计算物理第六次作业

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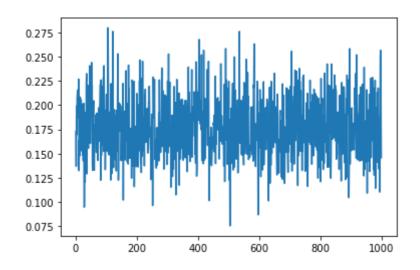
1.

1.1

```
import random
import numpy as np
import matplotlib.pyplot as plt
def f(x):
   return np.exp(-100 * (x - 0.5)**2)
def integral(num):
   sum = 0
   b = 1
   a = 0
   for i in range(num):
       x = random.random()
       sum += f(x)
    return sum * (b - a) / num
def plot(times, num):
   ctr = []
   int = []
    for i in range(times):
        ctr.append(i+1)
        int.append(integral(num))
    plt.plot(ctr,int)
    plt.show()
```

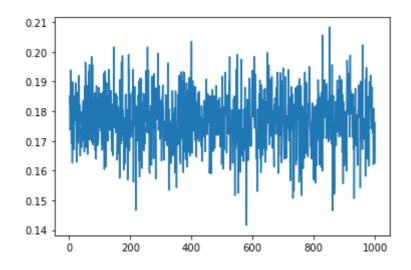
重复1000次,每次100个散点

```
plot(1000,100)
```



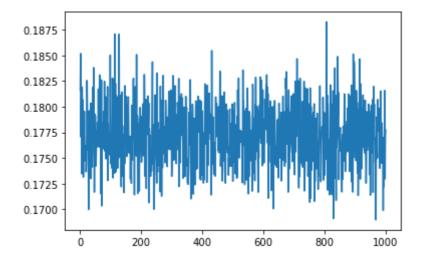
重复1000次,每次1000个散点

plot(1000, 1000)



重复1000次,每次10000个散点

plot(1000, 10000)

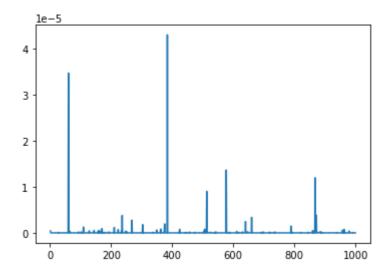


综合上面的结果可知: 随着散点数的增加,积分的波动范围变小,误差变小,符合大数定理。

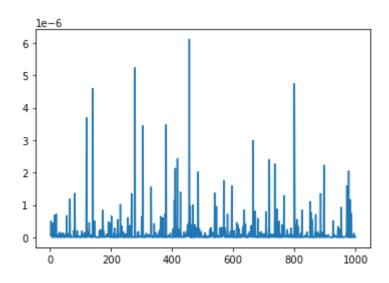
1.2

```
import random
import numpy as np
def f(x):
    return np.exp(-100 * (x - 0.5) @ (x - 0.5).T)
def multi_integral(num):
   sum = 0
   b = 1
    a = 0
    for i in range(num):
       x = np.random.rand(9)
        sum += f(x)
    return sum / num
def plot(times, num):
    ctr = []
    int = []
    for i in range(times):
        ctr.append(i + 1)
        int.append(multi_integral(num))
    plt.plot(ctr, int)
    plt.show()
    print('integral = {}'.format(np.mean(int)))
```

```
plot(1000, 1000)
plot(1000, 10000)
```



integral = 1.5750283682938318e-07



integral = 1.400362613097055e-07

2.

2.1

当我们对Potts model做一次 spin flip 的时候,系统能量的该变量只取决于这个被反转的 spin 以及它周围的四个 spins。

$$\begin{split} E' &= -J(\delta_{s's_l} + \delta_{s's_r} + \delta_{s's_t} + \delta_{s's_b}) \\ E &= -J(\delta_{ss_l} + \delta_{ss_r} + \delta_{ss_t} + \delta_{ss_b}) \\ \Delta E &= -J(\delta_{s's_l} + \delta_{s's_r} + \delta_{s's_t} + \delta_{s's_b}) + J(\delta_{ss_l} + \delta_{ss_r} + \delta_{ss_t} + \delta_{ss_b}) \\ &= -J(4 - (\delta_{ss_l} + \delta_{ss_r} + \delta_{ss_t} + \delta_{ss_b})) + J(\delta_{ss_l} + \delta_{ss_r} + \delta_{ss_t} + \delta_{ss_b}) \\ &= -4J + 2J(\delta_{ss_l} + \delta_{ss_r} + \delta_{ss_t} + \delta_{ss_b}) \end{split}$$

需要注意的是,对于 Potts Model, magnetization 的公式如下:

$$M=|\sum_{i,j}e^{2\pirac{s_{ij}}{q}}|$$

Potts model

```
import numpy as np
import random
import matplotlib.pyplot as plt
from tqdm import tqdm
class Potts():
   def __init__(self, size, J):
        self.size = size
        self.J = J
        self.lattice = np.ones((self.size, self.size),int)
        self.E = 0
   def set_initial(self):
        self.lattice = np.ones((self.size, self.size), int)
        self.E = self.totalE()
   def up(self, x, y):
       # 周期性边界条件
        if x == 0:
            return [self.size - 1, y]
        else:
            return [x - 1, y]
   def down(self, x, y):
        if x == self.size - 1:
            return [0, y]
        else:
            return [x + 1, y]
   def left(self, x, y):
        if y == 0:
            return [x, self.size - 1]
        else:
            return [x, y - 1]
   def right(self, x, y):
        if y == self.size - 1:
            return [x, 0]
        else:
            return [x, y + 1]
   def delta(self, x1, y1, x2, y2):
        if self.lattice[x1, y1] == self.lattice[x2, y2]:
            return 1
        else:
            return 0
   def totalE(self):
        E = 0
        for x in range(self.size):
            for y in range(self.size):
```

```
x1,y1 = self.left(x,y)
                xr,yr = self.right(x,y)
                xu,yu = self.up(x,y)
                xd,yd = self.down(x,y)
                E += self.delta(x, y, xl, yl) + self.delta(x, y, xr, yr) +
self.delta(x, y, xu, yu) + self.delta(x, y, xd, yd)
        E = -self.J * E / 2
        return E
    def totalM(self):
        return np.abs(np.sum(2 * self.lattice - 3))
   def avgE(self):
        return self.totalE() / self.size**2
   def avgM(self):
        return self.totalM() / self.size**2
   def deltaE(self,x,y):
        x1,y1 = self.left(x,y)
        xr,yr = self.right(x,y)
        xu, yu = self.up(x,y)
        xd,yd = self.down(x,y)
        deltaE = -4 * self.J + 2 * self.J * (
            self.delta(x, y, xl, yl) + self.delta(x, y, xr, yr) +
            self.delta(x, y, xu, yu) + self.delta(x, y, xd, yd))
        return deltaE
   def flip(self,temperature):
        x = random.randint(0, self.size-1)
        y = random.randint(0, self.size-1)
        deltaE = self.deltaE(x, y)
        if deltaE < 0:</pre>
            self.lattice[x,y] = 3 - self.lattice[x,y]
            self.E += deltaE
        else:
            if random.random() < np.exp(- deltaE / temperature):</pre>
                self.lattice[x, y] = 3 - self.lattice[x,y]
                self.E += deltaE
   # def equi(self, temperature, flip_num=1):
    #
          for flip_time in range(flip_num):
              self.flip(temperature)
          return self.totalE(),self.totalM()
    def output(self,t1,t2,step,start:int=100000, times:int=10000):
        t = t1
        templ = []
        E = []
        M = \lceil \rceil
        C = []
        X = []
        for i in tqdm(range(int((t2 - t1) / step + 1))):
            templ.append(t)
            E_t = []
            M_t = []
            self.set_initial()
```

```
P = Potts(10, 1)
temp, E_10, M_10, C_10, X_10 = P.output(0.1, 4, 0.1, times=100000)
P = Potts(40, 1)
temp, E_40, M_40, C_40, X_40 = P.output(0.1, 4, 0.1, times=100000)
P = Potts(80, 1)
temp, E_80, M_80, C_80, X_80 = P.output(0.1, 4, 0.1, times=100000)
```

```
100%| 40/40 [04:20<00:00, 6.52s/it]

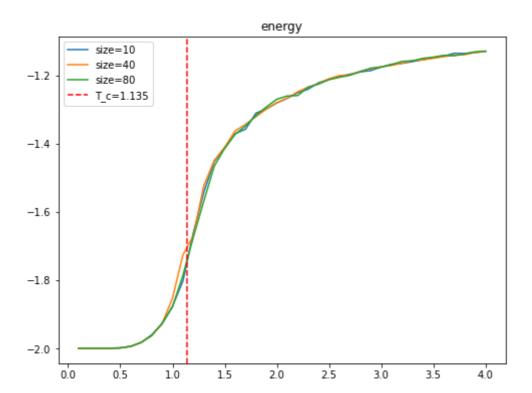
100%| 40/40 [04:53<00:00, 7.35s/it]

100%| 40/40 [06:25<00:00, 9.63s/it]
```

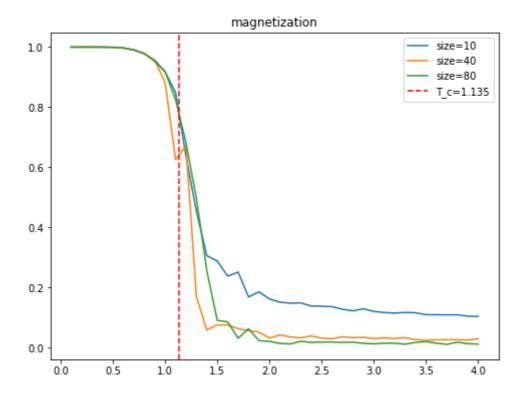
```
data_10 = np.c_[temp, E_10, M_10, C_10, X_10]
np.save('2_1_data_10', data_10)
data_40 = np.c_[temp, E_40, M_40, C_40, X_40]
np.save('2_1_data_40', data_40)
data_80 = np.c_[temp, E_80, M_80, C_80, X_80]
np.save('2_1_data_80', data_80)
```

```
data_10 = np.load('2_1_data_10.npy')
temp, E_10, M_10, C_10, X_10 = data_10[:, 0], data_10[:, 1], data_10[:, 2],
data_10[:, 3], data_10[:, 4]
data_40 = np.load('2_1_data_40.npy')
temp, E_40, M_40, C_40, X_40 = data_40[:, 0], data_40[:, 1], data_40[:, 2],
data_40[:, 3], data_40[:, 4]
data_80 = np.load('2_1_data_80.npy')
temp, E_80, M_80, C_80, X_80 = data_80[:, 0], data_80[:, 1], data_80[:, 2],
data_80[:, 3], data_80[:, 4]
```

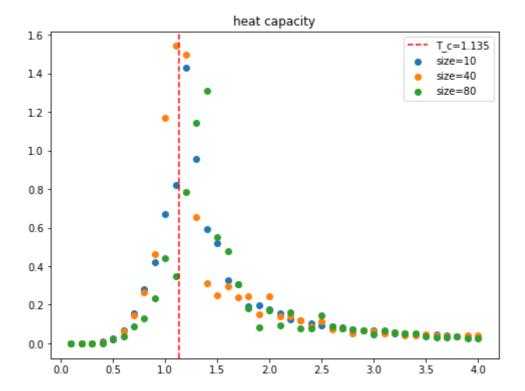
```
plt.figure(figsize=[8, 6])
plt.plot(temp, E_10, label='size=10')
plt.plot(temp, E_40, label='size=40')
plt.plot(temp, E_80, label='size=80')
plt.axvline(x=1.135, c='r', linestyle='--', label='T_c=1.135')
plt.title('energy')
plt.legend()
plt.show()
```



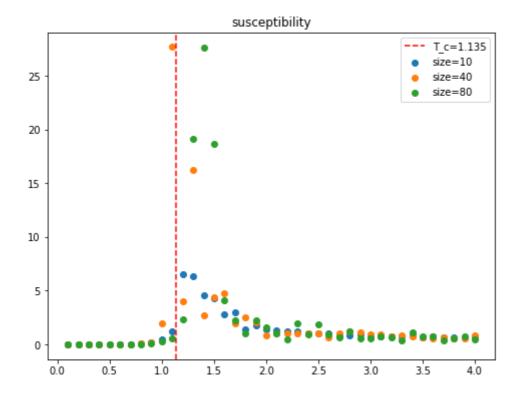
```
plt.figure(figsize=[8, 6])
plt.plot(temp, M_10, label='size=10')
plt.plot(temp, M_40, label='size=40')
plt.plot(temp, M_80, label='size=80')
plt.axvline(x=1.135, c='r', linestyle='--', label='T_c=1.135')
plt.title('magnetization')
plt.legend()
plt.show()
```



```
plt.figure(figsize=[8, 6])
plt.scatter(temp, C_10, label='size=10')
plt.scatter(temp, C_40, label='size=40')
plt.scatter(temp, C_80, label='size=80')
plt.axvline(x=1.135, c='r', linestyle='--', label='T_c=1.135')
plt.title('heat capacity')
plt.legend()
plt.show()
```



```
plt.figure(figsize=[8, 6])
plt.scatter(temp, X_10, label='size=10')
plt.scatter(temp, X_40, label='size=40')
plt.scatter(temp, X_80, label='size=80')
plt.axvline(x=1.135, c='r', linestyle='--', label='T_c=1.135')
plt.title('susceptibility')
plt.legend()
plt.show()
```



运行 p=2 的 Potts model 程序,可以发现,热容与磁导率作为温度的函数在 $T_C \approx 1.135$ 附近不连续,发生二级相变。

2.2

和Potts model一样,当我们对Ising model做一次 spin flip 的时候,系统能量的该变量也只取决于这个被反转的 spin 以及它周围的四个 spins。

$$E' = -J(s's_l + s's_r + s's_t + s's_b)$$
 $E = -J(ss_l + ss_r + ss_t + ss_b)$
 $\Delta E = -J(s's_l + s's_r + s's_t + s's_b) + J(ss_l + ss_r + ss_t + ss_b)$
 $= J(s_l + s_r + s_t + s_b)(s - s')$

```
import numpy as np
import random
import matplotlib.pyplot as plt
class Ising():
   def __init__(self, size, J):
        self.size = size
        self.J = J
        self.lattice = np.ones((self.size, self.size), int)
        self.E = 0
   def set_initial(self):
        self.lattice = np.ones((self.size, self.size), int)
        self.E = self.totalE()
   def up(self, x, y):
       # 周期性边界条件
        if x == 0:
            return [self.size - 1, y]
```

```
else:
            return [x - 1, y]
   def down(self, x, y):
        if x == self.size - 1:
            return [0, y]
        else:
            return [x + 1, y]
    def left(self, x, y):
       if y == 0:
            return [x, self.size - 1]
        else:
            return [x, y - 1]
    def right(self, x, y):
        if y == self.size - 1:
            return [x, 0]
        else:
            return [x, y + 1]
   def delta(self, x1, y1, x2, y2):
        return self.lattice[x1, y1] * self.lattice[x2, y2]
   def totalE(self):
        E = 0
        for x in range(self.size):
            for y in range(self.size):
                x1, y1 = self.left(x, y)
                xr, yr = self.right(x, y)
                xu, yu = self.up(x, y)
                xd, yd = self.down(x, y)
                E += self.delta(x, y, xl, yl) + self.delta(
                    x, y, xr, yr) + self.delta(x, y, xu, yu) + self.delta(
                        x, y, xd, yd)
        E = -self.J * E / 2
        return E
   def totalM(self):
        return np.abs(np.sum(self.lattice))
   def avgE(self):
        return self.totalE() / self.size**2
   def avgM(self):
        return self.totalM() / self.size**2
   def deltaE(self, x, y):
        x1, y1 = self.left(x, y)
        xr, yr = self.right(x, y)
        xu, yu = self.up(x, y)
        xd, yd = self.down(x, y)
        deltaE = self.J * (self.lattice[xl, yl] + self.lattice[xr, yr] +
                           self.lattice[xu, yu] + self.lattice[xd, yd]) * ( 2 *
self.lattice[x,y])
        return deltaE
   def flip(self, temperature):
```

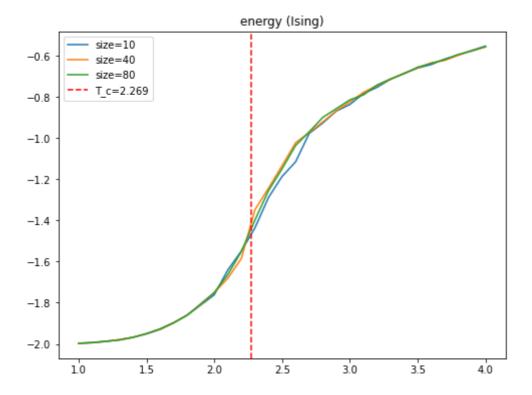
```
x = random.randint(0, self.size - 1)
    y = random.randint(0, self.size - 1)
    deltaE = self.deltaE(x, y)
    if deltaE < 0:</pre>
        self.lattice[x, y] = -self.lattice[x, y]
        self.E += deltaE
    else:
        if random.random() < np.exp(-deltaE / temperature):</pre>
            self.lattice[x, y] = -self.lattice[x, y]
            self.E += deltaE
def output(self, t1, t2, step, start: int = 100000, times: int = 1000):
    t = t1
    templ = []
    E = []
    M = []
   C = []
    X = []
    for i in tqdm(range(int((t2 - t1) / step + 1))):
        templ.append(t)
        E_t = []
        M_t = []
        self.set_initial()
        for i in range(start):
            self.flip(t)
        for time in range(times):
            self.flip(t)
            E_t.append(self.E)
            M_t.append(self.totalM())
        E.append(np.mean(E_t) / self.size**2)
        M.append(np.mean(M_t) / self.size**2)
        C.append((np.mean(np.array(E_t)**2) - np.mean(E_t)**2) /
                 (self.size**2 * t**2))
        X.append(
            (np.mean(np.array(M_t)**2) - np.mean(M_t)**2) / (self.size**2))
        t += step
    return templ, E, M, C, X
```

```
I = Ising(10, 1)
temp, E_10, M_10, C_10, X_10 = I.output(1, 4, 0.1, start=500000, times=500000)
I = Ising(40, 1)
temp, E_40, M_40, C_40, X_40 = I.output(1, 4, 0.1, start=500000, times=500000)
I = Ising(80, 1)
temp, E_80, M_80, C_80, X_80 = I.output(1, 4, 0.1, start=500000, times=500000)
```

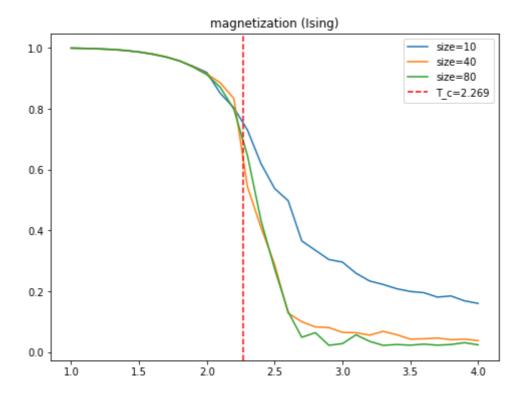
```
100%| 31/31 [08:24<00:00, 16.27s/it]
100%| 31/31 [17:40<00:00, 34.21s/it]
100%| 31/31 [19:17<00:00, 37.33s/it]
```

```
data_10 = np.c_[temp, E_10, M_10, C_10, X_10]
np.save('2_2_data_10', data_10)
data_40 = np.c_[temp, E_40, M_40, C_40, X_40]
np.save('2_2_data_40', data_40)
data_80 = np.c_[temp, E_80, M_80, C_80, X_80]
np.save('2_2_data_80', data_80)
```

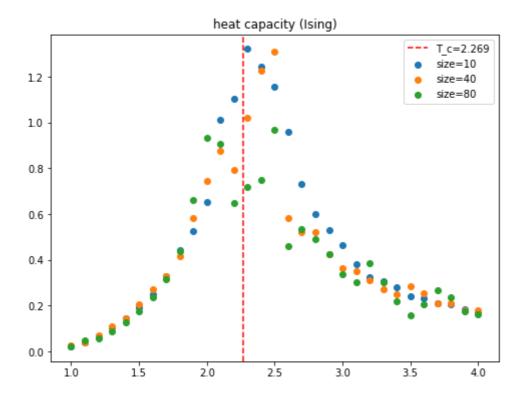
```
plt.figure(figsize=[8,6])
plt.plot(temp, E_10, label='size=10')
plt.plot(temp, E_40, label='size=40')
plt.plot(temp, E_80, label='size=80')
plt.axvline(x=2.269, c='r', linestyle='--', label='T_c=2.269')
plt.title('energy (Ising)')
plt.legend()
plt.show()
```



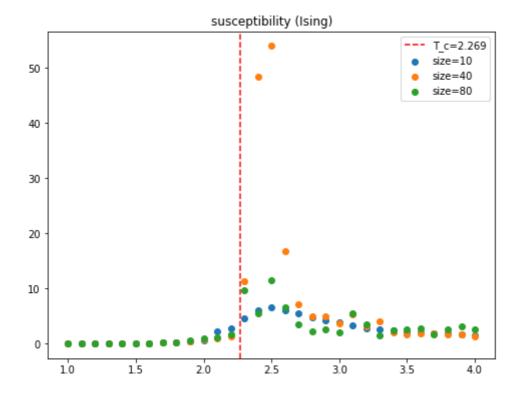
```
plt.figure(figsize=[8, 6])
plt.plot(temp, M_10, label='size=10')
plt.plot(temp, M_40, label='size=40')
plt.plot(temp, M_80, label='size=80')
plt.axvline(x=2.269, c='r', linestyle='--', label='T_c=2.269')
plt.title('magnetization (Ising)')
plt.legend()
plt.show()
```



```
plt.figure(figsize=[8, 6])
plt.scatter(temp, C_10, label='size=10')
plt.scatter(temp, C_40, label='size=40')
plt.scatter(temp, C_80, label='size=80')
plt.axvline(x=2.269, c='r', linestyle='--', label='T_c=2.269')
plt.title('heat capacity (Ising)')
plt.legend()
plt.show()
```



```
plt.figure(figsize=[8, 6])
plt.scatter(temp, X_10, label='size=10')
plt.scatter(temp, X_40, label='size=40')
plt.scatter(temp, X_80, label='size=80')
plt.axvline(x=2.269, c='r', linestyle='--', label='T_c=2.269')
plt.title('susceptibility (Ising)')
plt.legend()
plt.show()
```



运行 Ising model 程序,可以发现,热容与磁导率作为温度的函数在 $T_C \approx 2.269$ 附近不连续,发生二级相变。对比 q=2 的 Potts model 可以发现,Ising model 的二级相变温度大约是 Potts model 的 2 倍。

2.3 q=3,6,10

当我们对Potts model做一次 spin flip 的时候,系统能量的该变量只取决于这个被反转的 spin 以及它周围的四个 spins。

$$E' = -J(\delta_{s's_l} + \delta_{s's_r} + \delta_{s's_t} + \delta_{s's_b})
onumber \ E = -J(\delta_{ss_l} + \delta_{ss_r} + \delta_{ss_t} + \delta_{ss_b})
onumber \ \Delta E = -J(\delta_{s's_l} + \delta_{s's_r} + \delta_{s's_t} + \delta_{s's_b}) + J(\delta_{ss_l} + \delta_{ss_r} + \delta_{ss_t} + \delta_{ss_b})$$

initial				final				deltaE(-J)
1	1	1	1	0	0	0	0	-4
0	1	1	1	1	0	0	0	-2
				0	0	0	0	-3
0	0	1	1	1	1	0	0	0
				0	1	0	0	-1
				0	0	0	0	-2
0	0	0	1	1	1	1	0	2
				0	1	1	0	1
				0	0	1	0	0
				0	0	0	0	-1
0	0	0	0	1	1	1	1	4
				0	1	1	1	3
				0	0	1	1	2
				0	0	0	1	1
				0	0	0	0	0

q=3,6,10时, ΔE 上述值均可取到,即 $\pm 4J,\pm 3J,\pm 2J,\pm J,0$

```
import numpy as np
import random
import matplotlib.pyplot as plt
from tqdm import tqdm
class q_Potts():
   def __init__(self, size, J, q):
       self.size = size
        self.J = J
        self.lattice = np.ones((self.size, self.size), int)
        self.q = q
        self.E = 0
   def set_initial(self):
        self.lattice = np.ones((self.size, self.size), int)
        self.E = self.totalE()
   def up(self, x, y):
       # 周期性边界条件
        if x == 0:
           return [self.size - 1, y]
        else:
           return [x - 1, y]
```

```
def down(self, x, y):
    if x == self.size - 1:
        return [0, y]
    else:
        return [x + 1, y]
def left(self, x, y):
    if y == 0:
        return [x, self.size - 1]
    else:
        return [x, y - 1]
def right(self, x, y):
   if y == self.size - 1:
        return [x, 0]
    else:
        return [x, y + 1]
def delta(self, x1, y1, x2, y2):
    if self.lattice[x1, y1] == self.lattice[x2, y2]:
        return 1
    else:
        return 0
def Delta(self, s1, x2, y2):
    if s1 == self.lattice[x2, y2]: return 1
    else: return 0
def totalE(self):
    E = 0
    for x in range(self.size):
        for y in range(self.size):
            x1, y1 = self.left(x, y)
            xr, yr = self.right(x, y)
            xu, yu = self.up(x, y)
            xd, yd = self.down(x, y)
            E += self.delta(x, y, xl, yl) + self.delta(
                x, y, xr, yr) + self.delta(x, y, xu, yu) + self.delta(
                    x, y, xd, yd)
    E = -self.J * E / 2
    return E
def totalM(self):
    return np.sqrt(
        np.sum(np.cos(2 * np.pi * self.lattice / self.q))**2 +
        np.sum(np.sin(2 * np.pi * self.lattice / self.q))**2)
def avgE(self):
    return self.totalE() / self.size**2
def avgM(self):
    return self.totalM() / self.size**2
def deltaE(self, x, y, new_state):
    x1, y1 = self.left(x, y)
    xr, yr = self.right(x, y)
    xu, yu = self.up(x, y)
    xd, yd = self.down(x, y)
```

```
deltaE = -self.J * (
        self.Delta(new_state, xl, yl) + self.Delta(new_state, xr, yr) +
        self.Delta(new_state, xu, yu) +
        self.Delta(new_state, xd, yd)) + self.J * (
            self.delta(x, y, xl, yl) + self.delta(x, y, xr, yr) +
            self.delta(x, y, xu, yu) + self.delta(x, y, xd, yd))
    return deltaE
def flip(self, temperature):
    x = random.randint(0, self.size - 1)
    y = random.randint(0, self.size - 1)
    state = self.lattice[x, y]
    new_state = random.randint(1, self.q)
    deltaE = self.deltaE(x, y, new_state)
    if deltaE < 0:</pre>
        self.lattice[x, y] = new_state
        self.E += deltaE
    else:
        if random.random() < np.exp(-deltaE / temperature):</pre>
            self.lattice[x, y] = new_state
            self.E += deltaE
def output(self, t1, t2, step, start: int = 100000, times: int = 10000):
    t = t1
    templ = []
    E = []
    M = []
    C = []
    X = \lceil \rceil
    for i in tqdm(range(int((t2 - t1) / step + 1))):
        templ.append(t)
        E_t = []
        M_t = []
        self.set_initial()
        for i in range(start):
            self.flip(t)
        for time in range(times):
            self.flip(t)
            E_t.append(self.E)
            M_t.append(self.totalM())
        E.append(np.mean(E_t) / self.size**2)
        M.append(np.mean(M_t) / self.size**2)
        C.append((np.mean(np.array(E_t)**2) - np.mean(E_t)**2) /
                 (self.size**2 * t**2))
        X.append(
            (np.mean(np.array(M_t)**2) - np.mean(M_t)**2) / (self.size**2))
        t += step
    return templ, E, M, C, X
```

```
def plot(q, E, M, C, X):
    plt.figure(figsize=[10,10])

plt.subplot(221)
    plt.plot(temp, E, label='q=' + str(q))
    plt.title('energy')
    plt.legend()
```

```
plt.subplot(222)
plt.plot(temp, M, label='q=' + str(q))
plt.title('magnetization')
plt.legend()

plt.subplot(223)
plt.scatter(temp, C, label='q=' + str(q))
plt.title('heat capacity')
plt.legend()

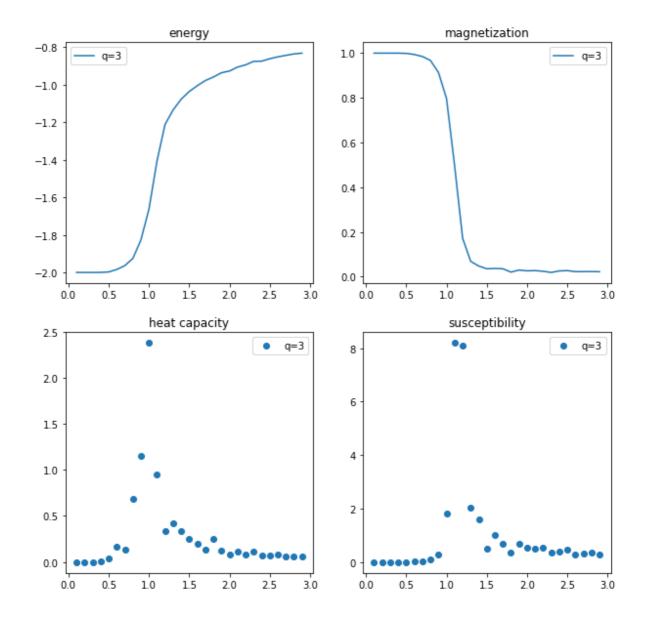
plt.subplot(224)
plt.scatter(temp, X, label='q=' + str(q))
plt.title('susceptibility')
plt.legend()

plt.show()
```

```
P3 = q_Potts(50, 1, 3)
temp, E, M, C, X = P3.output(0.1, 3, 0.1, times=100000)
```

```
100%| 29/29 [08:05<00:00, 16.74s/it]
```

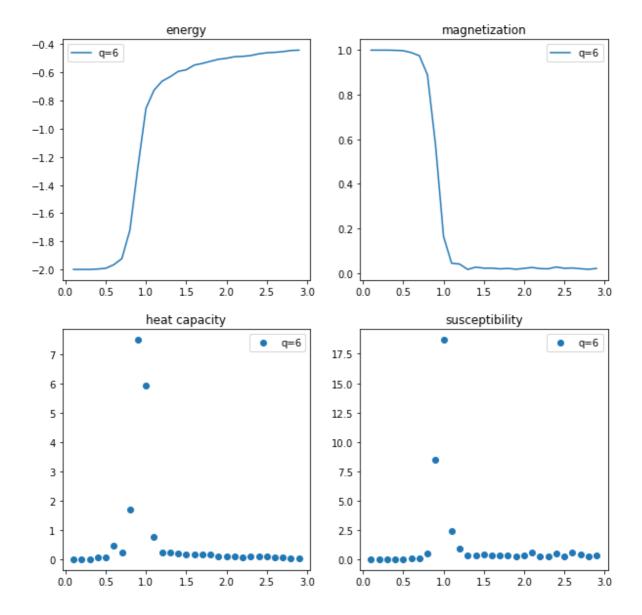
```
plot(3, E, M, C, X)
```



```
P6 = q_Potts(50, 1, 6)
temp, E, M, C, X = P6.output(0.1, 3, 0.1, times=100000)
```

```
100%| 29/29 [07:22<00:00, 15.27s/it]
```

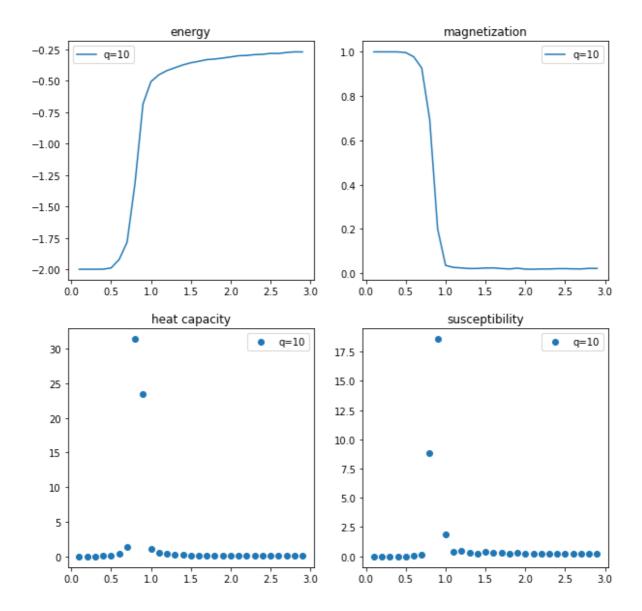
```
plot(6, E, M, C, X)
```



```
P10 = q_Potts(50, 1, 10)
temp, E, M, C, X = P10.output(0.1, 3, 0.1, times=100000)
```

```
100%| 29/29 [07:29<00:00, 15.52s/it]
```

```
plot(10, E, M, C, X)
```



缩小温度范围

$$q = 3$$

```
def plot_(q, E, M, C, X):
    plt.figure(figsize=[10, 10])

    plt.subplot(221)
    plt.plot(temp, E, '.-.', label='q=' + str(q))
    plt.title('energy')
    plt.legend()

    plt.subplot(222)
    plt.plot(temp, M, '.-.', label='q=' + str(q))
    plt.title('magnetization')
    plt.legend()

    plt.subplot(223)
    plt.scatter(temp, C, label='q=' + str(q))
    plt.title('heat capacity')
    plt.legend()
```

```
plt.subplot(224)
plt.scatter(temp, X, label='q=' + str(q))
plt.title('susceptibility')
plt.legend()

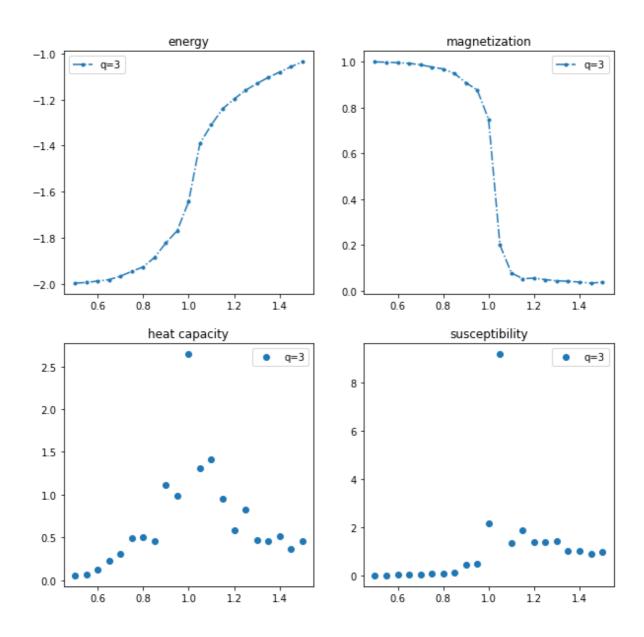
plt.show()
```

```
P3 = q_Potts(50, 1, 3)
temp, E, M, C, X = P3.output(0.5, 1.5, 0.05, start=500000, times=500000)
```

```
100%| 21/21 [23:57<00:00, 68.47s/it]
```

```
data = np.c_[temp, E, M, C, X]
np.save('2_3_q=3_data', data)
```

```
plot_(3, E, M, C, X)
```



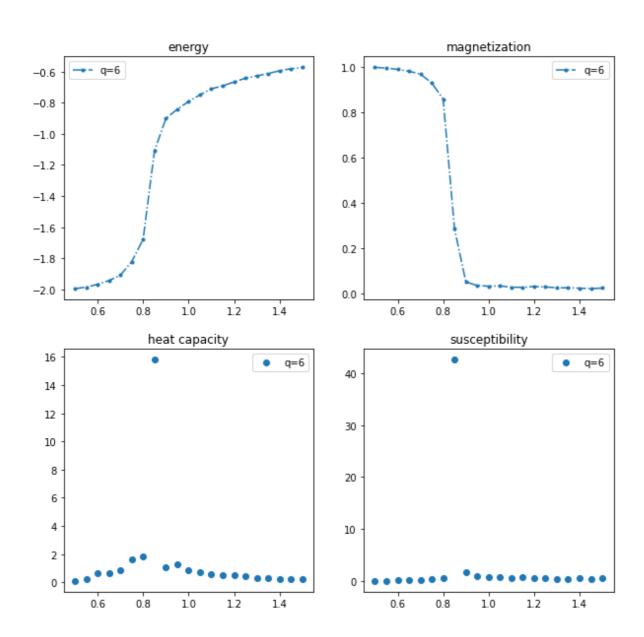
```
q = 6
```

```
P6 = q_Potts(50, 1, 6)
temp, E, M, C, X = P6.output(0.5, 1.5, 0.05, start=500000, times=500000)
```

```
100%| 21/21 [21:50<00:00, 62.38s/it]
```

```
data = np.c_[temp, E, M, C, X]
np.save('2_3_q=6_data', data)
```

```
plot_(6, E, M, C, X)
```



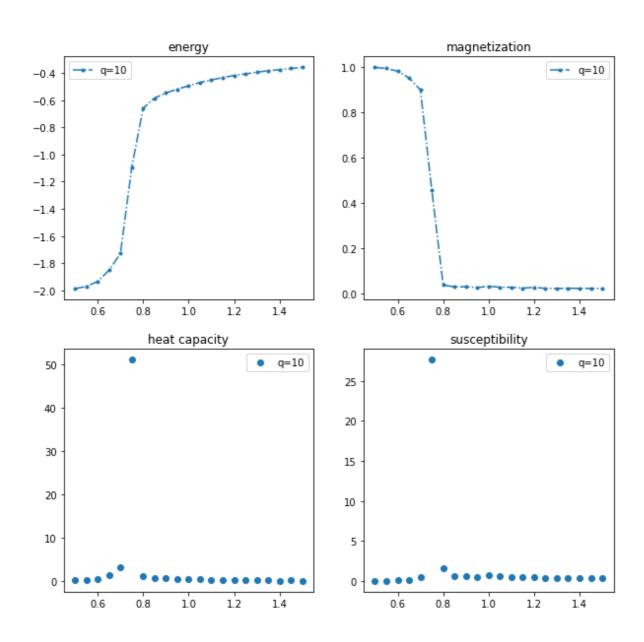
q=6 时,相变温度在 $\sim 0.85 K$

```
P10 = q_Potts(50, 1, 10)
temp, E, M, C, X = P10.output(0.5, 1.5, 0.05, start=500000, times=500000)
```

100%| 21/21 [21:24<00:00, 61.15s/it]

```
data = np.c_[temp, E, M, C, X]
np.save('2_3_q=10_data', data)
```

 $plot_{10}$, E, M, C, X)



q=10 时,相变温度在 $\sim 0.75 K$

与 q=2 相比,临界温度随 q 增大而减小。且一阶相变的情况越来越明显。