期末考试

截止时间：2021. 6. 16（周三）12:00

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成绩：________

- 通用符号：$T=$ 温度，$P=$ 压强，$V=$ 体积，$N=$ 粒子数，$\rho=$ 数密度，$\mu=$ 化学势，$k=$ Boltzmann 常数，$\hbar=$ Plank 常数.
- 热力学极限：

$$N\to\infty\quad V\to\infty\quad \rho=\frac{N}{V}\neq 0\text{且有限.}$$

第 1 题 得分: ________. 某一磁性物质对外界所做的微功为

$$\delta W=-H\mathrm{d}M$$

其中 H 和 M 为磁场强度和磁化强度. 体积固定且设为 1.
如果 H, M 和温度 T 的关系为

$$M=\frac{aH}{T-T_c}$$

a, T_c 为常数且 $T>T_c$.

1) 证明该物质的内能由下式给出：（10 分）

$$U(T,M)=U(T,0)-\frac{M^2T_c}{2a}.$$

2) 求该物质在 H 固定条件下的热容量，$C_H(T,M)$.（10 分）

解: 1) 由热力学第一定律的微分形式

$$\mathrm{d}U=\delta Q-\delta W=T\,\mathrm{d}S+H\,\mathrm{d}M.\tag{1}$$

以及 Helmholtz 自由能的定义

$$F=U-TS,\tag{2}$$

可得 Helmholtz 自由能的微分为

$$\mathrm{d}F=-S\,\mathrm{d}T+H\,\mathrm{d}M.\tag{3}$$

由上式可得

$$S=-\left(\frac{\partial F}{\partial T}\right)_M,\tag{4}$$

$$H=\left(\frac{\partial F}{\partial M}\right)_T.\tag{5}$$

以上两式分别关于磁化强度 M 和温度 T 求导可得

$$\left(\frac{\partial S}{\partial M}\right)_T=-\frac{\partial^2 F}{\partial M\partial T}=-\left(\frac{\partial H}{\partial T}\right)_M.\tag{6}$$

在给定温度下，磁性物质的内能关于磁化强度 M 的偏导为

$$\left(\frac{\partial U}{\partial M}\right)_T=T\left(\frac{\partial S}{\partial M}\right)_T+H.\tag{7}$$

将式 (6) 以及 H, M 和 T 的关系 $M=\frac{aH}{T-T_c}$，代入上式可得

$$\left(\frac{\partial U}{\partial M}\right)_T=-T\left(\frac{\partial H}{\partial T}\right)_M+H=-\frac{TM}{a}+\frac{(T-T_c)M}{a}=-\frac{T_cM}{a}.\tag{8}$$

因此，

$$U(T,M)=U(T,0)+\int_0^M\left(\frac{\partial U}{\partial M}\right)_T\mathrm{d}M=U(T,0)-\int_0^M\frac{T_cM'}{a}\,\mathrm{d}M'=U(T,0)-\frac{T_cM^2}{2a}.\tag{9}$$

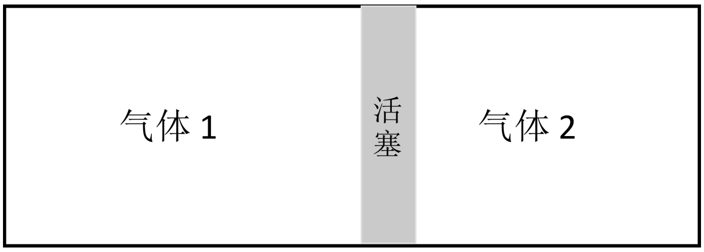
2) 该物质在 H 固定条件下的热容量为

$$C_H(T,M)=\lim_{\Delta T\to 0}\left(\frac{\Delta Q}{\Delta T}\right)_H=\lim_{\Delta T\to 0}\left(\frac{\Delta U-H\,\mathrm{d}M}{\Delta T}\right)_H=\frac{\mathrm{d}U(T,M=0)}{\mathrm{d}T}-\frac{T_cM}{a}\left(\frac{\partial M}{\partial T}\right)_H-H\left(\frac{\partial M}{\partial T}\right)_H \tag{10}$$

$$=\frac{\mathrm{d}U(T,M=0)}{\mathrm{d}T}+\left(\frac{T_cM}{a}+H\right)\frac{aH}{(T-T_c)^2}=\frac{\mathrm{d}U(T,M=0)}{\mathrm{d}T}+\frac{TM^2}{a(T-T_c)}. \tag{11}$$

□

第 2 题 得分: _________. 一温度为 T 的圆柱形容器被一活塞隔成两部分. 每部分放置一种非相对论 Fermi 气体. 活塞可以自由移动. 两种 Fermi 气体的分子质量相同，但自旋不同，分别为 j_1 和 j_2. 求 $T=0$ 和 $T\to\infty$ 条件下两种 Fermi 气体分子数密度的比值.（20 分）



解: 非简并情况下，非相对论 Fermi 气体的状态方程为

$$\frac{P}{kT}=\frac{\omega}{\lambda^3}\left(z-\frac{z^2}{2^{5/2}}+\cdots\right). \tag{12}$$

粒子数密度为

$$\rho=\frac{\omega}{\lambda^3}\left(z-\frac{z^2}{2^{3/2}}+\cdots\right). \tag{13}$$

其中热波长 $\lambda=\sqrt{\frac{2\pi}{mkT}}\hbar$，易逸度 $z=e^{\beta\mu}$. 在 $T\to\infty$ 条件下，$z\ll 1$，以上两式联立解得

$$\frac{P}{kT}=\rho\left(1+\frac{1}{2^{5/2}}\frac{\rho\lambda^3}{\omega}+\cdots\right). \tag{14}$$

容器温度给定，故两部分气体温度相等，$T_1=T_2$；活塞可以自由移动，故两部分气体压强相等，$P_1=P_2$. 故在$T\to\infty$ 条件下，两部分气体的分子数密度为

$$\boxed{\frac{\rho_1}{\rho_2}=1.} \tag{15}$$

非相对论气体的态密度为

$$D(\varepsilon)=\frac{(2j+1)m^{3/2}\varepsilon^{1/2}}{\sqrt{2}\pi^2\hbar^3}. \tag{16}$$

分子数密度为

$$\rho=\frac{N}{V}=\int_0^{\varepsilon_F}\mathrm{d}\varepsilon\,D(\varepsilon)=\int_0^{\varepsilon_F}\mathrm{d}\varepsilon\,\frac{(2j+1)m^{3/2}\varepsilon^{1/2}}{\sqrt{2}\pi^2\hbar^3}=\frac{2}{3}\frac{(2j+1)m^{3/2}\varepsilon_F^{3/2}}{\sqrt{2}\pi^2\hbar^3}, \tag{17}$$

$$\Longrightarrow \varepsilon_F=\left[\frac{3}{\sqrt{2}}\frac{\pi^2\hbar^3}{(2j+1)m^{3/2}}\frac{N}{V}\right]^{2/3}. \tag{18}$$

在 $T=0$ 下，非相对论 Fermi 气体的内能为

$$U=V\int_0^{\varepsilon_F}\mathrm{d}\varepsilon\,D(\varepsilon)\varepsilon=V\frac{2}{5}\frac{(2j+1)m^{3/2}\varepsilon_F^{5/2}}{\sqrt{2}\pi^2\hbar^3}. \tag{19}$$

因此

$$U\propto V^{-2/3}. \tag{20}$$

压强为

$$P=-\frac{\partial U}{\partial V}=\frac{2}{3}\frac{U}{V}=\frac{4}{15}\frac{(2j+1)m^{3/2}\varepsilon_F^{5/2}}{\sqrt{2}\pi^2\hbar^3}. \tag{21}$$

活塞可以自由移动，故两部分气体压强相等，$P_1=P_2$，即

$$\frac{4}{15}\frac{(2j_1+1)m^{3/2}\varepsilon_{F,1}^{5/2}}{\sqrt{2}\pi^2\hbar^3}=\frac{4}{15}\frac{(2j_2+1)m^{3/2}\varepsilon_{F,2}^{5/2}}{\sqrt{2}\pi^2\hbar^3}, \tag{22}$$

$$\Longrightarrow\frac{\varepsilon_{F,1}}{\varepsilon_{F,2}}=\left(\frac{2j_1+1}{2j_2+1}\right)^{-2/5}. \tag{23}$$

将上式代入式 (17) 中可得在 $\underline{T=0\text{ 条件下}}$，两部分气体的分子数密度比值为

$$\boxed{\frac{\rho_1}{\rho_2}=\frac{2j_1+1}{2j_2+1}\left(\frac{\varepsilon_{F,1}}{\varepsilon_{F,2}}\right)^{3/2}=\left(\frac{2j_1+1}{2j_2+1}\right)^{2/5}.} \tag{24}$$

综上，在 $T=0$ 和 $T\to\infty$ 条件下两种 Fermi 气体分子数密度的比值为

$$\boxed{\frac{\rho_1}{\rho_2}=\begin{cases}\left(\frac{2j_1+1}{2j_2+1}\right)^{2/5}, & T=0.\\ 1, & T\to\infty.\end{cases}} \tag{25}$$

□

第 3 题 得分: _________. 考虑一低密度的经典单原子非理想气体，原子之间的相互作用势能为

$$u(r)=\begin{cases}\infty, & r\leq a\\ -g, & a<r<b\\ 0, & r\geq b\end{cases}$$

1) 求精确到 ρ^2 的状态方程，即把 P/kT 展开到 ρ^2.（10 分）

2) 求该气体的化学势对理想气体化学势的领头阶修正.（5 分）

3) 求该气体的熵和内能对理想气体熵和内能的领头阶修正.（5 分）

解: 1) 根据原子之间的相互作用势能，有

$$f_{ij}(r)=e^{-\beta u_{ij}(r)}-1=\begin{cases}-1, & r\leq a,\\ e^{\beta g}-1, & a<r<b,\\ 0, & r\geq b.\end{cases} \tag{26}$$

利用 Mayer 第二定理对 $\frac{P}{kT}$ 按 ρ 的幂级数展开，有

$$\frac{P}{kT}=\rho\left[1-\frac{1}{2}\beta_1\rho+O(\rho^2)\right]. \tag{27}$$

其中 viral 系数

$$\beta_1=2b_2, \tag{28}$$

$$\begin{aligned}b_2=&\frac{1}{2!V}\int\mathrm{d}^3\vec{r}_2\int\mathrm{d}^3\vec{r}_1\,f_{12}(|\vec{r}_1-\vec{r}_2|)=2\pi\int_0^b\mathrm{d}r_{12}\,r_{12}^2f_{12}(r_{12})=2\pi\left[\int_0^a\mathrm{d}r_{12}\,r_{12}^2(-1)+\int_a^b\mathrm{d}r_{12}\,r_{12}^2(e^{\beta g}-1)\right]\\ =&2\pi\left[-\frac{a^3}{3}+(e^{\beta g}-1)(b^3-a^3)\right],\end{aligned} \tag{29}$$

故

$$\boxed{\frac{P}{kT}=\rho\left\{1-2\pi\left[-\frac{a^3}{3}+(e^{\beta g}-1)(b^3-a^3)\right]\rho+O(\rho^2)\right\}.} \tag{30}$$

2) 理想气体的状态方程为

$$\rho_0=\frac{P}{kT}. \tag{31}$$

上式与该非理想气体的状态方程联立得

$$\rho_0=\rho[1-b_2\rho+O(\rho^2)], \tag{32}$$

$$\Longrightarrow\rho=\rho_0\left[1+b_2\rho_0+O(\rho_0^2)\right], \tag{33}$$

其中

$$\rho=\sum_{l=1}^{\infty}lb_ly^l=y+2b_2y^2+O(y^3), \tag{34}$$

$$\rho_0=y_0. \tag{35}$$

从而

$$y_0=(y+2b_2y^2+O(y^3))[1-b_2(y+2b_2y^2+O(y^3))+O(y^2)]=y+b_2y^2+O(y^3), \tag{36}$$

$$\Longrightarrow y = y_0 - b_2 y_0^2 + O(y_0^3). \tag{37}$$

该气体的化学势为

$$\mu = kT \ln z = kT \ln[\lambda^3 y] = kT \ln\left[\lambda^3 (y_0 - b_2 y_0^2 + O(y_0^3))\right] \tag{38}$$

其中

$$y_0 = \frac{z_0}{\lambda^3} = \frac{e^{\beta\mu_0}}{\lambda^3} \Longrightarrow \mu_0 = kT \ln(\lambda^3 y_0), \tag{39}$$

μ_0 为理想气体的化学势，$\beta = \frac{1}{kT}$，故

$$\mu = \mu_0 + kT \ln(1 - b_2\rho_0 + O(\rho_0^2)) = \mu_0 - kT b_2 \rho_0 + O(\rho_0^2) = \mu_0 - kT b_2 \rho + O(\rho^2), \tag{40}$$

即该气体的化学势对理想气体化学势的领头阶修正为 $\underline{kTb_2\rho}$，其中 $b_2 = 2\pi\left[-\frac{a^3}{3} + (e^{\beta g} - 1)(b^3 - a^3)\right]$.

3) 理想气体的 Gibbs 势为

$$G_0 = N\mu_0. \tag{41}$$

理想气体的熵为

$$S_0 = -\frac{\partial G_0}{\partial T}. \tag{42}$$

理想气体的内能为

$$U_0 = G_0 + TS_0 - PV. \tag{43}$$

该气体的 Gibbs 势为

$$G = N\mu = G_0 + N[kTb_2\rho + O(\rho^2)]. \tag{44}$$

该气体的熵为

$$\begin{aligned}
S = -\frac{\partial G}{\partial T} &= S_0 + Nkb_2\rho + NkTb_2\frac{\partial \rho}{\partial T} \\
&= S_0 + Nkb_2\rho + NkTb_2\frac{\partial\{\rho_0[1 + b_2\rho_0 + O(\rho_0^2)]\}}{\partial T} \\
&= S_0 + Nkb_2\rho + NkTb_2(1 + 2b_2\rho_0 + O(\rho_0^2))\frac{\partial \rho_0}{\partial T} \\
&= S_0 + Nkb_2\rho + NkTb_2(1 + 2b_2\rho_0 + O(\rho_0^2))\frac{\partial\left(\frac{P}{kT}\right)}{\partial T} \\
&= S_0 + Nkb_2\rho + NkTb_2(1 + 2b_2\rho_0 + O(\rho_0^2))\left(-\frac{P}{kT^2}\right) \\
&= S_0 + Nkb_2\rho - Nkb_2\rho_0(1 + 2b_2\rho_0 + O(\rho_0^2)) \\
&= S_0 + Nkb_2\rho - Nkb_2\rho(1 - b_2\rho + O(\rho^2))[1 + 2b_2\rho(1 - b_2\rho + O(\rho^2)) + O(\rho^2)] \\
&= S_0 + O(\rho^2),
\end{aligned}$$

即该气体的熵对理想气体的熵的领头阶修正为 $\underline{0}$. 该气体的内能为

$$\begin{aligned}
U &= G + TS - PV = G_0 + N[kTb_2\rho + O(\rho^2)] + T[S_0 + O(\rho^2)] + PV = G_0 + NkTb_2\rho + TS_0 + O(\rho^2) \\
&= U_0 + NkTb_2\rho + O(\rho^2),
\end{aligned} \tag{45}$$

即该气体的内能对理想气体的内能的领头阶修正为 $\underline{NkTb_2\rho}$，其中 $b_2 = 2\pi\left[-\frac{a^3}{3} + (e^{\beta g} - 1)(b^3 - a^3)\right]$.

□

第 4 题 得分: ________. 用 Monte Carlo 方法数值求解零场下正方格点上的二维 Ising 模型. 假设最近邻铁磁耦合，且任何近邻对的耦合能量相同.

1) 写出 Hamiltonian 和计算程序的流程.（5 分）

2) 绘出磁化强度作为温度的函数的图像.（10 分）

3) 确定临界温度并与严格解比较.（5 分）

提示：要求格点至少为 10×10，并取周期性边界条件.

解: 1) Ising 模型的 Hamiltonian 为

$$H(\{S_i\})=-\frac{1}{2}J\sum_{\langle i,j\rangle}S_i\cdot S_j, \tag{46}$$

其中 J 为近邻对的耦合系数，S_i 为第 i 个格点的自旋且 $S_i\in\{\pm 1\}$，$\sum_{\langle i,j\rangle}$ 代表对相邻的格点对求和.

计算过程：

1. **初始化**：设定正方形晶格尺寸 $L\times L$，温度 T，耦合系数 J，所有自旋均向上，即$(S_i)_z=+1\quad\forall i$；
2. **Warming up**：随机选取晶格中的某个格点 i，利用上面的 Hamiltonian 计算该格点的自旋在翻转前和翻转后的能量差：
$$\Delta E=-JS_i\cdot\sum_{j\in\{\text{neighbors of i}\}}S_j. \tag{47}$$
若 $\Delta E<0$，则翻转该格点的自旋；否则生成一个在 $[0,1)$ 范围内均匀分布的随机数 r，比较 r 和 $e^{-E/kT}$，若 $r\leq e^{-\Delta E/kT}$，则翻转该格点的自旋，若 $r>e^{-\Delta E/kT}$，则不翻转（即按照 $e^{-E/kT}$ 的概率翻转该格点的自旋）. 重复这样的操作足够多步，使系统达到平衡态；
3. **演化和测量**：用与上一步相同的方法，随机选择格点并尝试翻转其自旋，每完成一步，就测量一次系统的磁化强度（这里假设单位晶胞的大小为 1）
$$M=\frac{1}{L\times L}\sum_i S_i. \tag{48}$$
重复这样的操作足够多次，然后计算磁化强度的平均值 $\langle M\rangle$.
4. 扫描温度 T，重复以上 2.、3. 步骤，从而得到磁化强度随温度的函数曲线.

2) 这里我们取各点数为 32×32，简单起见取 $k=1$，$J=1$，温度从 0.01 K 扫描到 5.00 K，步长为 0.01 K，得到如图 1 所示的磁化强度关于温度的函数曲线.

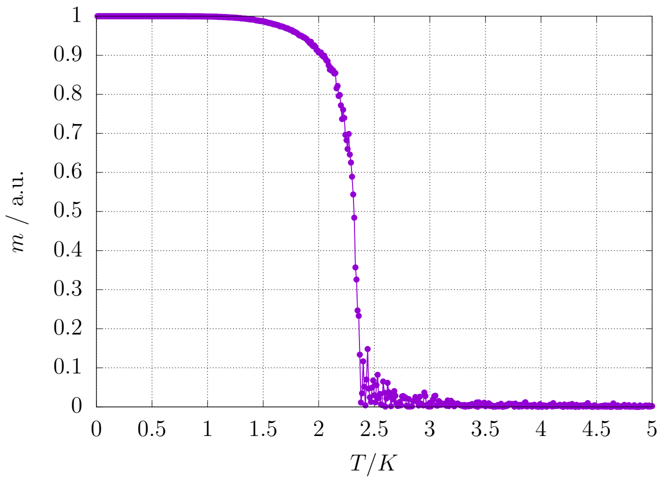


图 1: 32×32 格点的 Ising 模型磁化强度关于温度的函数曲线.

3) 由图 1 中可见，该 Ising 模型的临界温度约 2.3 K，利用平均场理论，临界温度的严格解为

$$\tanh^2 \frac{2J}{kT_c} = \frac{1}{2} \Longrightarrow T_c = \frac{2J}{k\ln(1+\sqrt{2})} = \frac{2\times 1}{1\times\ln(1+\sqrt{2})}\text{ K} = 2.269\text{ K}. \tag{49}$$

两者符合得较好.

附 Fortran 代码如下：

```
program main
    use mpi
    implicit none
    real(8), parameter :: pi = acos(-1.d0), kB = 1.d0
    integer :: ntasks, id, rc
    integer, allocatable :: status(:)
    integer :: i, n, clock
    integer, allocatable :: seed(:)
    real(8) :: r

    real(8) :: T = .01d0, dT = .01d0, T_final = 5.d0, beta
    integer, parameter :: L_x = 32, L_y = 32
    integer :: lattice(0:L_x - 1,0:L_y - 1) = 1
    integer :: x, y
    integer, parameter :: n_warmup = 10000, n_evol = 100000
    real(8) :: J = 1.d0, B = 0.d0
    real(8) :: M, M_sqr, E_tmp, E, E_sqr, M_ave, M_sqr_ave, chi, E_ave, E_sqr_ave, C

    ! initialize MPI environment
    call MPI_INIT(rc)
    call MPI_COMM_SIZE(MPI_COMM_WORLD, ntasks, rc)
    call MPI_COMM_RANK(MPI_COMM_WORLD, id, rc)
```

```
    allocate(status(MPI_STATUS_SIZE))

    ! initialize seeds for different processes
    if (id == 0) then
        call SYSTEM_CLOCK(clock)
        call RANDOM_SEED(size = n)
        allocate(seed(n))
        do i = 1, n
            seed(i) = clock + 37 * i
        end do
        call RANDOM_SEED(PUT = seed)
        deallocate(seed)
        do i = 1, ntasks - 1
            call RANDOM_NUMBER(r)
            clock = clock + Int(r * 1000000)
            call MPI_SEND(clock, 1, MPI_INTEGER, i, i, MPI_COMM_WORLD, rc)
        end do
    else
        call MPI_RECV(clock, 1, MPI_INTEGER, 0, id, MPI_COMM_WORLD, status, rc)
        call RANDOM_SEED(size = n)
        allocate(seed(n))
        do i = 1, n
            seed(i) = clock + 37 * i
        end do
        call RANDOM_SEED(PUT = seed)
        deallocate(seed)
    end if

    if (id == 0) then
        open(unit = 1, file = 'data.txt', status = 'unknown')
        write(*,'(4a20)') 'T', 'm', 'chi', 'C'
    end if

    do while (T < T_final)
        beta = 1.d0 / kB / T
        M = 0.d0
        M_sqr = 0.d0
        E = 0.d0
        E_sqr = 0.d0

        ! warm up
        do i = 1, n_warmup
```

```
            call EVOLUTION(lattice, L_x, L_y, beta, B, J)
        end do

        ! evolution
        do i = 1, n_evol
            call EVOLUTION(lattice, L_x, L_y, beta, B, J)
            M = M + sum(lattice)
            M_sqr = M_sqr + sum(lattice)**2
            E_tmp = 0.d0
            do x = 0, L_x - 2
                do y = 0, L_y - 2
                    E_tmp = E_tmp + lattice(x, y) * (lattice(x + 1, y) + lattice(x, y + 1))
                end do
            end do
            do x = 0, L_x - 2
                E_tmp = E_tmp + lattice(x, L_y - 1) * (lattice(x + 1, L_y - 1) + lattice(x, 0))
            end do
            do y = 0, L_y - 2
                E_tmp = E_tmp + lattice(L_x - 1, y) * (lattice(L_x - 1, y + 1) + lattice(0, y))
            end do
            E_tmp = E_tmp + lattice(L_x - 1, L_y - 1) * (lattice(0, L_y - 1) + Lattice(L_x - 1, 0))
            E_tmp = - E_tmp * J - B * sum(lattice)
            E = E + E_tmp
            E_sqr = E_sqr + E_tmp**2
        end do
        call MPI_REDUCE(M, M_ave, 1, MPI_REAL8, MPI_SUM, 0, MPI_COMM_WORLD, rc)
        call MPI_REDUCE(M_sqr, M_sqr_ave, 1, MPI_REAL8, MPI_SUM, 0, MPI_COMM_WORLD, rc)
        call MPI_REDUCE(E, E_ave, 1, MPI_REAL8, MPI_SUM, 0, MPI_COMM_WORLD, rc)
        call MPI_REDUCE(E_sqr, E_sqr_ave, 1, MPI_REAL8, MPI_SUM, 0, MPI_COMM_WORLD, rc)
        if (id == 0) then
            M_ave = M_ave / dble(ntasks * n_evol)
            M_sqr_ave = M_sqr_ave / dble(ntasks * n_evol)
            chi = beta * (M_sqr_ave - M_ave**2)
            E_ave = E_ave / dble(ntasks * n_evol)
            E_sqr_ave = E_sqr_ave / dble(ntasks * n_evol)
            C = kB * beta**2 / dble((L_x) * (L_y)) * (E_sqr_ave - E_ave**2)
```

```fortran
            write(*,'(4f20.10)') T, M_ave / dble((L_x) * (L_y)), chi, C
            write(1,'(4f20.10)') T, M_ave / dble((L_x) * (L_y)), chi, C
        end if
        T = T + dT
    end do

    if (id == 0) then
        close(1)
    end if

    ! done with MPI
    call MPI_FINALIZE(rc)
end program main

subroutine EVOLUTION(lattice, L_x, L_y, beta, B, J)
    implicit none
    integer, intent(in) :: L_x, L_y
    integer, intent(inout) :: lattice(0:L_x - 1, 0:L_y - 1)
    real(8), intent(in) :: beta, B, J
    real(8) :: r
    integer :: x, y
    real(8) :: dE

    call RANDOM_NUMBER(r)
    x = floor(r * dble(L_x))
    call RANDOM_NUMBER(r)
    y = floor(r * dble(L_y))

    dE = 0.d0
    dE = dE + 2.d0 * J * lattice(x,y) * (lattice(modulo(x - 1, L_x), y)&
        + lattice(modulo(x + 1, L_x), y)&
        + lattice(x, modulo(y - 1, L_y))&
        + lattice(x, modulo(y + 1, L_y)))&
        + 2.d0 * B * dble(lattice(x,y))

    call RANDOM_NUMBER(r)
    if (r < exp(-beta * dE)) then
        lattice(x,y) = -lattice(x,y)
    end if
end subroutine EVOLUTION
```

□

第 5 题 得分: ________. 弱耦合自旋为零玻色气体的相互作用算符为

$$\Omega=\frac{1}{2V}g\sum_{\vec{p}_1+\vec{p}_2=\vec{p}_1'+\vec{p}_2'}a_{\vec{p}_1'}^\dagger a_{\vec{p}_2'}^\dagger a_{\vec{p}_2}a_{\vec{p}_1}\quad g>0$$

其中 $a_{\vec{p}}$ 和 $a_{\vec{p}^\dagger}$ 为动量表象的湮灭产生算符，g 为耦合常数. 令 $|\{n_{\vec{p}}\}\rangle$ 为自由波色气体的能量本征态，其中 $n_{\vec{p}}$ 为动量 $\vec{p}$ 态的占据数.

1) 证明相互作用能密度的平均值

$$E[\{n_{\vec{p}}\}]\equiv\frac{1}{V}\langle\{n_{\vec{p}}\}|\Omega|\{n_{\vec{p}}\}\rangle=g\rho^2-\frac{g}{2V^2}\sum_{\vec{p}}n_{\vec{p}}^2-\frac{g\rho}{2V}$$

其中 ρ 玻色子的数密度.

2) 在热力学极限下比较有 Bose-Einstein 凝聚的上述平均值 E 和没有 Bose-Einstein 凝聚的上述平均值 E'，证明

$$E<E'$$ (5 分)

证: 1) 自由波色气体的能量本征态为

$$|\{n_{\vec{p}}\}\rangle=\prod_{\vec{p}}\frac{\left(a_{\vec{p}}^\dagger\right)^{n_{\vec{p}}}}{\sqrt{n_{\vec{p}}!}}|0\rangle.\tag{50}$$

相互作用能密度的平均值为

$$\begin{aligned}
&E[\{n_{\vec{p}}\}]=\frac{1}{V}\langle\{n_{\vec{p}}\}|\Omega|\{n_{\vec{p}}\}\rangle\\
=&\frac{g}{V^2}\prod_{\vec{p},\vec{p}'}\sum_{\vec{p}_1+\vec{p}_2=\vec{p}_1'+\vec{p}_2'}\frac{1}{\sqrt{n_{\vec{p}'}!}}\frac{1}{\sqrt{n_{\vec{p}}!}}\langle 0|\left(a_{\vec{p}'}\right)^{n_{\vec{p}}}a_{\vec{p}_1'}^\dagger a_{\vec{p}_2'}^\dagger a_{\vec{p}_2}a_{\vec{p}_1}\left(a_{\vec{p}}^\dagger\right)^{n_{\vec{p}}}|0\rangle\\
=&\frac{g}{V^2}\prod_{\vec{p},\vec{p}'}\sum_{\vec{p}_1+\vec{p}_2=\vec{p}_1'+\vec{p}_2'}\frac{1}{\sqrt{n_{\vec{p}'}!}}\frac{1}{\sqrt{n_{\vec{p}}!}}\langle 0|\left(a_{\vec{p}'}\right)^{n_{\vec{p}}}a_{\vec{p}_1'}^\dagger a_{\vec{p}_2'}^\dagger a_{\vec{p}_2}\left\{[a_{\vec{p}_1},a_{\vec{p}}^\dagger]+a_{\vec{p}}^\dagger a_{\vec{p}_1}\right\}\left(a_{\vec{p}}^\dagger\right)^{n_{\vec{p}}-1}|0\rangle\\
=&\frac{g}{V^2}\prod_{\vec{p},\vec{p}'}\sum_{\vec{p}_1+\vec{p}_2=\vec{p}_1'+\vec{p}_2'}\frac{1}{\sqrt{n_{\vec{p}'}!}}\frac{1}{\sqrt{n_{\vec{p}}!}}\langle 0|\left(a_{\vec{p}'}\right)^{n_{\vec{p}}}a_{\vec{p}_1'}^\dagger a_{\vec{p}_2'}^\dagger a_{\vec{p}_2}\left\{\delta_{\vec{p}_1\vec{p}}+a_{\vec{p}}^\dagger a_{\vec{p}_1}\right\}\left(a_{\vec{p}}^\dagger\right)^{n_{\vec{p}}-1}|0\rangle\\
=&\frac{g}{V^2}\prod_{\vec{p},\vec{p}'}\sum_{\vec{p}_1+\vec{p}_2=\vec{p}_1'+\vec{p}_2'}\frac{1}{\sqrt{n_{\vec{p}'}!}}\frac{1}{\sqrt{n_{\vec{p}}!}}\langle 0|\left(a_{\vec{p}'}\right)^{n_{\vec{p}}}a_{\vec{p}_1'}^\dagger a_{\vec{p}_2'}^\dagger a_{\vec{p}_2}\left\{\delta_{\vec{p}_1\vec{p}}+a_{\vec{p}}^\dagger\delta_{\vec{p}_1\vec{p}}+\left(a_{\vec{p}}^\dagger\right)^2a_{\vec{p}_1}\right\}\left(a_{\vec{p}}^\dagger\right)^{n_{\vec{p}}-2}|0\rangle\\
&\cdots\\
=&\frac{g}{V^2}\prod_{\vec{p},\vec{p}'}\sum_{\vec{p}_1+\vec{p}_2=\vec{p}_1'+\vec{p}_2'}\frac{1}{\sqrt{n_{\vec{p}'}!}}\frac{1}{\sqrt{n_{\vec{p}}!}}\langle 0|\left(a_{\vec{p}'}\right)^{n_{\vec{p}}}a_{\vec{p}_1'}^\dagger a_{\vec{p}_2'}^\dagger a_{\vec{p}_2}\left\{\delta_{\vec{p}_1\vec{p}}\sum_{n=0}^{n_{\vec{p}}-1}\left(a_{\vec{p}}^\dagger\right)^n+\left(a_{\vec{p}}^\dagger\right)^{n_{\vec{p}}}a_{\vec{p}_1}\right\}|0\rangle\\
=&\frac{g}{V^2}\prod_{\vec{p},\vec{p}'}\sum_{\vec{p}_1,\vec{p}_2,\vec{p}_1',\vec{p}_2'=\vec{p}_1+\vec{p}_2-\vec{p}_1'}\frac{1}{\sqrt{n_{\vec{p}'}!}}\frac{1}{\sqrt{n_{\vec{p}}!}}\langle 0|\left(a_{\vec{p}'}\right)^{n_{\vec{p}}}a_{\vec{p}_1'}^\dagger a_{\vec{p}_2'}^\dagger a_{\vec{p}_2}\left\{\delta_{\vec{p}_1\vec{p}}\sum_{n=0}^{n_{\vec{p}}-1}\left(a_{\vec{p}}^\dagger\right)^n+\left(a_{\vec{p}}^\dagger\right)^{n_{\vec{p}}}a_{\vec{p}_1}\right\}|0\rangle\\
=&\frac{g}{V^2}\prod_{\vec{p},\vec{p}'}\sum_{\vec{p}_2,\vec{p}_1',\vec{p}_2'=\vec{p}+\vec{p}_2-\vec{p}_1'}\frac{1}{\sqrt{n_{\vec{p}'}!}}\frac{1}{\sqrt{n_{\vec{p}}!}}\langle 0|\left(a_{\vec{p}'}\right)^{n_{\vec{p}}}a_{\vec{p}_1'}^\dagger a_{\vec{p}_2'}^\dagger a_{\vec{p}_2}\left\{\sum_{n=0}^{n_{\vec{p}}-1}\left(a_{\vec{p}}^\dagger\right)^n\right\}|0\rangle\\
=&\frac{g}{V^2}\prod_{\vec{p},\vec{p}'}\sum_{\vec{p}_1',\vec{p}_2'=2\vec{p}-\vec{p}_1'}\frac{1}{\sqrt{n_{\vec{p}'}!}}\frac{1}{\sqrt{n_{\vec{p}}!}}\langle 0|\left(a_{\vec{p}'}\right)^{n_{\vec{p}}}a_{\vec{p}_1'}^\dagger a_{\vec{p}_2'}^\dagger\left\{\sum_{n=0}^{n_{\vec{p}}-1}\sum_{m=0}^{n-1}\left(a_{\vec{p}}^\dagger\right)^m\right\}|0\rangle\\
=&\frac{g}{V^2}\prod_{\vec{p},\vec{p}'}\frac{1}{\sqrt{n_{\vec{p}'}!}}\frac{1}{\sqrt{n_{\vec{p}}!}}\langle 0|\left\{\sum_{l=0}^{n_{\vec{p}'}-1}\left(a_{\vec{p}'}\right)^l\right\}a_{2\vec{p}-\vec{p}'}^\dagger\left\{\sum_{n=0}^{n_{\vec{p}}-1}\sum_{m=0}^{n-1}\left(a_{\vec{p}}^\dagger\right)^m\right\}|0\rangle\\
=&\frac{g}{V^2}\prod_{\vec{p},\vec{p}'}\frac{1}{\sqrt{n_{\vec{p}'}!}}\frac{1}{\sqrt{n_{\vec{p}}!}}\langle 0|\left\{\sum_{l=0}^{n_{\vec{p}}-1}\sum_{k=0}^{l-1}\left(a_{\vec{p}'}\right)^k\delta_{\vec{p}',2\vec{p}-\vec{p}'}\right\}\left\{\sum_{n=0}^{n_{\vec{p}}-1}\sum_{m=0}^{n-1}\left(a_{\vec{p}}^\dagger\right)^m\right\}|0\rangle
\end{aligned}$$

$$
\begin{aligned}
=&\frac{g}{V^2}\prod_{\vec{p},\vec{p}'}\frac{1}{\sqrt{n_{\vec{p}'}!}}\frac{1}{\sqrt{n_{\vec{p}}!}}\langle 0|\left\{\sum_{l=0}^{n_{\vec{p}}-1}\sum_{k=0}^{l-1}\left(a_{\vec{p}'}\right)^k\delta_{\vec{p},\vec{p}'}\right\}\left\{\sum_{n=0}^{n_{\vec{p}}-1}\sum_{m=0}^{n-1}\left(a_{\vec{p}}^\dagger\right)^m\right\}|0\rangle\\
=&\frac{g}{V^2}\prod_{\vec{p},\vec{p}'}\frac{1}{\sqrt{n_{\vec{p}'}!}}\frac{1}{\sqrt{n_{\vec{p}}!}}\langle 0|\left\{\sum_{l=0}^{n_{\vec{p}'}-1}\left(n_{\vec{p}'}-l-1\right)\left(a_{\vec{p}'}\right)^l\delta_{\vec{p},\vec{p}'}\right\}\left\{\sum_{n=0}^{n_{\vec{p}}-1}\left(n_{\vec{p}}-n-1\right)\left(a_{\vec{p}}^\dagger\right)^n\right\}|0\rangle\\
=&g\rho^2-\frac{g}{2V^2}\sum_{\vec{p}}n_{\vec{p}}^2-\frac{g\rho}{2V}.
\end{aligned}
\tag{51}
$$

□