蒙特卡洛模拟-伊辛模型

代码实现

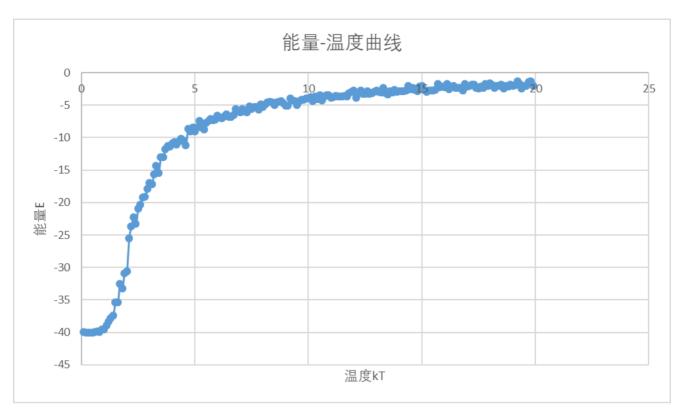
```
import numpy as np
import matplotlib.pyplot as plt
from numba import jit,int8,float32
                                                     #初始化参数
J = 1
kT = 1
ising = np.zeros((7,7))
                                                     #初始化模型
def init():
   for i in range(1,6):
       for j in range(1,6):
            np.random.seed()
            a = np.random.random_sample()
            if a>=0.5:
                ising[i][j]=1
            else:
                ising[i][j]=-1
init()
@jit(float32(int8,int8,int8[::]))
def H(i,j,A=ising):
                                                     #定义能量
    e_{ij} = -J/2*(A[i][j]*(A[i-1][j]+A[i+1][j]+A[i][j-1]+A[i][j+1]))
    return e_ij
@jit(float32(int8,int8,int8[::]))
                                                     #计算翻转概率
def P(i,j,A=ising):
    delta_h = -4*H(i,j)
    p = np.exp(-delta_h/kT)
    return p
@jit(float32(int8[::]))
                                                     #计算模型能量
def calc_energy(A=ising):
    e = 0
    for i in range(1,6):
       e_i = 0
        for j in range(1,6):
            e_{ij} = H(i,j)
            e_i = e_i + e_{ij}
        e = e + e_i
   return e
                                                     #蒙特卡洛模拟
energy_list = np.array([])
for _ in range(100000):
   if %100 == 0:
        print(_)
        np.random.seed()
    i = np.random.randint(1,5)
    j = np.random.randint(1,5)
   ran = np.random.random_sample()
    p = P(i,j)
   if ran < p:</pre>
        ising[i][j] = -ising[i][j]
    else:
        pass
    e = calc_energy()
    energy_list = np.append(energy_list,e)
                                                    #计算能量平均值
energy = np.average(energy_list)
print(energy)
```

由于python的计算速度过慢,后改用go语言实现并编译成可执行文件(输出的是不同温度对应的不同能量的列表)

```
package main
import (
   "math/rand"
   "math"
   "time"
   "fmt"
)
var J = 1.0
var kT float64
func H(i, j int)float64{
   e_ij := -J/2*float64(ising[i][j]*(ising[i-1][j]+ising[i+1][j]+ising[i][j-1]+ising[i][j+1]))
   return e ij
}
func P(i, j int)float64{
   delta_h := -4*H(i,j)
   p := math.Exp(-delta_h/kT)
   return p
}
func calc_energy()float64{
   e := 0.0
   for i:=1;i<6;i++{
       e_i := 0.0
       for j:=1;j<6;j++ {
           e_{ij} := H(i,j)
           e_i = e_i + e_{ij}
       }
       e = e + e_i
   }
   return e
}
func random_int(a, b int)int{
   var x int
   for b>0{
       x = rand.Intn(b+1)
       if x>a-1{
           break;
       }
   return x
func main(){
var energy_list [100000] float64
var energy,ran,p,sum_energy float64
var m,n int
for i:=1;i<6;i++{
       for j:=1;j<6;j++{</pre>
           rand.Seed(int64(time.Now().Nanosecond()))
           a:=rand.Float64()
```

```
if a \ge 0.5
                  ising[i][j]=1
             }else{
                  ising[i][j]=-1
             }
         }
    }
for kT = 0.1; kT<20; kT = kT+0.1{
for k:=0; k<100000; k++{}
    if k%100 == 0{
         rand.Seed(int64(time.Now().Nanosecond()))
    }
    m = random_int(1,5)
    n = random_int(1,5)
    ran = rand.Float64()
    p = P(m,n)
    if ran<p{</pre>
         ising[m][n] = -ising[m][n]
    energy_list[k] = calc_energy()
}
sum_energy = 0
for 1:=0;1<100000;1++{}
    sum_energy = sum_energy + energy_list[1]
energy = sum_energy/100000
fmt.Println(energy)
}
}
```

绘制E-kT图像



可观测到在2到3出出现明显的相变潜热