Ising Model with Metropolis MC Method

QIANG YIHUA

2D Ising model

Structure(E-T, M)

Heat capacity(C)

Entropy (S)

Helmholtz free energy(F)

How it works

- ✓ Set desired T and H.
- ✓ Initialize all spins.
- ✓ Calculate $E_{flip}=E_2-E_1$, if $\exp[-E_{flip}/k_BT]$.lt. random number, leave it undisturbed or flip the spin ($s_i=-s_i$), i.e. state 1→state 2.
- ✓ After each sweep, record the new energy, magnetization, etc.
- ✓ Plot the recorded thermodynamic quantities.

Why it works

A Monte Carlo spin flip connects 2 microstates; let us call their energies E_1 and E_2 and assume that $E_1 > E_2$. Then $W(1\rightarrow2)=1$, $W(2\rightarrow1)=\exp[-(E_1 - E_2)/k_BT]$.

When equilibrium state is reached, $P_1W(1\rightarrow2)=P_2\,W(2\rightarrow1)$, where P_1 and P_2 are the probabilities of the system being found in these two microstates.

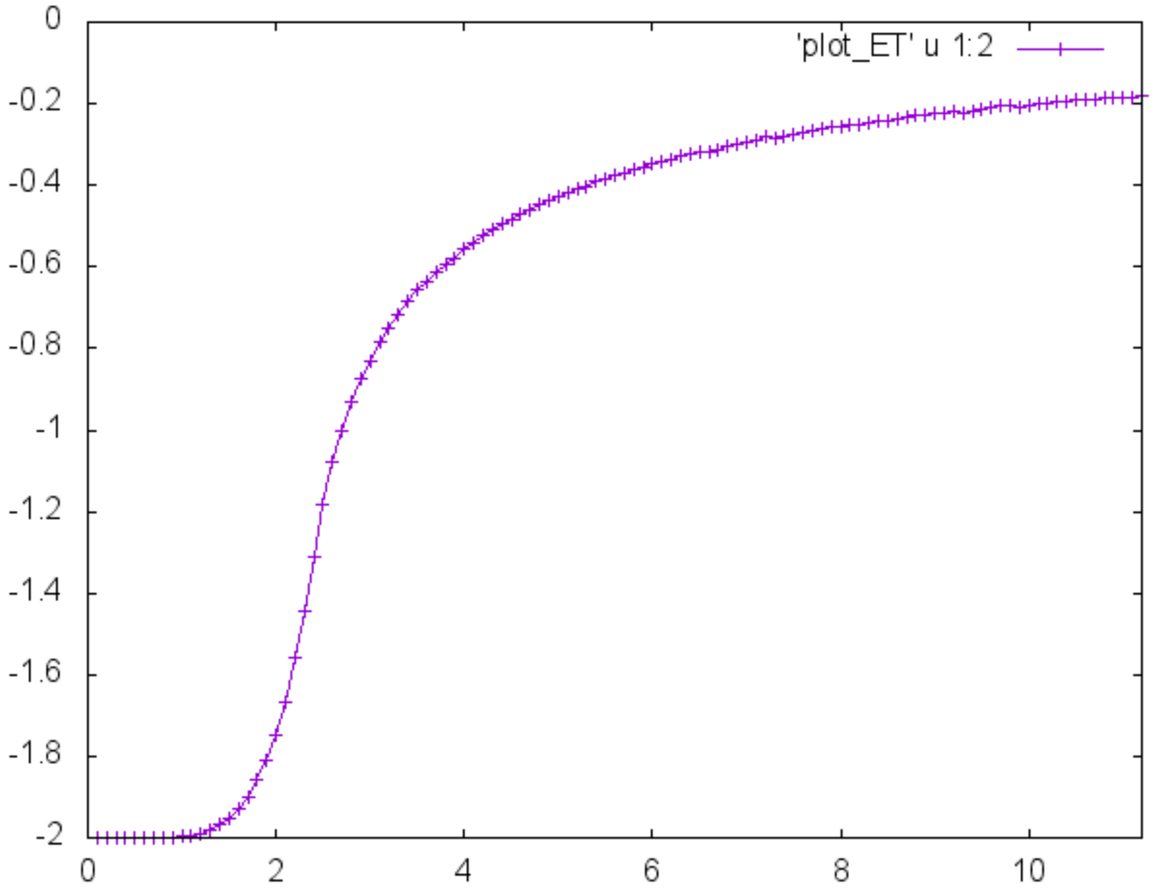
$$\frac{P_2}{P_1} = \exp[-(E_1 - E_2)/k_BT]$$

This is what we expected in a canonical ensemble.

E-T: I’m not alien.

$$T_c = \frac{2}{\ln(1+\sqrt{2})} \approx 2.27$$

Fluctuation at rather high temperature.
Solution:
add warm and measurement steps.



$$M = \sum s_i$$

Structure

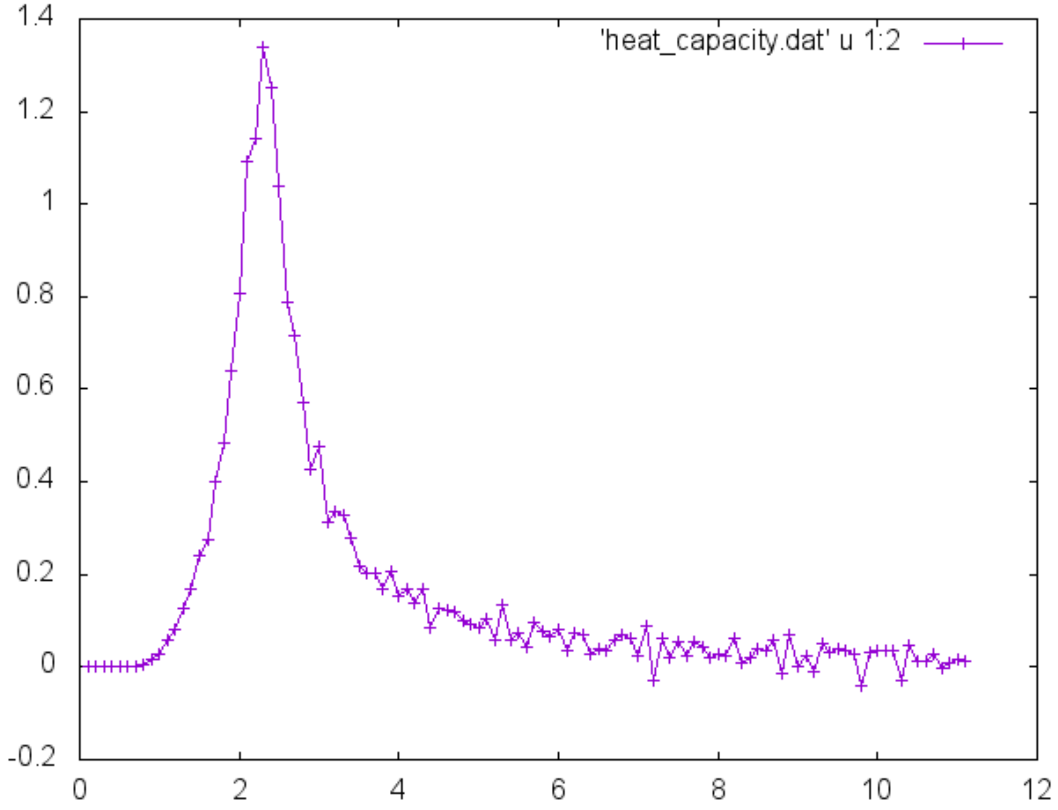
```
-1.00 -1.00  1.00 -1.00 -1.00 -1.00  1.00  1.00  1.00  1.00
 1.00  1.00  1.00 -1.00  1.00 -1.00  1.00  1.00  1.00  1.00
-1.00  1.00  1.00  1.00  1.00 -1.00 -1.00 -1.00 -1.00 -1.00
 1.00  1.00  1.00 -1.00  1.00  1.00  1.00 -1.00 -1.00 -1.00
 1.00  1.00 -1.00 -1.00  1.00  1.00 -1.00 -1.00 -1.00 -1.00
-1.00  1.00  1.00 -1.00  1.00  1.00 -1.00 -1.00 -1.00 -1.00
 1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00 -1.00 -1.00
 1.00  1.00 -1.00 -1.00  1.00 -1.00 -1.00 -1.00 -1.00  1.00
-1.00 -1.00 -1.00 -1.00  1.00  1.00  1.00  1.00  1.00  1.00
-1.00  1.00  1.00 -1.00  1.00  1.00  1.00  1.00  1.00  1.00
  5.0000000000000000       -0.42732199999999992        2.2321787983128746E-003  0.13999999999999999
```

Reduced Temperature   Mean energy   Error bar   Magnetization per lattice

$$C = \frac{\partial E}{\partial T}$$

At high temperature C→0

FDM



$$S = S_\infty + \frac{E(T)}{T} - \int_T^\infty \frac{E(T')}{T'^2} dT'$$

The entropy is calculated by $S_b - S_a = \int_a^b \frac{dQ}{T}$, and with fixed volume for lattice model we have $dQ = dE$. So we have

$$S(\infty) - S(T) = \int_T^\infty \frac{dE}{T'} = \left(\frac{E(T')}{T'}\right) |_T^\infty + \int_T^\infty \frac{E(T')}{T'^2} dT' \tag{55}$$

where $E(T)$ denotes the average total energy (internal energy) per particle at temperature T.

There is an upper limit for total energy, so we have $\lim_{T \to \infty} \frac{E(T)}{T} = 0$. So we have

$$S(T) = S(\infty) + \frac{E(T)}{T} - \int_T^\infty \frac{E(T')}{T'^2} dT' \tag{56}$$

Entropy

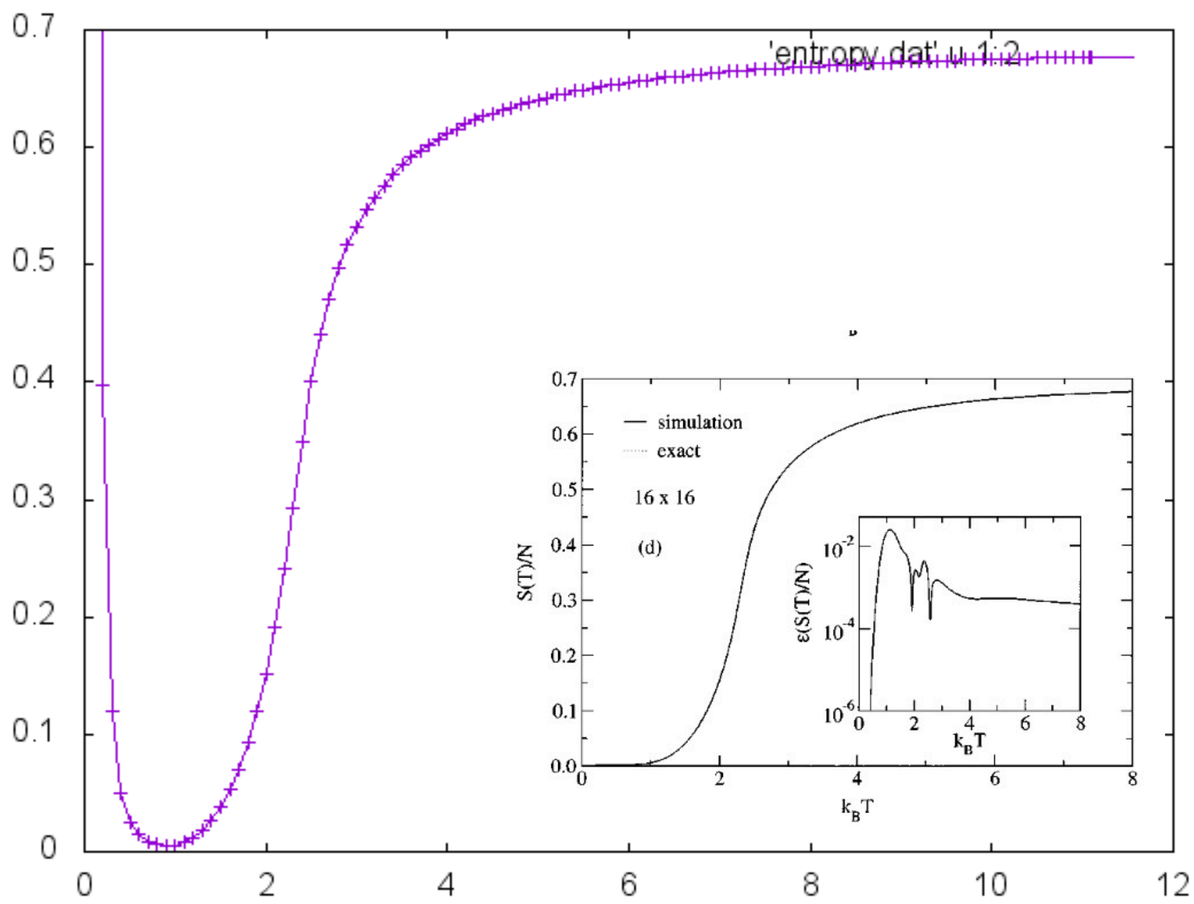
```
In[1]:= Integrate[0.01727 * Exp[-0.2233 * x] / x^2, {x, 11.1, Infinity}]
Out[1]= 0.0000316425
```

Divergent at T=0

S→ln2 as T→ ∞

$$\int_{11.1}^{\infty} \frac{E(T')}{T'^2} dT'$$

negligible



$F = E - TS$

Wang-Landau

$$F(T) = -k_B T \ln(Z) = -k_B T \ln\left(\sum_E g(E) e^{-E/k_B T}\right), \quad (8)$$

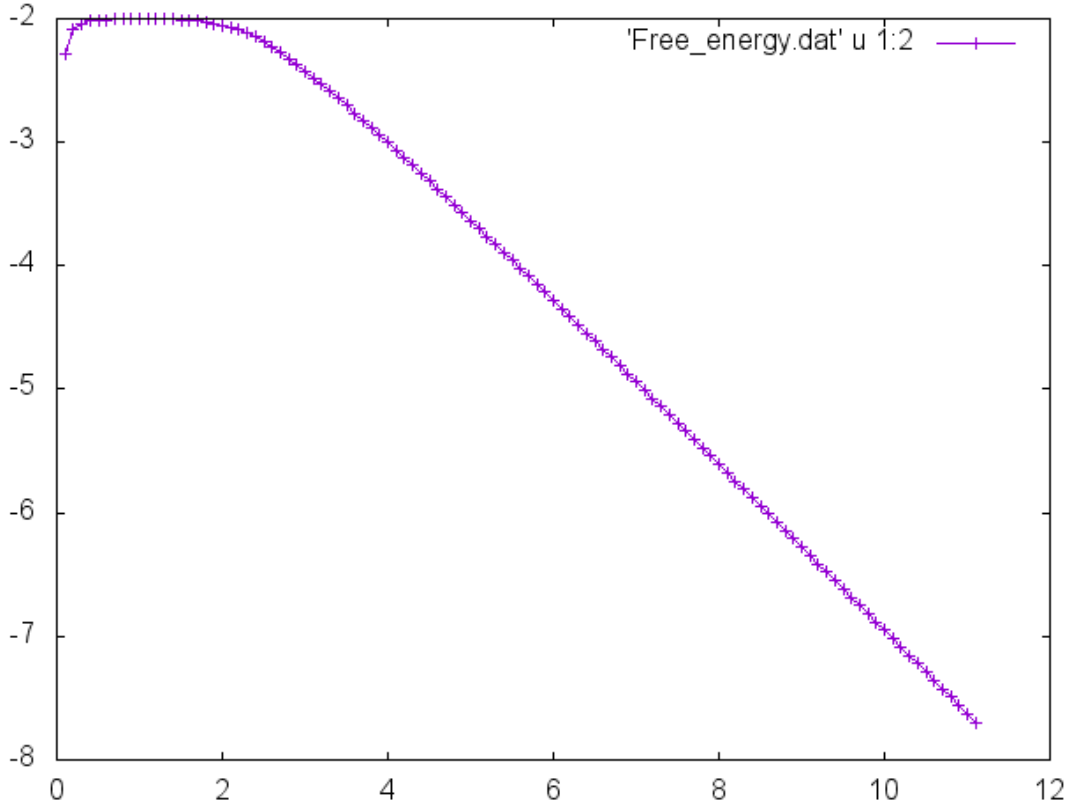
and the entropy can then be easily computed by

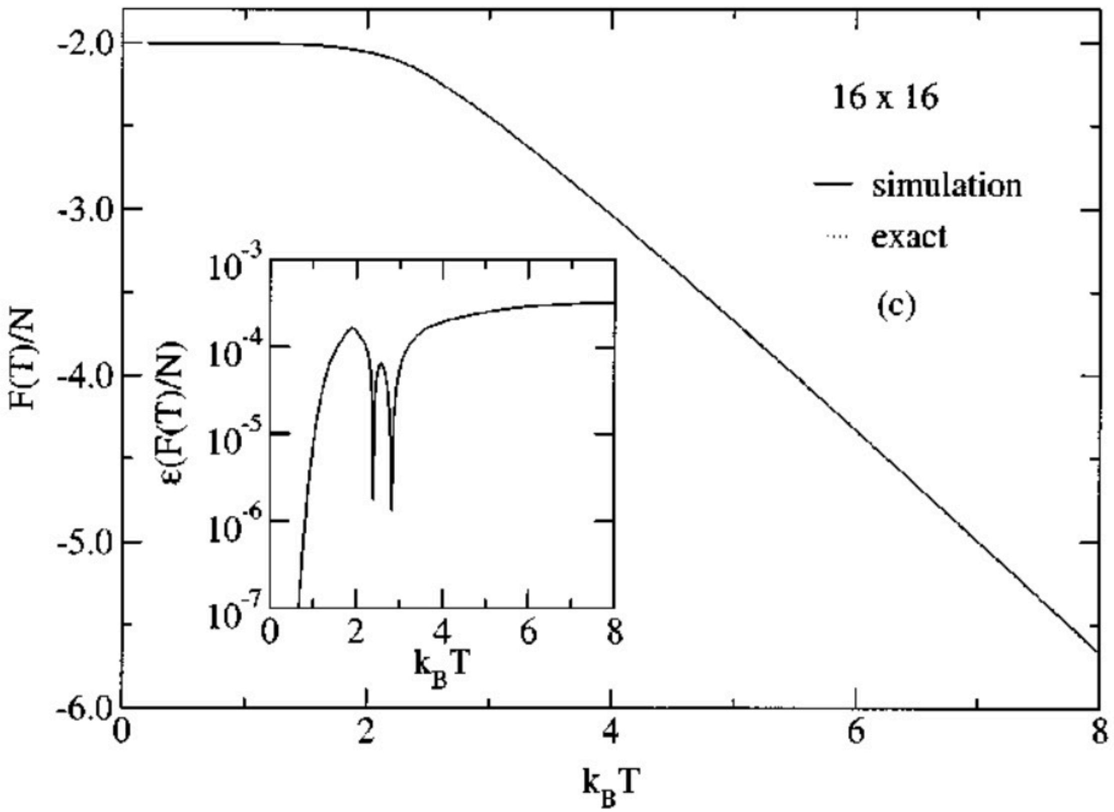
$$S(T) = \frac{U(T) - F(T)}{T}. \quad (9)$$

My curt way

$$F = E - TS$$

Free energy


'Free_energy.dat' u 1:2
-2
-3
-4
-5
-6
-7
-8
0
2
4
6
8
10
12


16 x 16
simulation
exact
(c)
F(T)/N
-2.0
-3.0
-4.0
-5.0
-6.0
0
2
4
6
8
$k_B T$
$\varepsilon(F(T)/N)$
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
0
2
4
6
8
$k_B T$

About computing

MC method:

$$\varepsilon \propto \frac{1}{\sqrt{n}}$$

Coding and solving:

$$L \times L$$

How about $\frac{1}{l} \to 0$?

Thanks