计算物理第六次作业

- 请提交一个 PDF 格式的作业解答，其中可以描述相应的解题步骤，必要的图表等 (建议用 LaTeX 进行排版)。
- 请提交程序的源文件 (格式:python,Fortran,c/c++)，并请提交一个源文件的说明文档 (任意可读格式), 主要说明源程序如何编译、输入输出格式等方面的事宜。请保证它们能够顺利编译通过，同时运行后产生你的解答中的结果。
- 所有文件打包为压缩文件夹后发送到课程的公邮 (num_phys2022@163.com)。压缩包的文件名和邮件题目请取为 "**学号 + 姓名 + 第几次作业**"。作业收到后自动回复。

1.

选取某种程序自带的随机数产生方法, 产生一组 $[0-1]$ 之间均匀分布的随机数.

1.1

利用随机数, 编写程序对下列积分进行蒙特卡洛计算。重复上述步骤多次 (如: 1000 次), 给出积分值的分布曲线, 讨论该分布与撒点数的关系。

$$\int_0^1 dx \exp[-100 \times (x-0.5)^2]$$

1.2

利用随机数，编写程序对下列多维积分进行蒙特卡洛估算:

$$\int_0^1 \cdots \int_0^1 dx_1 \cdots dx_9 \exp\left[-100 \times \sum_{i=1}^{i=9} (x_i - 0.5)^2\right]$$

2.

The Potts model has been, in addition to the Ising model, widely used in studies of phase transitions in statistical physics. The so-called two-dimensional q-state Potts model has an energy given by

$$E = -J \sum_{<kl>}^{N} \delta_{s_l, s_k}$$

(the symbol < kl > indicates that we sum over nearest neighbours only.) where the spin s_k at lattice position k can take the values $1, 2, \ldots, q$. The Kroneckr delta function δ_{s_l,s_k} equals unity if the spins are equal and is zero otherwise. N is the total number of spins. For $q = 2$ the Potts model corresponds to the Ising model. To see that we can rewrite the last equation as

$$E = -\frac{J}{2}\sum_{<kl>}^{N} 2\left(\delta_{s_l,s_k} - \frac{1}{2}\right) - \sum_{<kl>}^{N}\frac{J}{2}.$$

Now, $2\left(\delta_{s_l,s_k} - \frac{1}{2}\right)$ is $+1$ when $s_l = s_k$ and -1 when they are different. This model is thus equivalent to the Ising model except a trivial difference in the energy minimum given by a an additional constant and a factor $J \to J/2$. One of the many applications of the Potts model is to helium absorbed on the surface of graphite.

The Potts model exhibits a second order phase transition for low values of q and a first order transition for larger values of q. Using Eherenfest's definition of a phase transition, a second order phase transition has second derivatives of the free energy that are discontinuous or diverge (the heat capacity and susceptibility in our case) while a first order transition has first derivatives like the mean energy that are discontinuous or diverge. Since the calculations are done with a finite lattice it is always difficult to find the order of the phase transitions. In this project we will limit ourselves to find the temperature region where a phase transition occurs and see if the numerics allows us to extract enough information about the order of the transition.

2.1

Write a program which simulates the $q = 2$ Potts model for two-dimensional lattices with $10 \times 10, 40 \times 40$ and 80×80 spins and compute the average energy and specific heat. Establish an appropriate temperature range for where you see a sudden change in the heat capacity and susceptibility. Make the analysis first for few Monte Carlo cycles and smaller lattices in order to narrow down the region of interest. To get appropriate statistics afterwards you should allow for at least 10^5 Monte Carlo cycles. In setting up this code you need to find an efficient way to simulate the energy differences between different microstates. In doing this you need also to find all possible values of ΔE.

2.2

Compare these results with those obtained with the twodimensional Ising model. The exact critical temperature for the Ising model is Tc = 2.269. Tip when comparing results with the Ising model: remove the constant term. The first step is thus to check that your algorithm for the Potts model gives the same results as the Ising model. Note that critical temperature

for the $q = 2$ Potts model is half of that for the Ising model.

2.3

Extend the calculations to the Potts model with $q = 3, 6$ and $q = 10$. Make a table of the possible values of ΔE for each value of q. Establish first the location of the peak in the specific heat and study the behavior of the mean energy and magnetization as functions of q. Do you see a noteworthy change in behavior from the $q = 2$ case? For larger q values you may need lattices of at least 50×50 in size. For $q = 3$ and higher you can then proceed as follows: - Do a calculation with a small lattice first over a large temperature region. Use typical temperature steps of 0.1. - Establish a small region where you see the heat capacity and the susceptibility start to increase. - Decrease the temperature step in this region and perform calculations for larger lattices as well.

For $q = 6$ and $q = 10$ we have a first order phase transition, the energy shows a discontinuity at the critical temperature.