①. MCMC 2D Ising:

$$H=-J\sum_{<ij>} s_i s_j \quad (s=\pm 1) \Rightarrow Z=\sum_{\{s_i\}} e^{-\beta H}=\sum_{\{s_i\}}\prod_{<ij>} e^{\beta J s_i s_j} \xlongequal{\text{设}J=1} \sum_{\{s_i\}}\prod_{<ij>} e^{\beta s_i s_j}$$

Metropolis Algorithm:

$$\begin{cases} \pi(a)P(a\to b)=\pi(b)P(b\to a) \\ P(a\to b)=\min\left[1, \frac{\pi(b)}{\pi(a)}\right] \end{cases}$$

其中 $\pi(a)=e^{-\beta H_a}$, $\pi(b)=e^{-\beta H_b}$

*观测量

def: $m=\frac{1}{N}\sum_i s_i \qquad e=\frac{1}{N}H$

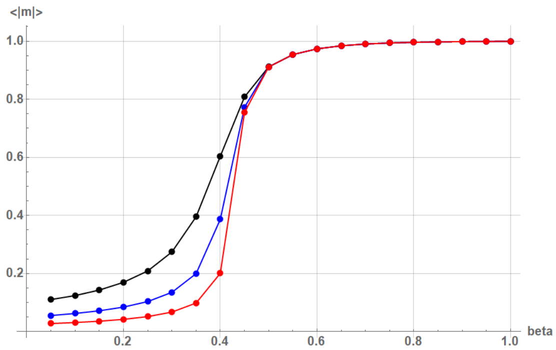
从而有:

$$\langle C_v\rangle = N\beta^2(\langle e^2\rangle-\langle e\rangle^2)$$

$$\langle \chi\rangle = N\beta(\langle m^2\rangle-\langle m\rangle^2)$$

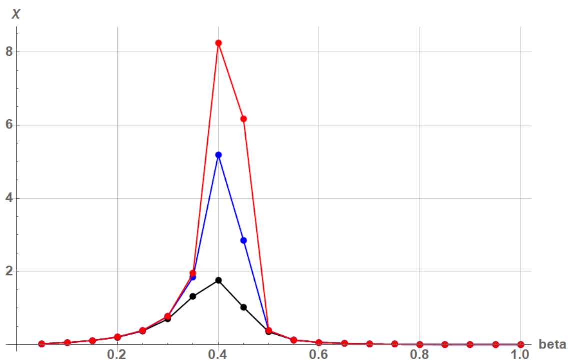
分别取$L=8, 16, 32$进行了MC模拟,计算结果如下:

$\langle |m|\rangle$



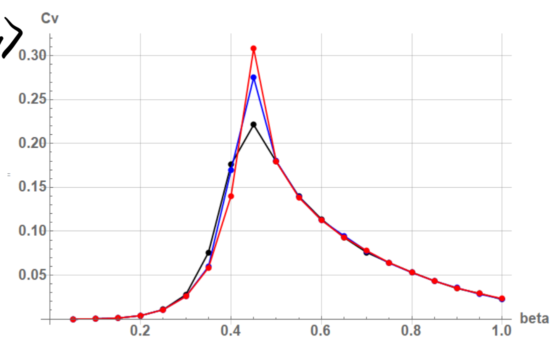
β

$\langle \chi\rangle$



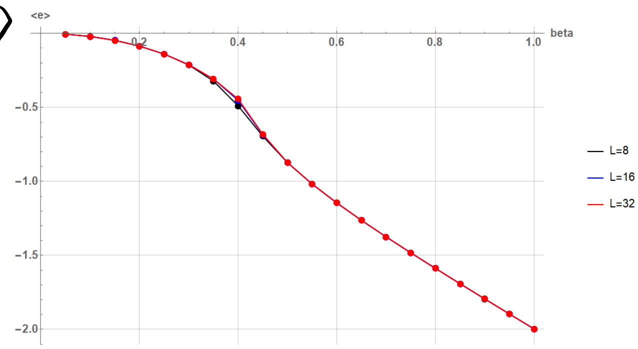
β

$\langle C_v\rangle$



β

$\langle e\rangle$



β

可以看到,在$\beta=0.44$附近,物理量都出现了突变,且该区域与L有关,从而出现有限尺度效应.

当$L\to\infty$时,则会出现热力学极限下的奇异性.利用如下关系,可以粗略得到临界指数γ:

L	χ
200	349.40 ± 0.081
100	103.89 ± 0.041
50	30.306 ± 0.040
20	6.03 ± 0.013
10	1.78 ± 0.014

def: $t=\frac{\beta_c-\beta}{\beta_c} \qquad \chi\sim t^{-\gamma} \quad (\beta\to\beta_c)$

假设关联长度$\xi(t,L)\sim L$ 则有 $t\sim L^{-1/\nu}$ (2D中$\nu=1$)

从而有: $\chi\sim L^{\gamma}$ 利用 $\frac{\chi_{L'}}{\chi_L}=a^{\gamma}$ 得到: $\gamma=1.76\pm 0.023$ 与$\gamma=1.75$相吻合

② Onsager 给出了正方格子 2D Ising 解，单格点自由能为：

$$-\beta f = \ln(2\cosh(2\beta J)) + \frac{1}{\pi}\int_0^{\pi/2} dw \ln\left[\frac{1}{2}\left(1+\sqrt{1-K^2\sin^2(w)}\right)\right] \quad 其中 \ K = \frac{2\sinh(2\beta J)}{[\cosh(2\beta J)]^2}$$

每个格点内能为：

$$u(0,T) = \frac{d}{d\beta}[\beta f(0,T)] = -2J\tanh(2\beta J) + \frac{K}{\pi}\frac{dK}{d\beta}\underbrace{\int_0^{\pi/2} dw \frac{\sin^2 w}{\Delta(1+\Delta)}}_{-\frac{\pi}{K^2}+\frac{1}{K}\int_0^{\pi/2}\frac{dw}{\Delta}} \quad \left(\Delta = \sqrt{1-K^2\sin^2 w}\right)$$

可以得到 $u(0,T) = -J\coth 2\beta J\left[1+\frac{2}{\pi}\frac{dK}{d\beta}K_1(K)\right]$ 其中 $K_1(K) = \int_0^{\frac{\pi}{2}}\frac{d\varphi}{\sqrt{1-K^2\sin^2\varphi}}$ 为第一类全椭圆积分.

对于比热 $C(0,T)$ 有：

$$\frac{1}{K}C(0,T) = \frac{1}{K}\frac{\partial u(0,T)}{\partial T} = \frac{2}{\pi}(\beta J\coth 2\beta J)^2\left\{2K_1(K) - 2E_1(K) - (1-K')\left[\frac{\pi}{2}+K'K_1(K)\right]\right\}$$

其中 $K' = \frac{dK}{d\beta} = 2\tanh^2 2\beta J - 1$，$E_1(K) = \int_0^{\frac{\pi}{2}} d\varphi\sqrt{1-K^2\sin^2\varphi}$ 为第二类全椭圆积分.

当 $K'=0$，有奇异性即：

$$2\tanh^2\frac{2J}{k_BT} = 1 \Rightarrow k_BT_c = \frac{2}{\ln(\sqrt{2}+1)}$$ 从而热容有：

$$\frac{1}{K}C(0,T) \simeq \frac{2}{\pi}\left(\frac{2J}{k_BT_c}\right)^2\left[-\ln\left|1-\frac{T}{T_c}\right| + \ln\left(\frac{k_BT_c}{2J}\right) - \left(1+\frac{\pi}{4}\right)\right]$$

可见热容在 T_c 处以对数地发散.