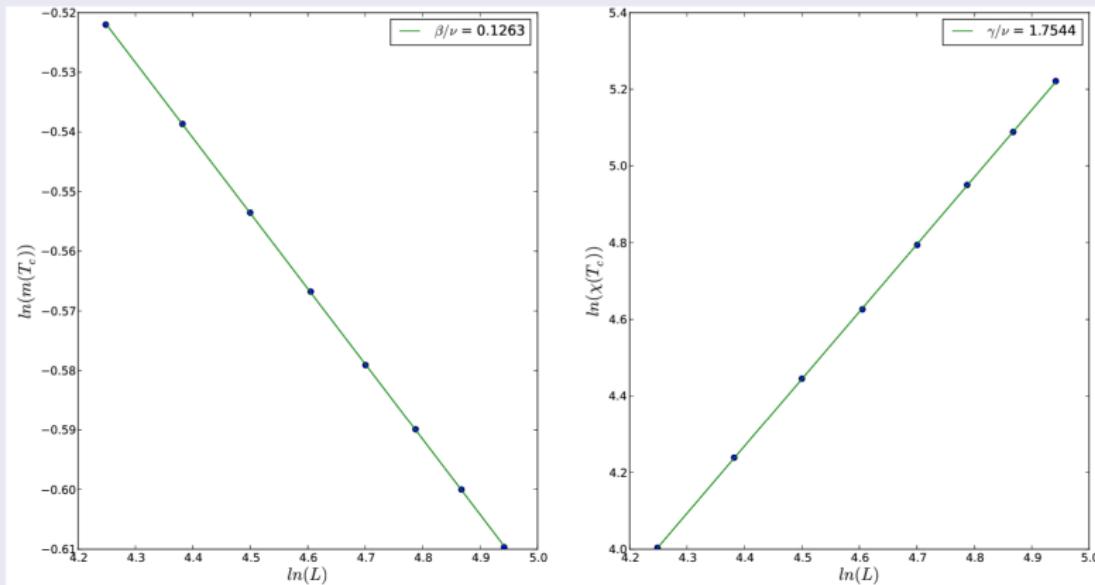


Figure: 利用相变点处相关物理量得到 $\beta/\nu$ 和 $\gamma/\nu$

# 有限尺寸标度分析

## 数据坍缩

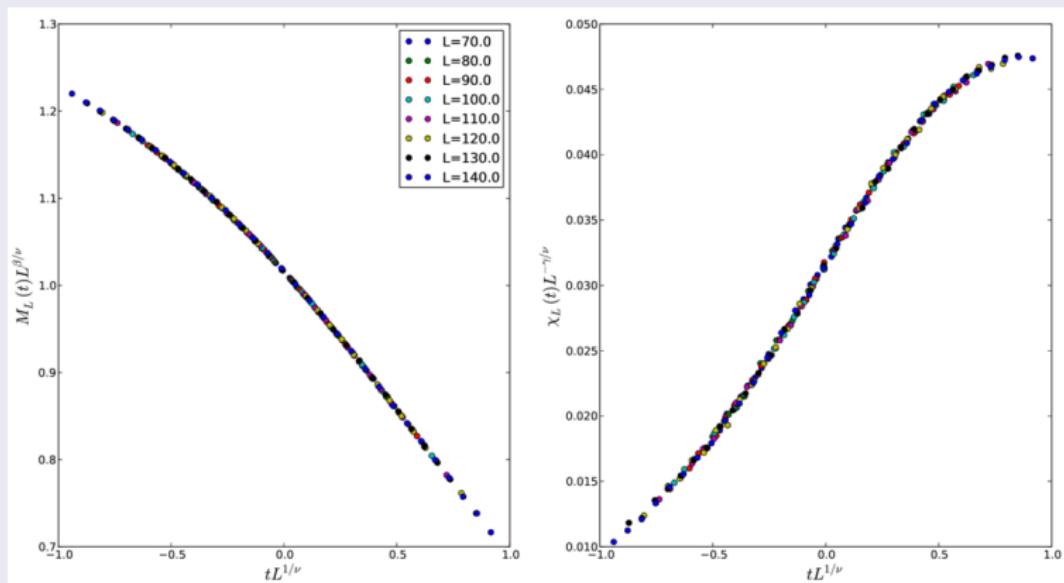
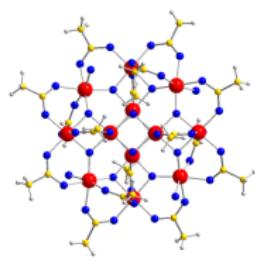


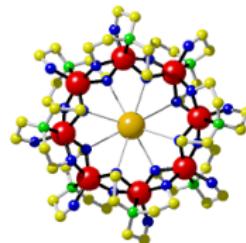
Figure: 磁化强度与磁化率的数据坍缩图

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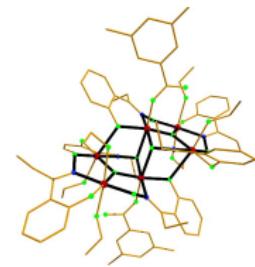
# 分子磁体



$Mn_{12}$



$Fe_8$



$Mn_6$

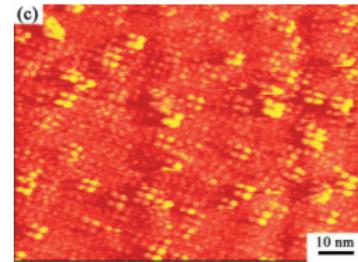
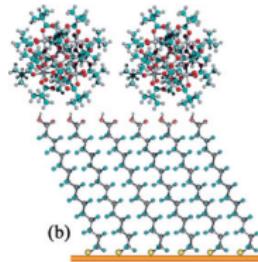
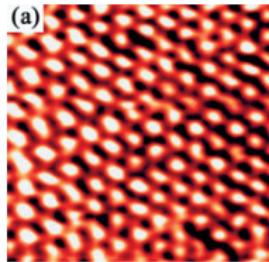


Figure:  $Au(111)$ 面上  $Mn_{12}Piv_{16}$  单层膜的STM图像(Adv.Mater. 17, 1612)

# 自旋模型

大自旋→视为经典自旋模型

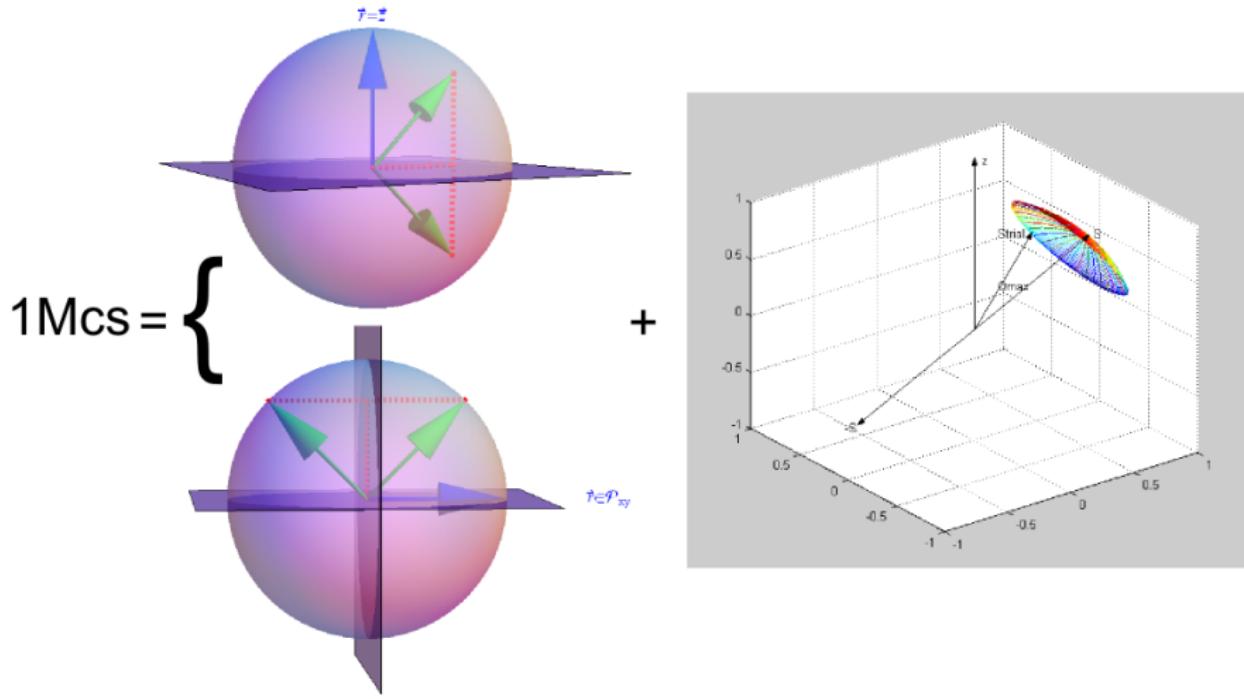
$$H = -K \sum_i (S_i^z)^2 - \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

物理量

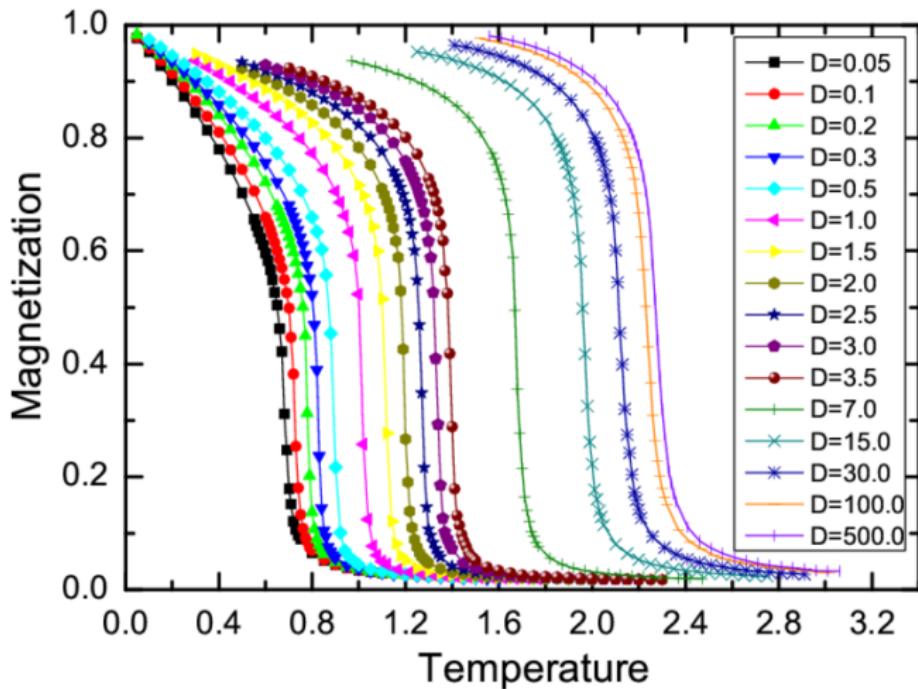
$$\begin{cases} M = \langle |\vec{s}| \rangle \\ U_4 = 1 - \langle \vec{s}^4 \rangle / (3 \langle \vec{s} \rangle^2) \\ C_\nu = (\langle H^2 \rangle - \langle H \rangle^2) / T^2 \\ \chi = (\langle \vec{s}^2 \rangle - \langle |\vec{s}| \rangle^2) / T \end{cases}$$

# 模拟细节

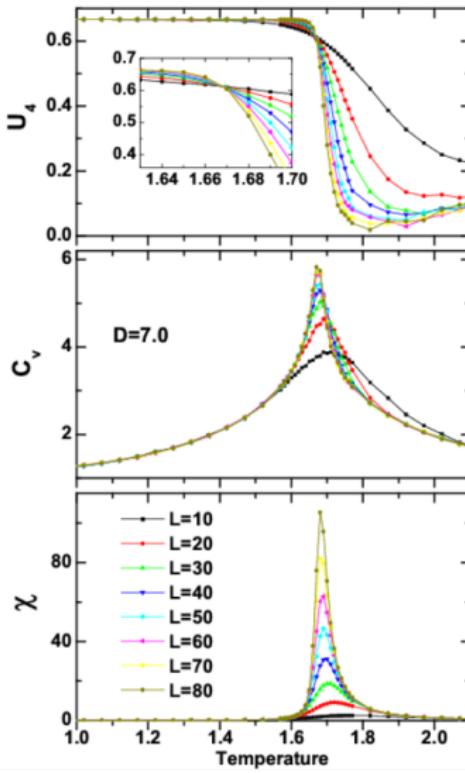
令  $k_B = 1$ ,  $D = K/J$  衡量单轴各向异性强度,  $1\text{bin} = 50000\text{Mcs}$ , 10 bins



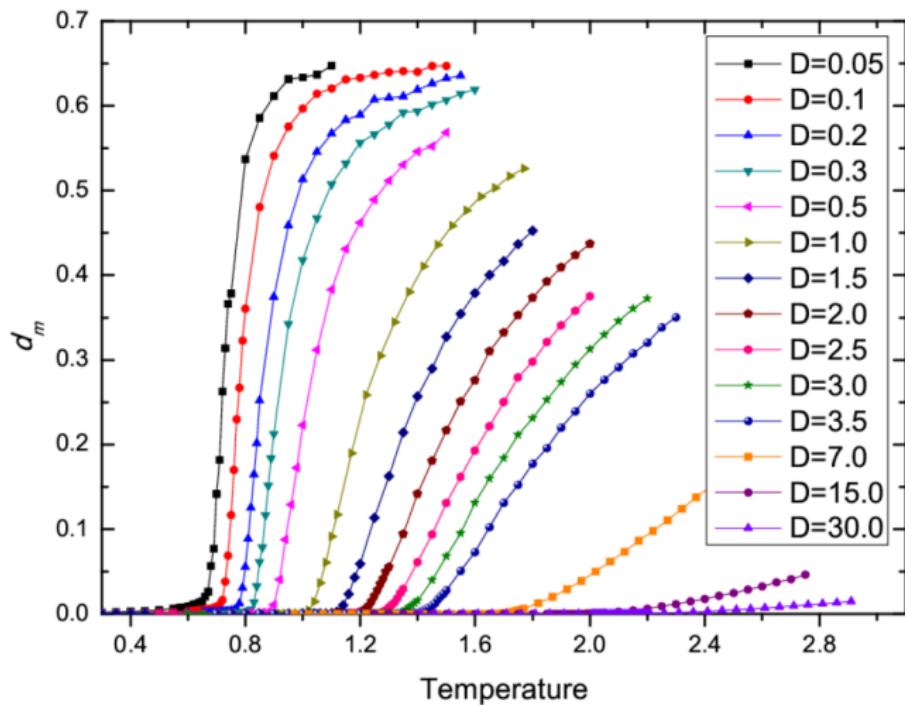
# 模拟结果



# 模拟结果

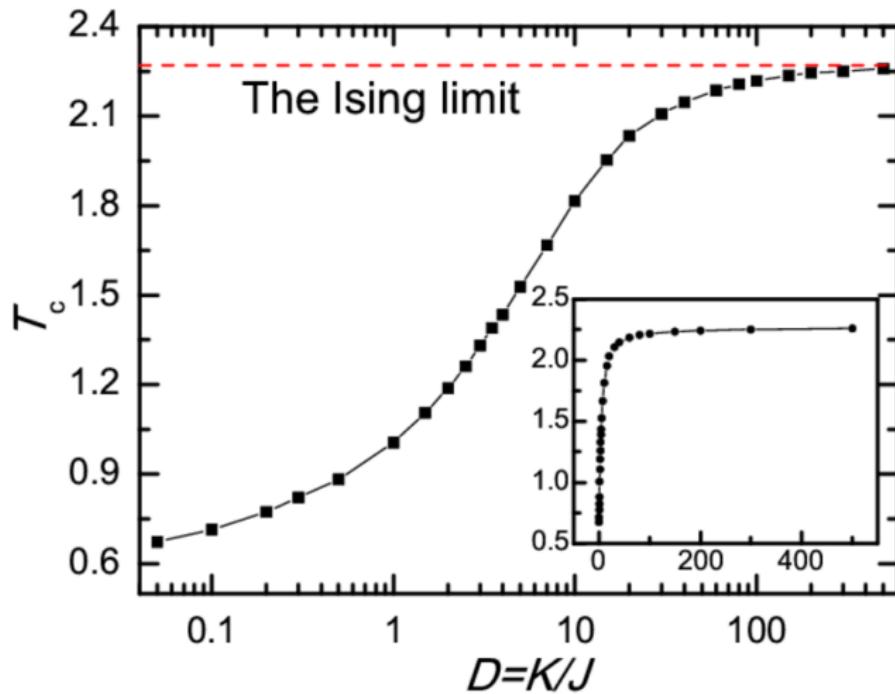


# 模拟结果



$$d_m = 1 - \langle (s^z)^2 \rangle / \langle \vec{s}^2 \rangle$$

# 模拟结果



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# 理论基础

## 配分函数的路径积分形式

- 经典

$$Z = \sum_x e^{-\beta E(x)}$$

- 量子

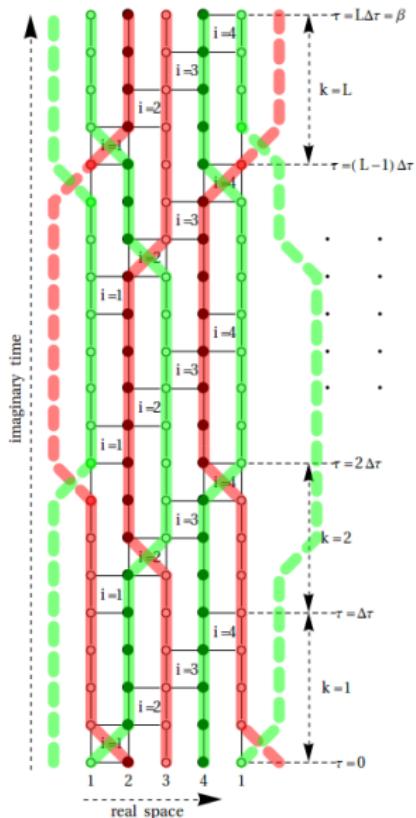
$$Z = Tr\{e^{-\beta H}\} = \sum_{\alpha} \langle \alpha | e^{-\beta H} | \alpha \rangle$$

$$H = \sum_{i=1}^M H_i$$

$$e^{-\beta H} = \lim_{L \rightarrow \infty} [\prod_{i=1}^M e^{-\Delta \tau H_i}]^L = \lim_{L \rightarrow \infty} \prod_{k=1}^L \prod_{i=1}^M e^{-\Delta \tau H_i}$$

$$Z = \lim_{L \rightarrow \infty} \sum_{\{\psi_i(k)\}} \prod_{k=1}^L \prod_{i=1}^M \langle \psi_{i+1}(k) | e^{-\Delta \tau H_i} | \psi_i(k) \rangle$$

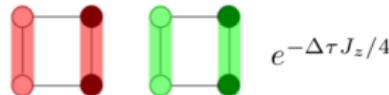
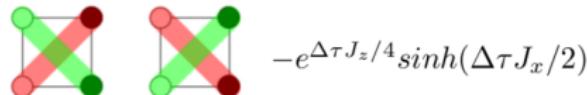
# 世界线组态



# 方块权重

对于 $XXZ$ 模型

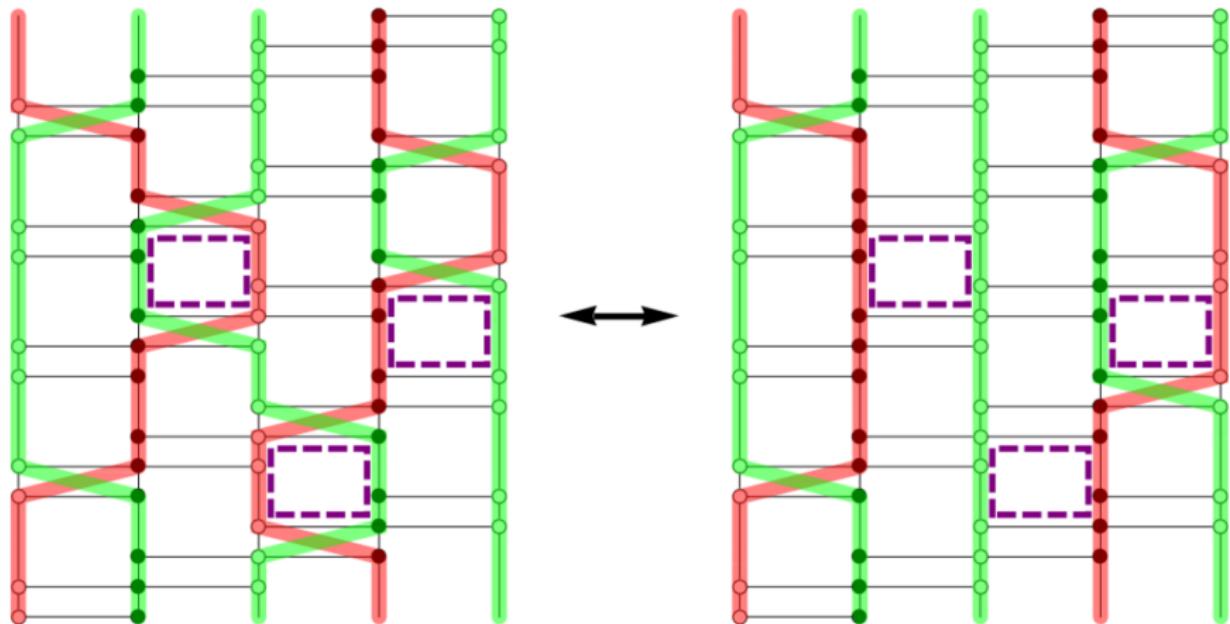
$$H_{two\ sites} = J_x(S_1^x S_2^x + S_1^y S_2^y) + J_z S_1^z S_2^z = \frac{J_x}{2}(S_1^+ S_2^- + S_1^- S_2^+) + J_z S_1^z S_2^z$$



## 符号问题

$$\langle A \rangle = \frac{\langle sign[W(\{\psi_i(k)\})]A(\{\psi_i(k)\}) \rangle_{|W|}}{\langle sign[W(\{\psi_i(k)\})] \rangle_{|W|}}$$

# 局域更新方式

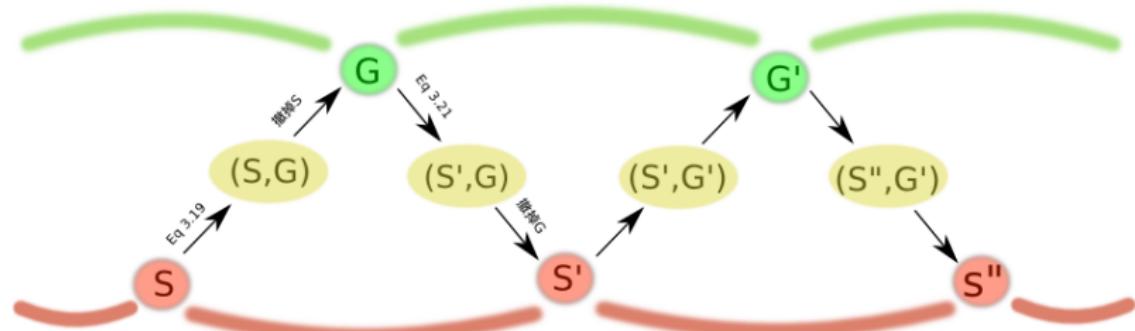


# 对偶蒙特卡洛方法

$$W(S) = \exp(K \sum_{\langle i,j \rangle} \sigma_i \sigma_j) = \prod_u w(S_u) \quad w(S_u) = \sum_{G_u} w(S_u, G_u)$$

$$W(S) = \sum_G W(S, G) \quad W(G) = \sum_S W(S, G) \quad W(S, G) = \prod_u w(S_u, G_u)$$

$$T(S \rightarrow (S, G)) = \frac{W(S, G)}{W(S)} \quad T(G \rightarrow (S, G)) = \frac{W(S, G)}{W(G)}$$



# 方块权重的图形分解

Fortuin-Kasteleyn theorem

$$w(S_u, G_u) = \begin{cases} e^{-K} & (G_u = 0) \\ e^K - e^{-K} & (\sigma_i = \sigma_j \text{ and } G_u = 1) \\ 0 & (\sigma_i \neq \sigma_j \text{ and } G_u = 1) \end{cases}$$

$$\begin{aligned} \langle \Omega_1 | w(S_u) | \Omega_2 \rangle &= \begin{pmatrix} e^K & e^{-K} \\ e^{-K} & e^K \end{pmatrix} \\ &= e^{-K} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + (e^K - e^{-K}) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ &= w(S_u, G_u = 0) \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + w(S_u, G_u = 1) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ &= w(S_u, G_u = 0) \hat{G}_0 + w(S_u, G_u = 1) \hat{G}_1 \end{aligned}$$

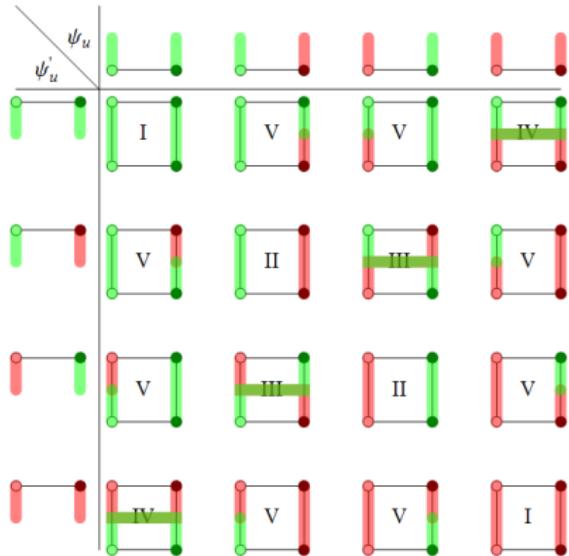
# 方块权重的图形分解

对于XXZ模型

$$H_{i,j} = -J(S_i^x S_j^x + S_i^y S_j^y + (\frac{1}{4} - S_i^z S_j^z))$$

$$\begin{aligned} w(S_u) &= \langle \psi'_u | 1 - \Delta\tau H_u | \psi_u \rangle \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 + \frac{J\Delta\tau}{2} & \frac{J\Delta\tau}{2} & 0 \\ 0 & \frac{J\Delta\tau}{2} & 1 + \frac{J\Delta\tau}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + \frac{J\Delta\tau}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ &= \hat{g}_V + \frac{J\Delta\tau}{2} \hat{g}_H \end{aligned}$$

# 可能的方块及分解方式



$$\hat{g}_C \begin{array}{c} \diagup \\ \diagdown \end{array} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{array}{c} \diagdown \\ \diagup \end{array} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

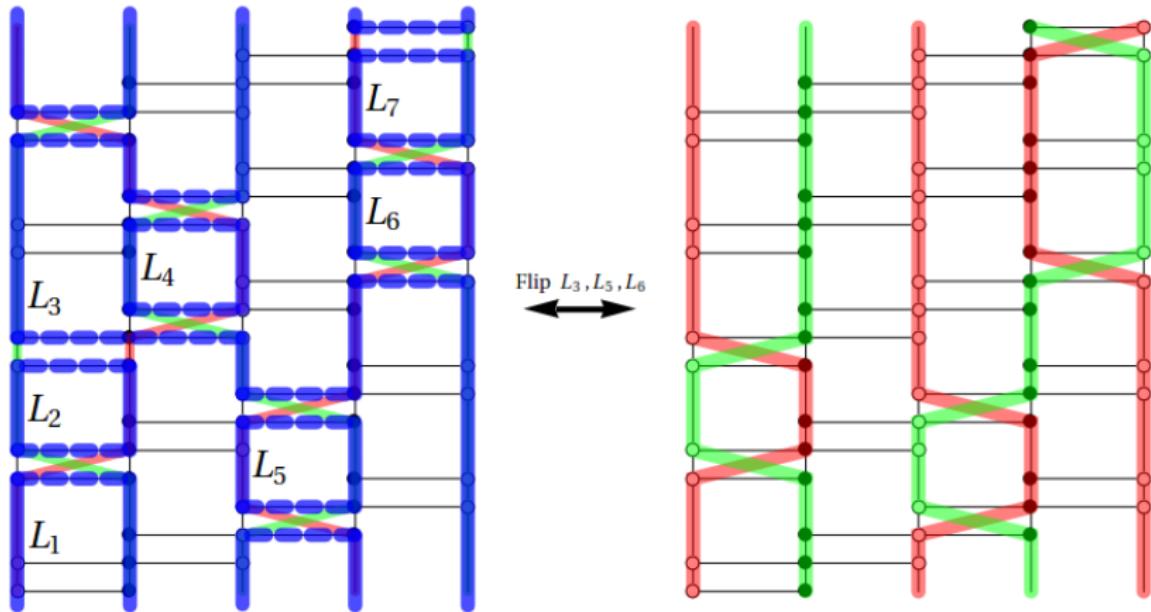
$$\hat{g}_H \begin{array}{c} \square \\ \square \end{array} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \begin{array}{c} \square \\ \square \end{array} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\hat{g}_B \begin{array}{c} \diagup \\ \diagdown \end{array} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{array}{c} \diagdown \\ \diagup \end{array} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$H_{ij} = \sum_{\hat{g}} H_{ij}(\hat{g}) = \sum_{\hat{g}} -a(\hat{g})\hat{g}$$

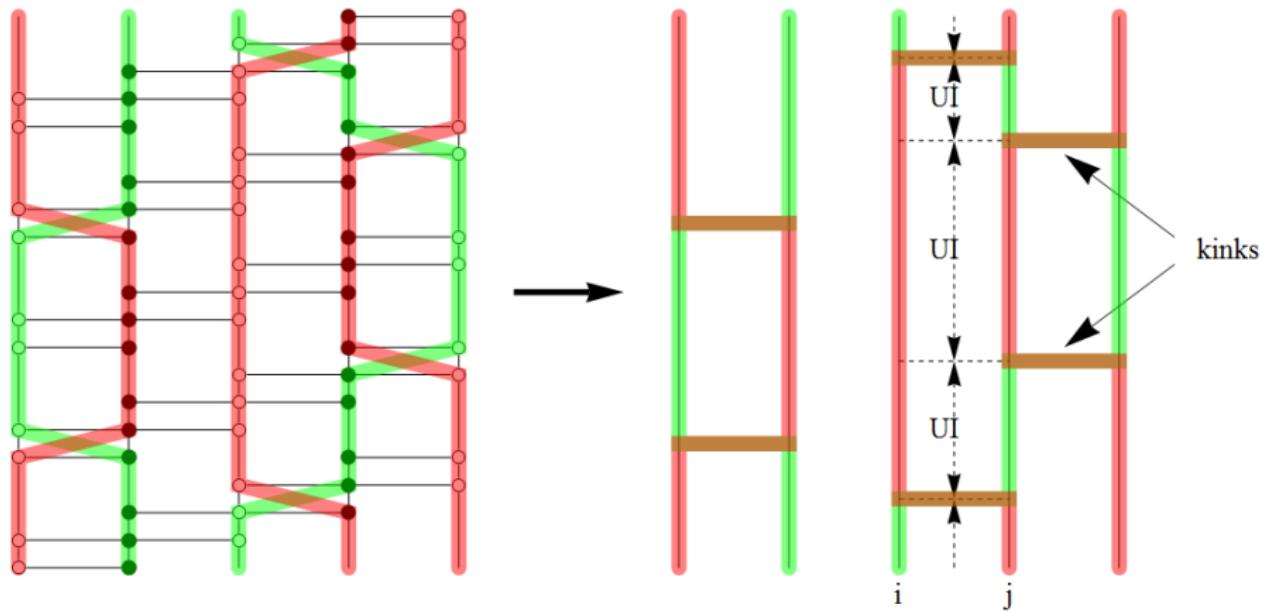
$$1 - \Delta\tau H_{ij} = \hat{g}_V + \sum_{\hat{g}} a(\hat{g})\Delta\tau\hat{g}$$

# 环算法



# 连续时间极限

粗粒化



# 生成泊松分布

考虑虚时长度为I的稳定间隔，其中的 $I/\Delta\tau$ 个重复方块分裂后有 $n$ 个 $g$ 图样的概率为

$$C_{I/\Delta\tau}^n ((\Delta\tau)a(g))^n (1 - (\Delta\tau)a(g))^{I/(\Delta\tau)-n}$$

当 $\Delta\tau \rightarrow 0$

$$\frac{1}{n!} (Ia(g))^n e^{-Ia(g)}$$

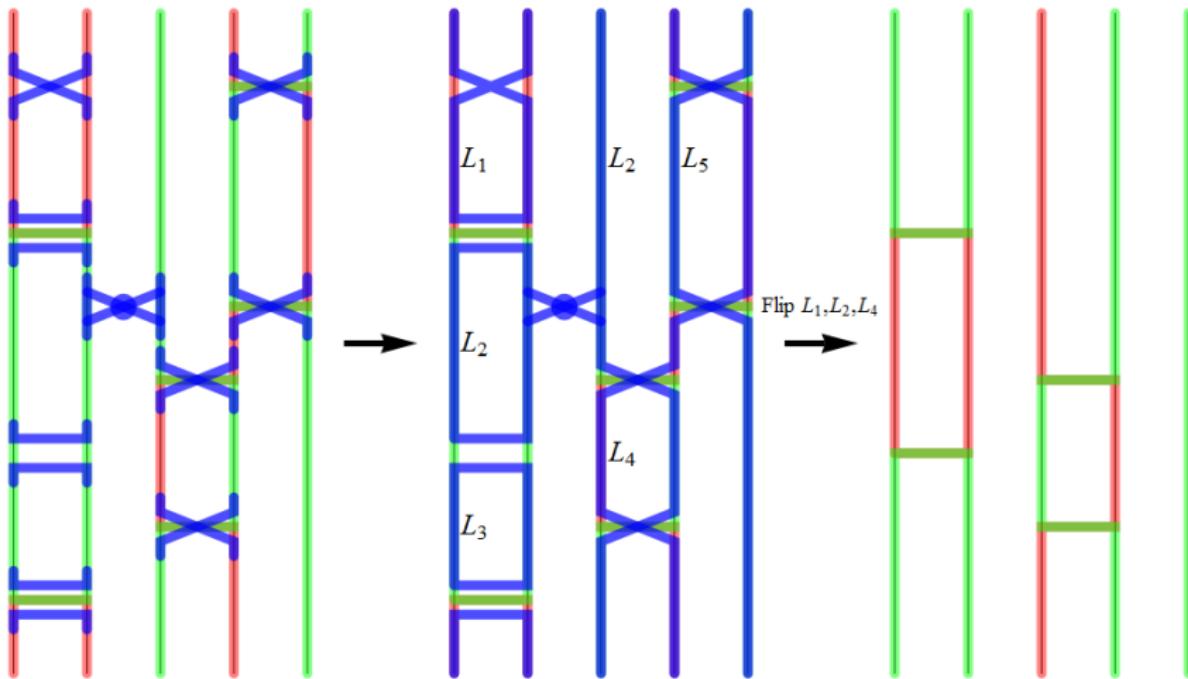
$P(t)$ 表示两个相邻事件发生的时间间隔为 $t$ 的概率密度函数

$$P(t) = a(g)e^{-a(g)t}$$

$$\int_0^t P(t)dt = 1 - e^{-a(g)t}$$

$-\ln(r)/a(g)$ 即为满足所要求泊松分布的时间间隔

# 连续时间极限环算法



# 物理量统计方式

S表象

$$\langle O \rangle = Tr(e^{-\beta H} O) / Z = \sum_S \frac{W(S)}{Z} \frac{\langle \psi'_u | O | \psi_u \rangle}{\langle \psi'_u | 1 - \Delta\tau H_u | \psi_u \rangle}$$

$$O(S) = \frac{1}{\beta/\Delta\tau} \sum_u \frac{\langle \psi'_u | O | \psi_u \rangle}{\langle \psi'_u | 1 - \Delta\tau H_u | \psi_u \rangle} = \frac{1}{\beta} \sum_u O(S_u)$$

$$O(S_u) = \frac{\langle \psi'_u | \Delta\tau O | \psi_u \rangle}{\langle \psi'_u | 1 - \Delta\tau H_u | \psi_u \rangle} = \begin{cases} \Delta\tau \langle \psi_u | O | \psi_u \rangle & (\psi_u = \psi'_u) \\ \frac{\langle \psi'_u | O | \psi_u \rangle}{\langle \psi'_u | -H_u | \psi_u \rangle} & (\psi_u \neq \psi'_u) \end{cases}$$

$$H(S) = H^{diag}(S) - \frac{1}{\beta} n_{kink}(S)$$

$$C = \beta^2 [\langle H_{diag}^2(S) \rangle - \langle H_{diag}(S) \rangle^2] + \langle n_{kink}^2 \rangle - \langle n_{kink} \rangle^2 - \langle n_{kink} \rangle$$

# 物理量统计方式

G表象

$$O(G) = \sum_S W(S, G) O(S) / W(G)$$

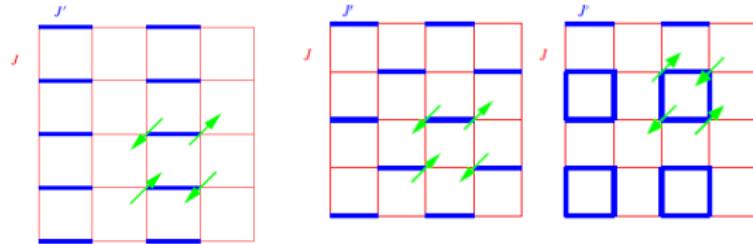
$$\chi_{zz}(S) = N^{-1} \int_0^\beta d\tau \langle M_z(\tau) M_z(0) \rangle = (N\beta)^{-1} (\int dX S^z(X))^2$$

$$\chi_{zz}(G) = (N\beta)^{-1} \sum_l (m_l)^2$$

$$\chi_{xx}(G) = \frac{1}{4N\beta} \sum_l (V_l)^2$$

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# VBS-Neel相变



$$J\text{-Q模型: } H = J \sum_{\langle ij \rangle} S_i \cdot S_j - Q \sum_{\langle i j k l \rangle} (S_i \cdot S_j - \frac{1}{4})(S_k \cdot S_l - \frac{1}{4})$$

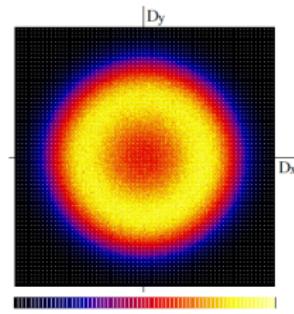


Figure: A.W. Sandvik, PRL 98, 227202 (2007)

# 非常规相变点

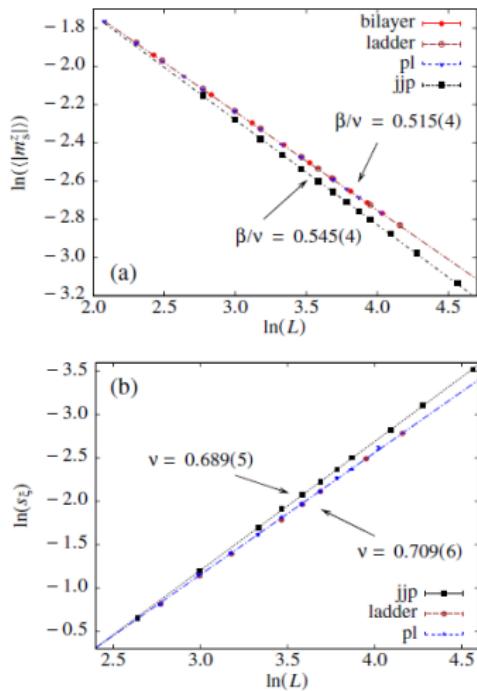
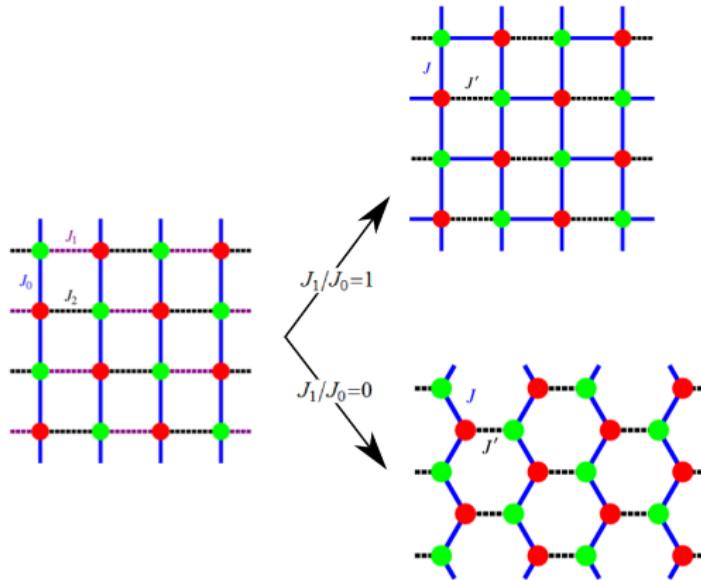


Figure: S. Wenzel, PRL 101, 127202 (2008)

# $J_0 - J_1 - J_2$ 模型

$$H = J_0 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_1 \sum_{\langle i,j \rangle'} S_i \cdot S_j + J_2 \sum_{\langle i,j \rangle''} S_i \cdot S_j$$



# 模拟细节

$$m_s = \frac{1}{N} \sum_i^N (-1)^{x_i + y_i} S_i$$

$$Q_2 = \frac{\langle (M_s^z)^4 \rangle}{\langle (M_s^z)^2 \rangle^2}$$

$$\rho_s = \frac{3}{4\beta N} \langle W_x^2 + W_y^2 \rangle$$

标度关系

$$\mathcal{O}_L(t) = L^{\lambda/\nu} [1 + c(tL^{1/\nu})L^{-\omega}] g_{\mathcal{O}}(tL^{1/\nu})$$

$$Q_2, \rho_s L : \lambda = 0 \quad |m_s^z| : \lambda/\nu \rightarrow -\beta/\nu \quad L^2 m_s^2 : \lambda/\nu \rightarrow d - z - \eta$$

$c(x)$ 可近似为常数

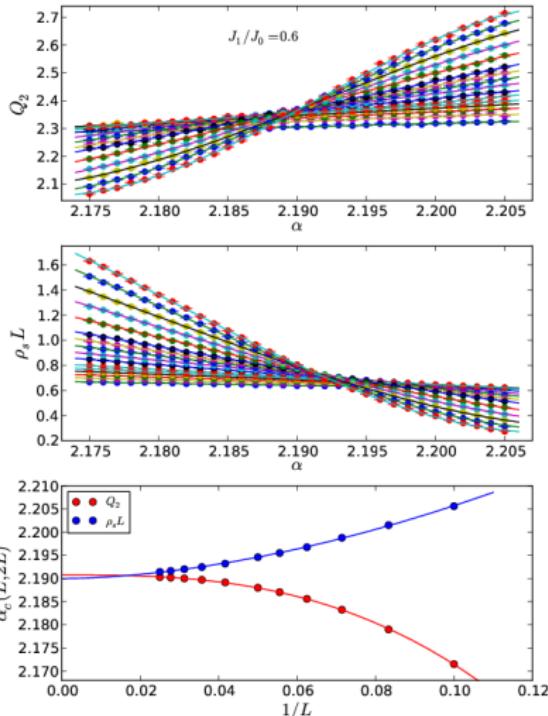
$$\mathcal{O}_L(t) = L^{\lambda/\nu} (1 + cL^{-\omega}) g_{\mathcal{O}}(x)$$

Taylor展开

$$\mathcal{O}_L(t) = L^{\lambda/\nu} (1 + cL^{-\omega}) (g_0 + g_1 x + g_2 x^2 + g_3 x^3 + g_4 x^4 + \dots)$$

# 确定临界耦合强度 $\alpha_c$ ( $\alpha = J_2/J_0$ )

$$\alpha_c(L, 2L) = \alpha_c + \frac{b}{L^{1/\nu+\omega}}$$

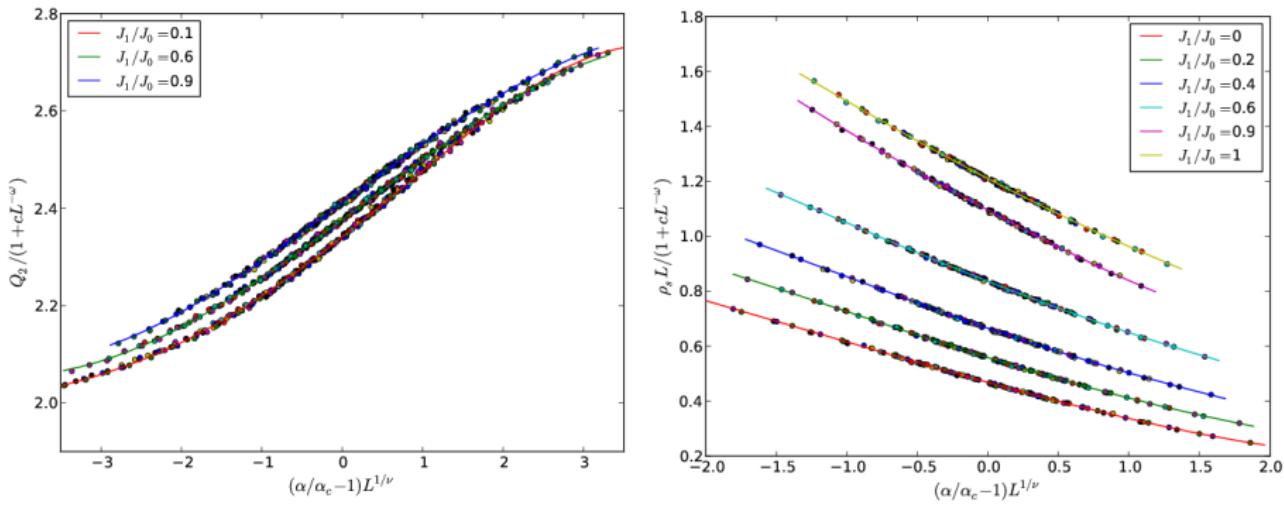


# 拟合结果 $\alpha_c$ 与 $\nu$

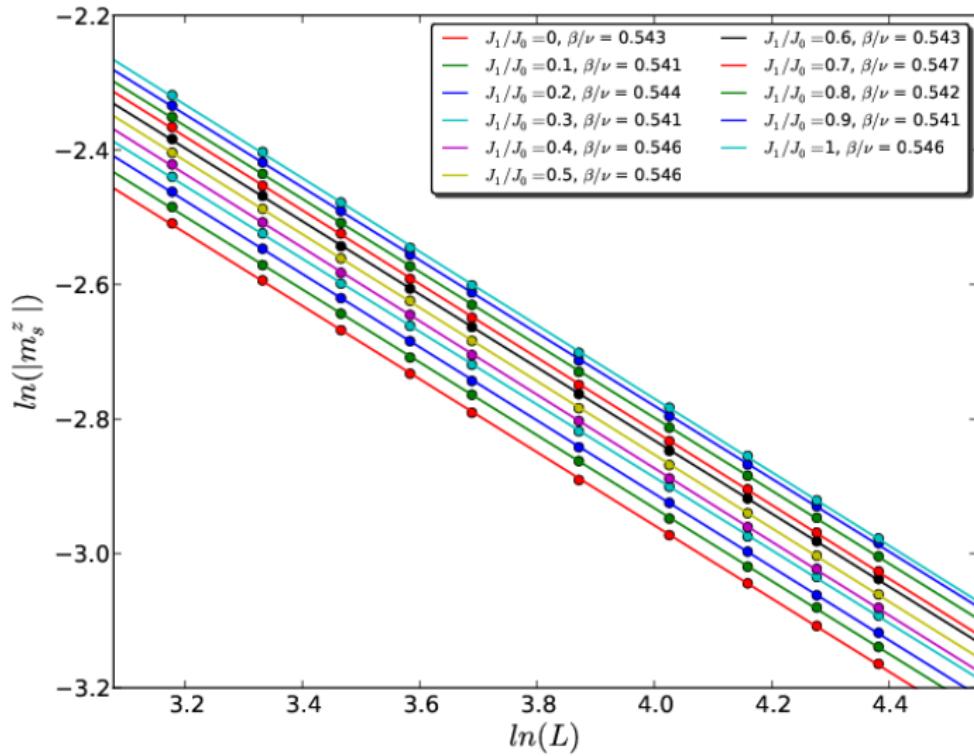
Table: Fitting results of  $\alpha_c$  and  $\nu$

$J_1/J_0$	$\alpha_c$ from Equ.5.9	fitting results of $Q_2$			fitting result of $\rho_s L$		
		$L_{min}$	$\alpha_c$	$\nu$	$L_{min}$	$\alpha_c$	$\nu$
0.0	1.7355(2)	24	1.7357(3)	0.712	28	1.7358(3)	0.680
0.1	1.8067(3)	28	1.8070(3)	0.708	36	1.8065(4)	0.697
0.2	1.8802(2)	28	1.8804(3)	0.707	28	1.8804(3)	0.687
0.3	1.9553(3)	28	1.9555(2)	0.707	28	1.9553(3)	0.691
0.4	2.0326(3)	32	2.0326(2)	0.711	28	2.0326(2)	0.687
0.5	2.1110(3)	24	2.1108(3)	0.705	24	2.1106(4)	0.688
0.6	2.1904(4)	28	2.1904(3)	0.710	24	2.1904(2)	0.685
0.7	2.2715(2)	28	2.2713(2)	0.706	28	2.2714(2)	0.687
0.8	2.3531(4)	28	2.3532(3)	0.701	28	2.3525(5)	0.693
0.9	2.4358(2)	24	2.4360(3)	0.711	32	2.4358(2)	0.701
1.0	2.5198(4)	40	2.5196(3)	0.705	24	2.5194(2)	0.689

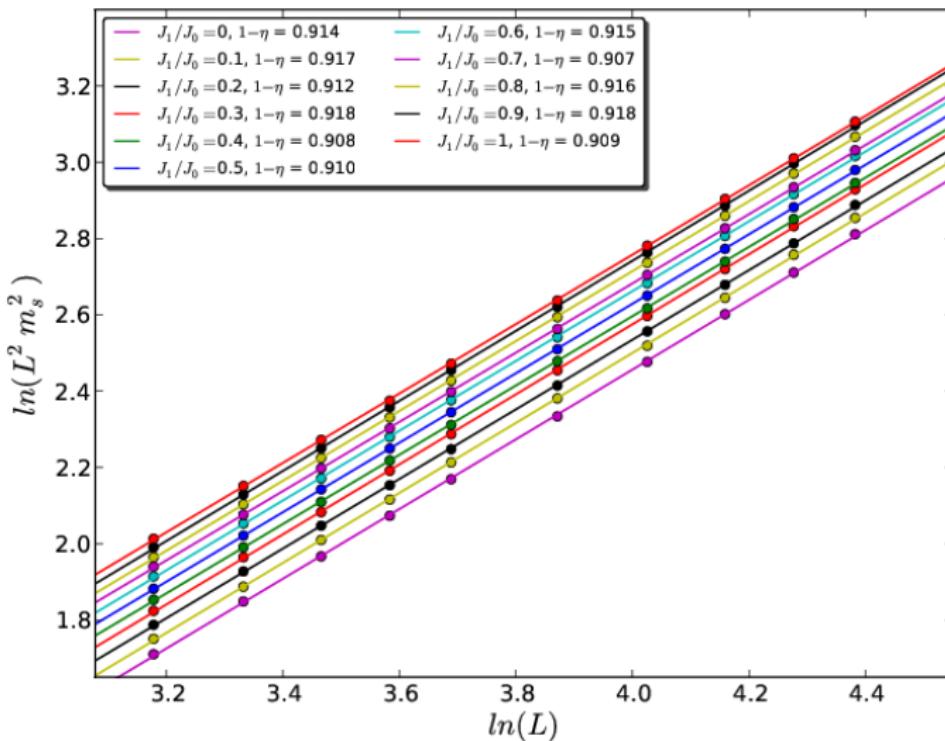
# 数据坍缩



# 临界指数 $\beta/\nu$



# 临界指数 $1 - \eta$



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# 反铁磁体系基态

Lieb-Mattis theorem

无阻挫，反铁磁系统，基态 $|\psi_0\rangle$ 必须满足

$$S = 0$$

Marshall sign rule

在 $S^z$ 表象下对 $\psi_0$ 进行展开

$$|\psi_0\rangle = \sum_{\alpha} (-1)^{\Gamma(\alpha)} f_{\alpha} |\sigma_{\alpha}\rangle$$

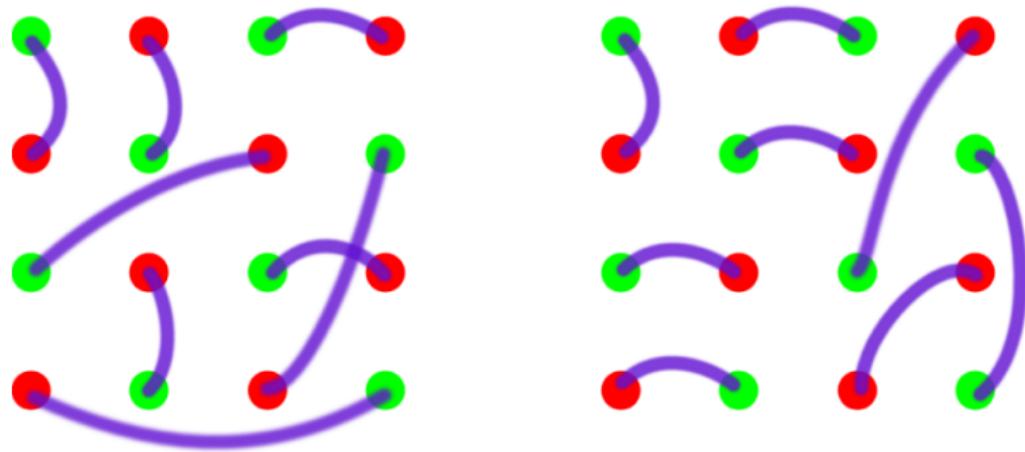
$|\sigma_{\alpha}\rangle$ 是 $S^z$ 表象下的一个基矢， $\Gamma(\alpha)$ 是 $|\sigma_{\alpha}\rangle$ 中A子格子中自旋朝下的数目， $f_{\alpha}$ 非负

# 价键基矢 $|V_\alpha\rangle$

$$(a, b) = (|\uparrow_a \downarrow_b\rangle - |\downarrow_a \uparrow_b\rangle)/\sqrt{2}$$

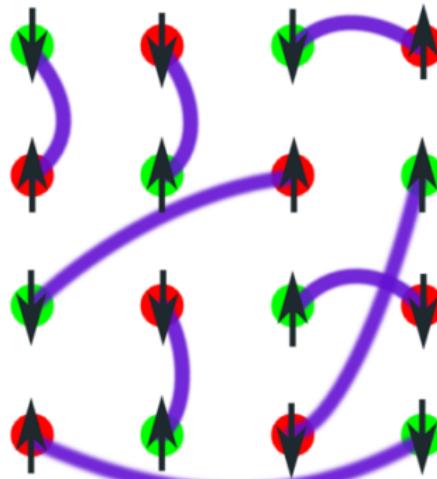
$$|\psi_0\rangle = \sum_{\alpha} f_{\alpha} |(a_1^{\alpha}, b_1^{\alpha}) \dots (a_{N/2}^{\alpha}, b_{N/2}^{\alpha})\rangle = \sum_{\alpha} f_{\alpha} |V_{\alpha}\rangle$$

$$(a, c)(b, d) = (a, b)(c, d) - (a, d)(c, b) \quad (a, c \in A, \quad b, d \in B)$$



# 联合表象 $|Z_i^\alpha\rangle$

$$|V_\alpha\rangle = \frac{1}{2^{N/4}} \sum_{i=1}^{2^{N/2}} (-1)^{A_{\downarrow}(\alpha, i)} |S_1^z(\alpha, i), \dots, S_N^z(\alpha, i)\rangle = \frac{1}{2^{N/4}} \sum_{i=1}^{2^{N/2}} (-1)^{A_{\downarrow}(\alpha, i)} |Z_i^\alpha\rangle$$



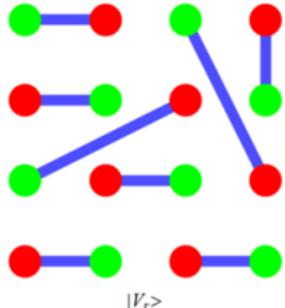
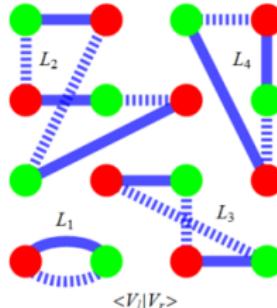
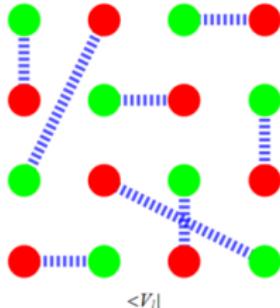
# VBS性质

$$(N/2)! > \frac{N!}{(N/2)!(N/2+1)!}$$

$$\langle V_l | V_r \rangle = \frac{1}{2^{N/2}} \sum_{i,j} \langle Z_j^l | Z_i^r \rangle (-1)^{A_{\downarrow}(r,i) + A_{\downarrow}(l,j)} = 2^{N_{loop} - N/2}$$

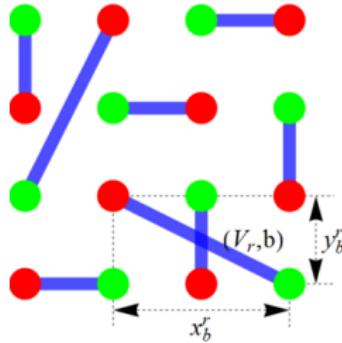
$$|\psi_0\rangle = \sum_r w_r |V_r\rangle$$

$$\frac{\langle V_l | S_i \cdot S_j | V_r \rangle}{\langle V_l | V_r \rangle} = \begin{cases} +3/4, & \text{if } i, j \in \text{ same loop, same sublattice.} \\ -3/4, & \text{if } i, j \in \text{ same loop, different sublattices.} \\ 0, & \text{if } i, j \in \text{ different loops.} \end{cases}$$



# 变分幅度乘积态

$$w_r = \prod_{b=1}^{N/2} h(x_b^r, y_b^r)$$

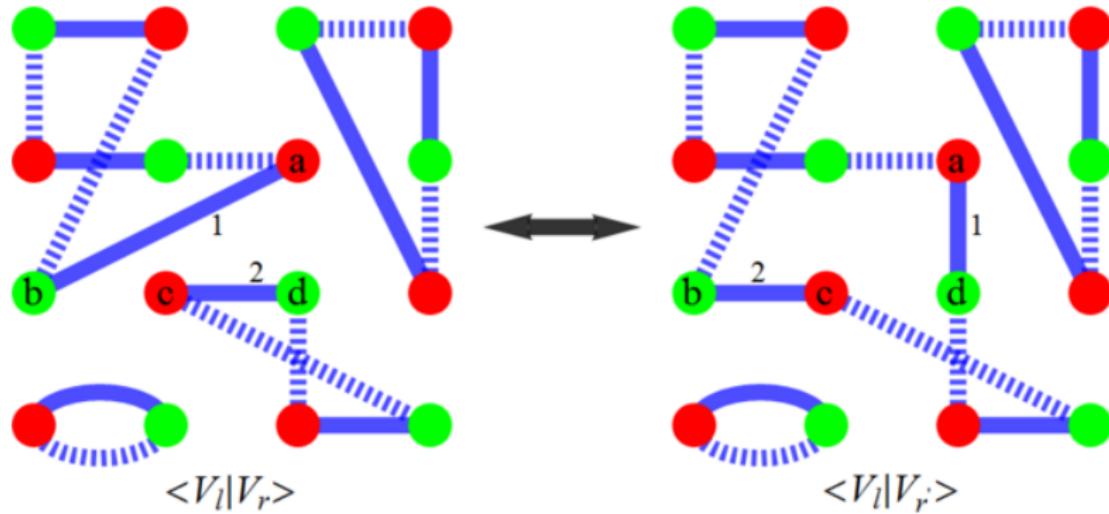


Manhattan length  $l_b^r = x_b^r + y_b^r$

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\sum_{lr} W_{lr} E_{lr}}{\sum_{lr} W_{lr}} \quad W_{lr} = w_l w_r \langle V_l | V_r \rangle$$

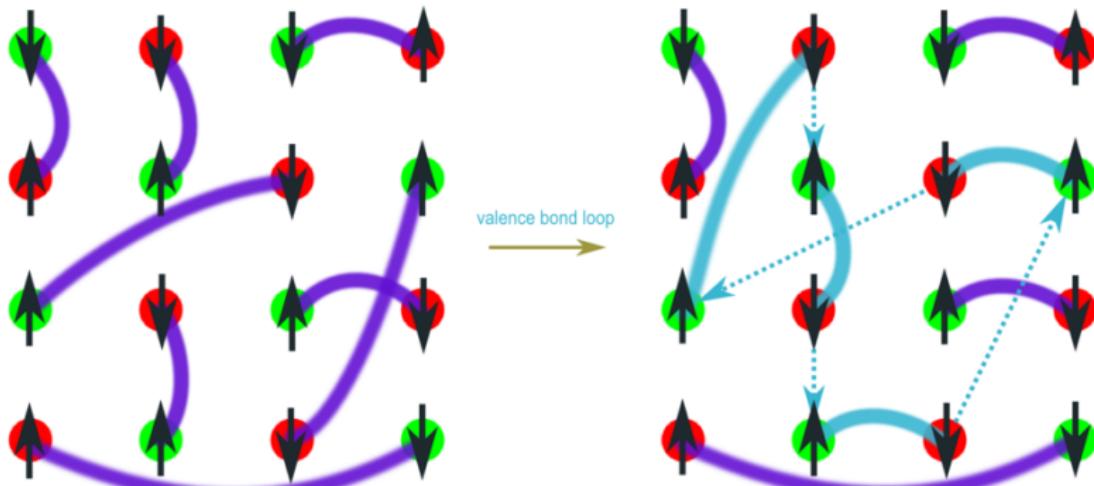
$$E_{lr} = \frac{\langle V_l | H | V_r \rangle}{\langle V_l | V_r \rangle}$$

# 两键重新配对翻转方式



$$P_{accept} = \min\left[\frac{h(x_1^{r'}, y_1^{r'})h(x_2^{r'}, y_2^{r'})}{h(x_1^r, y_1^r)h(x_2^r, y_2^r)} 2^{N_{loop}^{\langle l|r' \rangle} - N_{loop}^{\langle l|r \rangle}}\right]$$

# 价键环翻转方式



$$P_{accept} = \min\left[\frac{h(x_1^{r'}, y_1^{r'})h(x_2^{r'}, y_2^{r'})}{h(x_1^r, y_1^r)h(x_2^r, y_2^r)}\delta_{\langle l|r' \rangle, Z}\right]$$

# 价键基矢投影算法

$$(C - H)^m |\psi\rangle = c_0(C - E_0)^m[|0\rangle + \sum_n \frac{c_n}{c_0} (\frac{C - E_n}{C - E_0})^m |n\rangle]$$

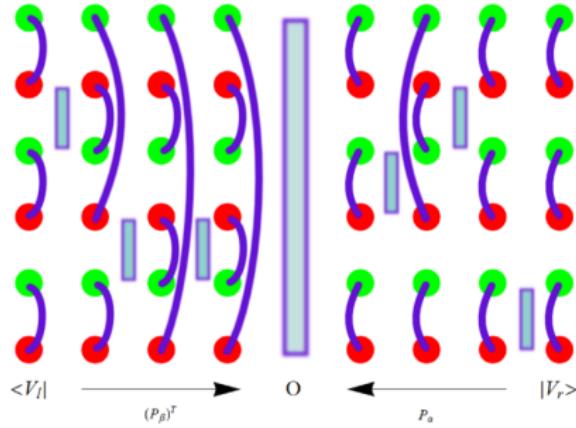
$$C = N_{bond}/4 \quad C - H = \sum_{\langle a,b \rangle} H_{ab} \quad H_{ab} = 1/4 - S_a \cdot S_b$$

$$(C - H)^m = \sum_{\alpha} \prod_{i=1}^m H_{a_i^{\alpha} b_i^{\alpha}} = \sum_{\alpha} P_{\alpha}$$

$$H_{ab} |\cdots (a, b) \cdots \rangle = |\cdots (a, b) \cdots \rangle$$

$$H_{bc} |\cdots (a, b) \cdots (c, d) \cdots \rangle = \frac{1}{2} |\cdots (c, b) \cdots (a, d) \cdots \rangle$$

# 价键基矢投影算法



$$P_\alpha |V_r\rangle = \left(\frac{1}{2}\right)^{o_\alpha^r} |V_r(\alpha)\rangle$$

$$\langle O \rangle = \frac{\langle \psi | (C - H)^m O (C - H)^m | \psi \rangle}{\langle \psi | (-H)^{2m} | \psi \rangle} = \sum_{lr\alpha\beta} W_{lr}^{\alpha\beta} O_{lr}^{\alpha\beta} / \sum_{lr\alpha\beta} W_{lr}^{\alpha\beta}$$

$$W_{lr}^{\alpha\beta} = w_l w_r \langle V_l(\beta) | V_r(\alpha) \rangle 2^{-(o_r^\alpha + o_l^\beta)} \quad O_{lr}^{\alpha\beta} = \langle V_l(\beta) | O | V_r(\alpha) \rangle / \langle V_l(\beta) | V_r(\alpha) \rangle$$

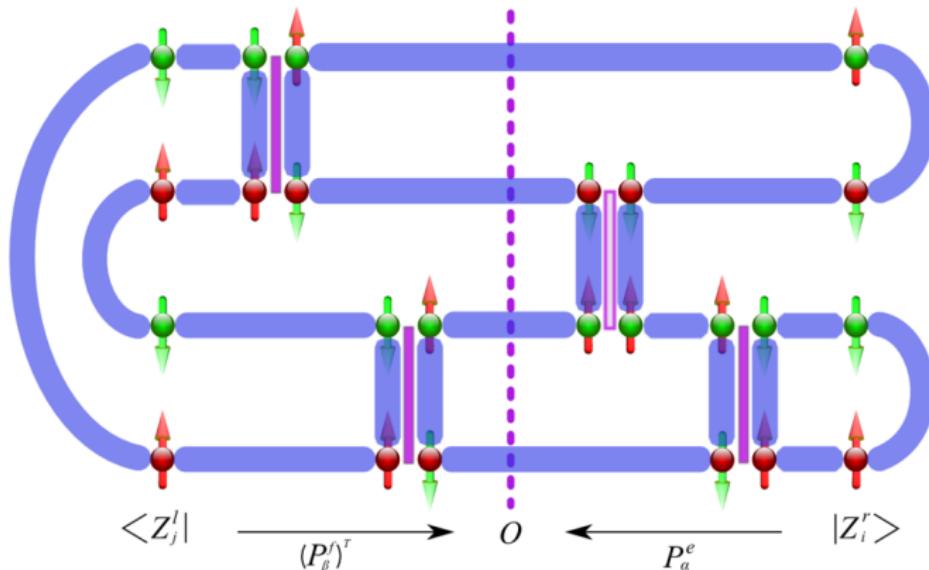
$$P_{accept} = \min[1, \frac{\langle V_l(\beta') | V_r(\alpha') \rangle 2^{-(o_r^{\alpha'} + o_l^{\beta'})}}{\langle V_l(\beta) | V_r(\alpha) \rangle 2^{-(o_r^\alpha + o_l^\beta)}}]$$

# 联合表象下的投影算法

$$H_{ab}(1) = \frac{1}{4} - S_a^z S_b^z$$

$$H_{ab}(2) = -\frac{1}{2}(S_a^+ S_b^- + S_a^- S_b^+)$$

$$W_{lr,ij}^{\alpha\beta,ef} = w_l w_r (\frac{1}{2})^{2m+N/2} \delta_{P_\alpha^e |Z_i^r\rangle, P_\beta^f |Z_j^l\rangle}$$



*Thank you!*