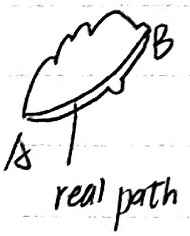
理力热统初步

一、拉格朗日力学 Lagrange Mechanics

1) Lagrange方程的推导

Lagrange 最小作用量原理 (哈密顿原理)



实际路程取极值

$$S=\int_A^B dt\ L(q_\alpha,\dot q_\alpha)$$

q_α:广义坐标 $\dot q_\alpha$:广义速度 (广义速度与广义坐标不一定具有微分关系).

$L(q_\alpha,\dot q_\alpha)=T$(动能)$-U$(势能) (广泛运用)

$\Delta S=S_{q+\delta q}$(猜想)$-S_q$(实际)

$$=\int_A^B dt[L(q+\delta q,\dot q+\delta\dot q)-L(q,\dot q)]$$

泰勒展开 $L(q+\delta q,\dot q+\delta\dot q)=L(q,\dot q)+\frac{\partial L}{\partial q}\delta q+\frac{\partial L}{\partial\dot q}\cdot\delta\dot q$

$$\delta\dot q=\delta\frac{d}{dt}q=\frac{d}{dt}(\delta q)$$

$$\Delta S=\int_A^B dt\left(\frac{\partial L}{\partial q}\delta q+\frac{\partial L}{\partial\dot q}\frac{d}{dt}(\delta q)\right)$$

第二项分部积分 $\int_A^B dt\left[\frac{\partial L}{\partial\dot q}\cdot\frac{d}{dt}(\delta q)\right]$

$$=\int_A^B\frac{\partial L}{\partial\dot q}d(\delta q)$$

$$=\delta q\frac{\partial L}{\partial\dot q}\Big|_A^B-\int_A^B\delta q\frac{d}{dt}\left(\frac{\partial L}{\partial\dot q}\right)dt$$

若δq出现在A、B处，则起始/终了位置改变 故 $\delta q(A/B)=0$

即第一项为0

故 $\Delta S=\int_A^B dt\left(\frac{\partial L}{\partial q}\delta q-\delta q\frac{d}{dt}\left(\frac{\partial L}{\partial\dot q}\right)\right)$

δq可以出现在A、B间任何一处

由于猜想路径与实际路径非常接近

故$\Delta S=0$ 即 $\int_A^B dt\left(\frac{\partial L}{\partial q}\delta q-\delta q\frac{d}{dt}\left(\frac{\partial L}{\partial\dot q}\right)\right)=\int_A^B dt\left(\frac{\partial L}{\partial q}-\frac{d}{dt}\left(\frac{\partial L}{\partial\dot q}\right)\right)\delta q=0$

即 $\frac{d}{dt}\left(\frac{\partial L}{\partial\dot q}\right)-\frac{\partial L}{\partial q}=0$

推广到n个自由度

$i=1,2,\cdots,n,\quad \frac{d}{dt}\left(\frac{\partial L}{\partial\dot q_i}\right)-\frac{\partial L}{\partial q_i}=0$ (Lagrange方程)

二、守恒定律

1. energy conservation $\Leftrightarrow$ time symmetry
能量守恒定律 $\Leftrightarrow$ 时间对称性

$t \to t+\delta t$，L不变

即 $L(q_i,\dot{q}_i,t) = L(q_i,\dot{q}_i,t+\delta t) = L(q_i,\dot{q}_i,t) + \frac{\partial L}{\partial t}\delta t$

$$\frac{dL}{dt} = \frac{\partial L}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial L}{\partial \dot{q}_i}\frac{d\dot{q}_i}{dt} + \frac{\partial L}{\partial t}$$

定义 $\boxed{p \equiv \frac{\partial L}{\partial \dot{q}_i}}$ $\Rightarrow$ 由Larange方程 $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i}$ 即 $\frac{dp}{dt} = \frac{\partial L}{\partial q_i} = \dot{p}$

$$\frac{dL}{dt} = \dot{p}\frac{dq_i}{dt} + \frac{\partial L}{\partial \dot{q}_i}\frac{d\dot{q}_i}{dt} + \frac{\partial L}{\partial t}$$

$$= \dot{p}\dot{q}_i + p\frac{d\dot{q}_i}{dt} + \frac{\partial L}{\partial t}$$ $\quad p\frac{d\dot{q}_i}{dt} = \frac{d}{dt}(p\dot{q}_i) - \dot{q}_i\frac{dp}{dt} = \frac{d}{dt}(p\dot{q}_i) - \dot{q}_i\dot{p}$

$$= \dot{p}\dot{q}_i + \frac{d}{dt}(p\dot{q}_i) - \dot{p}\dot{q}_i + \frac{\partial L}{\partial t}$$

$$= \frac{d}{dt}(p\dot{q}_i) + \frac{\partial L}{\partial t} \Rightarrow -\frac{\partial L}{\partial t} = \frac{d}{dt}(p\dot{q}_i) - \frac{dL}{dt} = \frac{d}{dt}(p\dot{q}_i - L)$$

定义哈密顿量 $H = p\dot{q}_i - L$ $\quad (p\dot{q}_i = \sum_i p_i\dot{q}_i = p_x\dot{q}_x + p_y\dot{q}_y + p_z\dot{q}_z)$

$$-\frac{\partial L}{\partial t} = \frac{d}{dt}H$$

若 $\frac{\partial L}{\partial t} = 0 \Rightarrow H$不变

$L = \frac{1}{2}m\dot{q}_i^2 - U(q_i)$，$p \equiv \frac{\partial L}{\partial \dot{q}_i} = m\dot{q}_i$（广义动量）

$$H = p\dot{q}_i - L = m\dot{q}_i^2 - \left[\frac{1}{2}m\dot{q}_i^2 - U(q_i)\right]$$
$$= \frac{1}{2}m\dot{q}_i^2 + U(q_i)$$

2. spatical homogenity $\Leftrightarrow$ momentum conservation
空间均匀性 $\Leftrightarrow$ 动量守恒

$q_\beta \to q_\beta + \delta q_\beta$，L不变

$$L(q_\beta+\delta q_\beta, \dot{q}_\beta, t) - L(q_\beta, \dot{q}_\beta, t) = \frac{\partial L}{\partial q_\beta}\delta q_\beta = 0 \Rightarrow \frac{\partial L}{\partial q_\beta} = 0$$

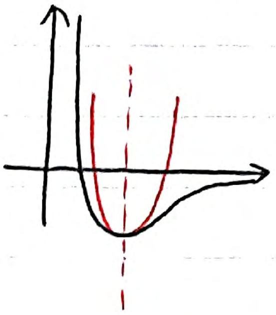
$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_\beta}\right) - \frac{\partial L}{\partial q_\beta} = 0 \Rightarrow \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_\beta}\right) = 0 \Rightarrow \frac{\partial L}{\partial \dot{q}_\beta} = p_\beta \text{不变}$$

Harmonic oscillation

有完 $\omega\to\omega_0$时, $\xi\to+\infty$

solution ① dissipation due to friction (摩擦力引起耗散)

② unharmonic osscillation (展开到更高阶项)



$$U=U(\rho=\rho_0)+\frac{1}{2}k(\rho-\rho_0)^2+\frac{1}{3!}\beta(\rho-\rho_0)^3+\cancel{O(\rho-\rho_0)}$$

$$L=\frac{1}{2}m\dot\rho^2-\frac{1}{2}k(\rho-\rho_0)^2-\frac{1}{6}\beta(\rho-\rho_0)^3$$

$$\left(\text{define } \frac{d^2}{d\rho^2}\Big|_{\rho=\rho_0}\equiv k,\ \frac{d^3}{d\rho^3}\Big|_{\rho=\rho_0}\equiv\beta\right)$$

define $\xi=\rho-\rho_0,\ \dot\xi=\dot\rho$

$$L=\frac{1}{2}m\dot\xi^2-\frac{1}{2}k\xi^2-\frac{1}{6}\beta\xi^3$$

$$\frac{\partial L}{\partial\xi}=-k\xi-\frac{1}{2}\beta\xi^2,\quad \frac{\partial L}{\partial\dot\xi}=m\dot\xi,\quad \frac{d}{dt}\left(\frac{\partial L}{\partial\dot\xi}\right)=m\ddot\xi$$

Lagrange equation $\Rightarrow m\ddot\xi=-k\xi-\frac{1}{2}\beta\xi^2$

即 $\ddot\xi+\omega_0^2\xi+\frac{1}{2}\bar\beta\xi^2=0$ (*)

$\left(\omega_0^2\equiv\frac{k}{m},\ \bar\beta\equiv\frac{\beta}{m}\right)$ 很小,否则展开无意义

微扰展开(由于$\bar\beta$很小,ξ可对$\bar\beta$幂级数展开)

$$\xi=\bar\beta^{(0)}\xi^{(0)}+\bar\beta^{(1)}\xi^{(1)}+\bar\beta^{(2)}\xi^{(2)}+\cancel{\xi^{(n)}}(\text{高阶})$$

$\bar\beta^{(0)}\approx1$

$$\Leftarrow=\bar\beta^{(0)}\xi^{(0)}+\bar\beta\xi^{(1)}+\bar\beta^{(2)}\xi^{(2)}$$

略去大于2阶 $\xi^2=\bar\beta^{(0)2}\xi^{(0)2}+2\bar\beta^{(1)}\xi^{(0)}\xi^{(1)}$

代入(*) $\bar\beta^{(0)}\ddot\xi^{(0)}+\bar\beta\ddot\xi^{(1)}+\bar\beta^{(2)}\ddot\xi^{(2)}$

$+\omega_0^2(\bar\beta^{(0)}\xi^{(0)}+\bar\beta\xi^{(1)}+\bar\beta^{(2)}\xi^{(2)})$

$+\frac{1}{2}\bar\beta^{(1)}(\bar\beta^{(0)2}\xi^{(0)2}+2\cancel{\bar\beta}\xi^{(0)}\xi^{(1)})=0$ 略去二次方项

化简 $\bar\beta^{(0)}[\ddot\xi^{(0)}+\omega_0^2\xi^{(0)}]+\bar\beta^{(1)}[\ddot\xi^{(1)}+\omega_0^2\xi^{(1)}+\frac{1}{2}\xi^{(0)2}\bar\beta^{(0)}]$

$+\bar\beta^{(2)}[\ddot\xi^{(2)}+\omega_0^2\xi^{(2)}]=0$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot\theta}\right)-\frac{\partial L}{\partial \theta}=0 \text{ 即 } -mgR\sin\theta=\frac{3}{2}m\ddot\theta R^2$$

$$\Rightarrow \ddot\theta+\frac{2g}{3R}\sin\theta=0$$

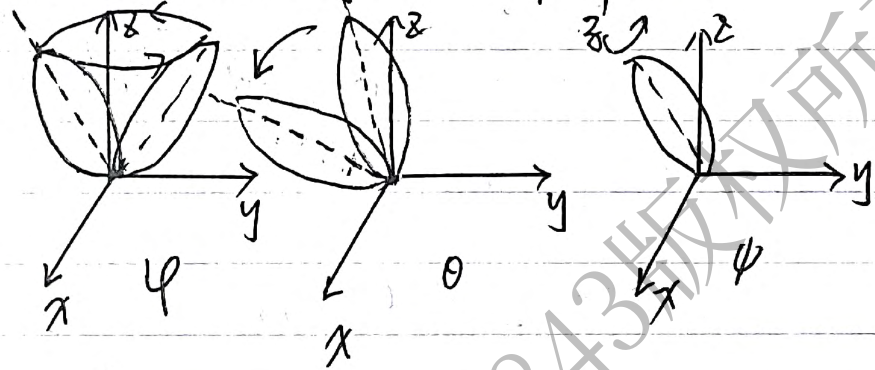
θ小 $\Rightarrow \sin\theta\approx\theta \Rightarrow \ddot\theta+\frac{2g}{3R}\theta=0$

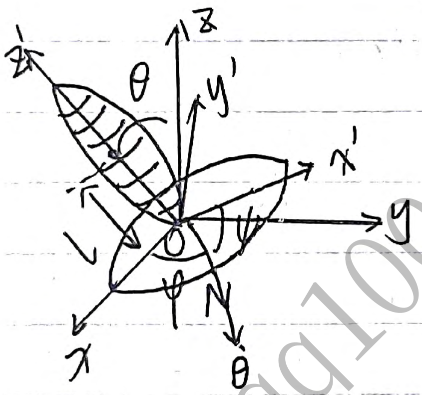
$$\omega_0^2=\frac{2g}{3R},\ \omega_0=\sqrt{\frac{2g}{3R}}$$

陀螺运动

Eulerian angles 欧拉角

主要是描述对称陀螺 symmetric top 三个角运动





平面$x'y'\perp oz'$，θ为oz与oz'夹角

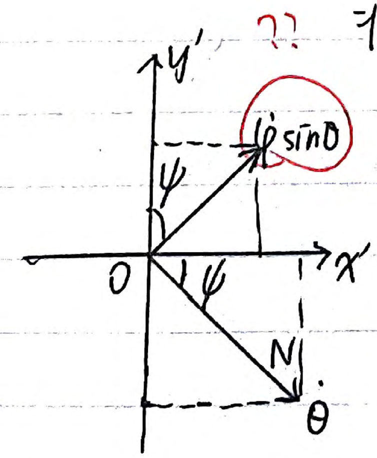
设ON为平面$x'y'$与平面xy的交线

$\Rightarrow ON\perp oz',\ ON\perp oz$

$\dot\theta$ 以ON为旋转轴

$\dot\varphi$ 以oz为旋转轴

$\dot\psi$ 以oz'为旋转轴



?? 将$\dot\theta,\dot\varphi,\dot\psi$投影到$x'y'$平面上

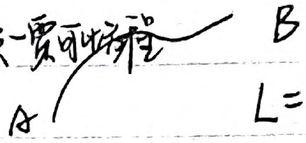
$\omega_{z'}=\cos\theta\cdot\dot\varphi+\dot\psi$??

$$\left.\begin{aligned}\omega_{x'}&=\cos\psi\,\dot\theta+\sin\psi(\dot\varphi\sin\theta)\\ \omega_{y'}&=-\sin\psi\cdot\dot\theta+\cos\psi(\dot\varphi\sin\theta)\end{aligned}\right\}\text{投影}$$

在$x'y'z'$坐标下

$$I=\begin{pmatrix} I_{xx} & 0 & 0\\ 0 & I_{yy} & 0\\ 0 & 0 & I_{zz}\end{pmatrix}=\begin{pmatrix} I_{xx} & 0 & 0\\ 0 & I_{xx} & 0\\ 0 & 0 & I_{zz}\end{pmatrix}.$$

八、Hamilton-Jacobi equation 哈密顿-贾可比方程



$S=\int L(q_i,\dot q_i)dt$ $L=\frac{dS}{dt}$

$\Delta S = \frac{\partial L}{\partial \dot q_i}\Delta q_i\Big|_A^B + \int_A^B\left[\frac{\partial L}{\partial q_i}-\frac{d}{dt}\left(\frac{\partial L}{\partial \dot q_i}\right)\right]\Delta q_i\,dt$

假设A固定，B不固定 ⇒ $\Delta q_i|_{q_i=A}=0$

由Lagrange equation知第二项为0

故 $\Delta S = \frac{\partial L}{\partial \dot q_i}\Delta q_i|_{q=B} - 0 = \frac{\partial L}{\partial \dot q_i}\Delta q_i|_{q_i=B}$

又 $\frac{\partial L}{\partial \dot q_i}=p_i$，且 $\frac{\partial S}{\partial q_i}=\frac{\partial L}{\partial \dot q_i}=p_i$

$L=\frac{dS}{dt}$ ($S=(q_i,t)$))

$=\frac{\partial S}{\partial q_i}\frac{dq_i}{dt}+\frac{\partial S}{\partial t}$

哈密顿-贾可比方程

$=p_i\dot q_i+\frac{\partial S}{\partial t} \Rightarrow -\frac{\partial S}{\partial t}=p_i\dot q_i - L$ 即 $-\frac{\partial S}{\partial t}=H(q_\alpha,p_\alpha,t)$

$\vec p=\nabla S$ (梯度)

$H=E$ (能量) $=-\frac{\partial S}{\partial t}$

$(\vec p, E)=(\nabla S, -\frac{\partial}{\partial t}S)$

做等S线，S线的极值 ⇒ 运动方向

△ 静电场 $\vec E=-\nabla\varphi$

粒子看作$\lambda\to\infty$的波

e.g. 在Hamonic oscillator中

$-\frac{\partial S}{\partial t}=H=\frac{p_x^2}{2m}+\frac12 kx^2$

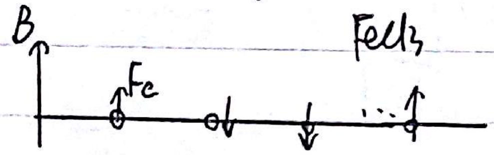
$p_x=\frac{\partial S}{\partial x} \Rightarrow -\frac{\partial S}{\partial t}=\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2+\frac12 kx^2$

猜测 $S=-E_0t+S_1(x)$；$\frac{\partial S}{\partial t}=E_0$，$\left(\frac{\partial S}{\partial x}\right)^2=\left(\frac{dS_1}{dx}\right)^2$

故 $E_0=\frac{1}{2m}\left(\frac{dS_1}{dx}\right)^2+\frac12 kx^2$

⇒ $\frac{dS_1}{dx}=\sqrt{(E_0-\frac12 kx^2)2m}$

Dilute Magnetism Cooling：稀磁制冷



忽略相互作用

μ_B为玻尔磁子，$\mu_B = 9.27\times10^{-24} J\cdot T^{-1}$

$H = -\sum_i \mu_B \cdot B \cdot n_i$ ($n_i = 1$ 或 -1) 当向上自旋时 $n_i = 1$，$H<0$

N 个 Fe 原子，$Z = \sum_i \Omega(\varepsilon_i) e^{-\beta\varepsilon_i}$

	$\Omega(\varepsilon_i)$	ε_i
$\uparrow\uparrow\cdots\uparrow\uparrow$	1	$-N\mu_B B$
$\uparrow\downarrow\cdots\uparrow\uparrow$	N	$-(N-2)\mu_B\cdot B$
$\uparrow\downarrow\downarrow\cdots\uparrow\uparrow$	$\frac{N(N-1)}{2}$	$-(N-4)\mu_B B$
$\vdots$	$\vdots$	$\vdots$
$\downarrow\downarrow\cdots\downarrow\downarrow$	1	$N\mu_B B$

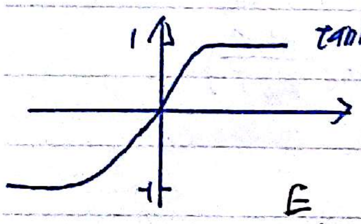
$$Z = \sum_i \Omega(\varepsilon_i) e^{-\beta\varepsilon_i}$$

$$= 1\cdot e^{\beta N\mu_B B} + N\cdot e^{\beta(N-2)\mu_B B} + \cdots + 1\, e^{-\beta N\mu_B B}$$

$$= (e^{\beta\mu_B B} + e^{-\beta\mu_B B})^N,\ \ln Z = N\ln(e^{\beta\mu_B B} + e^{-\beta\mu_B B}) = N\ln[2\cosh(\beta\mu_B B)]$$

$$F = -k_B T\ln Z = -Nk_B T\ln[2\cosh(\frac{\mu_B B}{k_B T})]$$

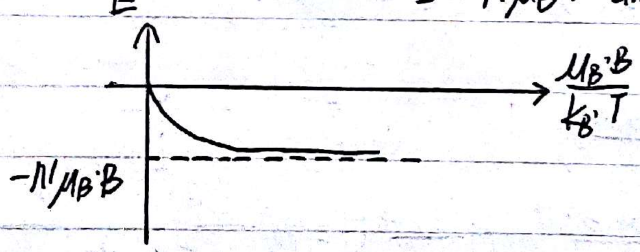
$$dF = -SdT - MdB,\ E = k_B T^2\frac{\partial}{\partial T}(\ln Z).$$



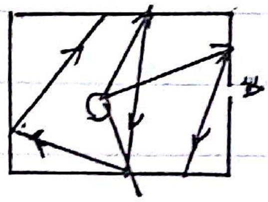
$\tanh(x) = \frac{1-e^{-2x}}{1+e^{-2x}}$

$$= k_B T^2 \frac{\sinh(\beta\mu_B B)}{\cosh(\beta\mu_B B)}\cdot(-\frac{\mu_B B}{k_B T^2})$$

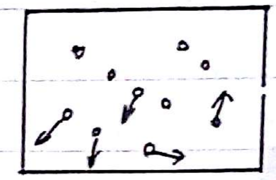
$$= -N\mu_B\cdot B\tanh(\frac{\mu_B\cdot B}{k_B T})$$



黑体辐射



$\Longleftrightarrow$



黑体辐射发光体

Ideal gas of quantom version of Boson gas

量子力学化的理想气体→光子气体 photons

photons model:

$$\nabla\times\vec{E}=-\frac{\partial}{\partial t}\vec{B} \quad ①$$

$$\nabla\times\vec{H}=\vec{j}+\frac{\partial}{\partial t}\vec{D} \quad ② \quad \text{真空中}\ \vec{H}=\frac{\vec{B}}{\mu_0},\ \vec{D}=\varepsilon_0\vec{E},\ \vec{j}=0$$

由① $\nabla\times\nabla\times\vec{E}=-\nabla\times\frac{\partial}{\partial t}\vec{B}$　　$\mu_0\varepsilon_0=\frac{1}{c^2}$

由② $\nabla\times\frac{\vec{B}}{\mu_0}=\frac{\partial}{\partial t}\varepsilon_0\vec{E}$ 即 $\nabla\times\vec{B}=\mu_0\varepsilon_0\frac{\partial}{\partial t}\vec{E}=\frac{1}{c^2}\frac{\partial}{\partial t}\vec{E}$

故 $\frac{\partial}{\partial t}(\nabla\times\vec{B})=\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\vec{E}$

$\Rightarrow \nabla\times\nabla\times\vec{E}=-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\vec{E}$

波动方程 $\vec{E}=\vec{E_0}e^{i\vec{k}\cdot\vec{r}-i\omega t}$

代入 $\nabla\times\nabla\times\vec{E}=-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\vec{E}$ 可得 $i\vec{k}\times i\vec{k}\times\vec{E_0}=-\frac{1}{c^2}(i\omega)^2\vec{E_0}=\frac{\omega^2}{c^2}\vec{E_0}$

?? $\Rightarrow \omega^2=-c^2k^2,\ \omega=ck,\ E=\hbar\omega=\hbar ck$

周期性边界条件 $\vec{E}(\vec{r},t)=\vec{E}(\vec{r}+\vec{L},t)$，$L^3$ 为 size of cavity 孔径大小

$$e^{i\vec{k}\cdot\vec{r}-i\omega t}=e^{i\vec{k}(\vec{r}+\vec{L})-i\omega t}$$

$\Rightarrow e^{i\vec{k}\vec{L}}=1$ 即 $\vec{k}\cdot\vec{L}=2\pi\cdot n\ (n=0,\pm1,\pm2,\cdots)$

故 $k_xL=2n_x\pi,\ k_yL=2n_y\pi,\ k_zL=2n_z\pi$

$$\vec{k}=\frac{2\pi}{L}(n_x,n_y,n_z),\ (n_x,n_y,n_z=0,\pm1,\pm2,\cdots)$$

$$\hat{Z}=\prod_{E_i}\left[\frac{1}{1-e^{\beta(E_i-\mu)}}\right]=\prod_{\varepsilon_i}\left[\frac{1}{1-e^{\beta(\varepsilon_i-\mu)}}\right]$$

Bose-Einstein condensation 玻色-爱因斯坦凝聚

$\hat{H}=\sum_i \frac{\vec{p_i}^2}{2m}$，$p=\frac{h}{\lambda}=\frac{h}{2\pi}\cdot\frac{2\pi}{\lambda}=\hbar k$

故 $\hat{H}=\sum_i \frac{(\hbar k_i)^2}{2m}=E$，$k=\frac{\sqrt{2mE}}{\hbar}$，$\Delta k=\frac{\sqrt{2m}}{2\hbar}\cdot\frac{\Delta E}{\sqrt{E}}$

$\Delta n=\frac{4\pi k^2\Delta k}{(\frac{2\pi}{L})^3}=\frac{L^3 4\pi\cdot 2mE}{2\cdot 8\pi^3\hbar^2}\cdot\frac{\sqrt{2m}}{2\hbar}\cdot\frac{\Delta E}{\sqrt{E}}$

$D(E)=\frac{\Delta n}{\Delta E}=\frac{L^3\sqrt{2m}\cdot m\sqrt{E}}{2\pi^2\hbar^3}=\frac{V(2m)^{\frac{3}{2}}}{4\pi^2\hbar^3}\sqrt{E}=C_1\sqrt{E}$

对于Bose气体 $A=-k_BT\ln\tilde{Z}=k_BT\sum_E\ln(1-e^{-\beta(E-\mu)})$

$=k_BT\int_0^{+\infty}dE[D(E)\ln(1-e^{-\beta(E-\mu)})]$

$dA=-SdT-pdV-Nd\mu$

$N=-\frac{dA}{d\mu}=-k_BT\int_0^{+\infty}dE[D(E)\frac{-\beta e^{-\beta(E-\mu)}}{1-e^{-\beta(E-\mu)}}]$

$=\int_0^{+\infty}dE\, C_1\sqrt{E}\frac{e^{-\beta(E-\mu)}}{1-e^{-\beta(E-\mu)}}=\int_0^{+\infty}\frac{C_1\sqrt{E}}{e^{\beta(E-\mu)}-1}dE$

$f^{B\cdot E}=\frac{1}{e^{\beta(E-\mu)}-1}$

$E=0$时，$f^{BE}(E=0)=\frac{1}{e^{-\beta\mu}-1}$（平均粒子数$>0$）$\Rightarrow e^{-\beta\mu}-1=e^{(-k_BT)\cdot\mu}-1>0$

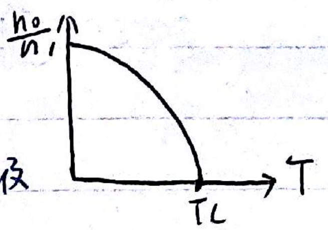
$\Rightarrow \mu<0$

再看 $N=\int_0^{+\infty}dE\frac{C_1\sqrt{E}}{e^{\beta(E-\mu)}-1}$，其中$e^{\beta(E-\mu)}=\underbrace{e^{\beta E}}_{\geq 1}\cdot\underbrace{e^{-\beta\mu}}_{>1}>1$，$\frac{1}{e^{\beta(E-\mu)}-1}$ 收敛

令$x=\beta E$，$N=\int_0^{+\infty}\frac{C_1\sqrt{\frac{x}{\beta}}}{e^{x-\beta\mu}-1}d\frac{x}{\beta}=\frac{1}{\beta^{\frac{3}{2}}}\int_0^{+\infty}\frac{C_1\sqrt{x}}{e^x e^{-\beta\mu}-1}dx=(k_BT)^{\frac{3}{2}}\cdot M$ 有限大小的常数

$T\to 0$时，$N=(k_BT)^{\frac{3}{2}}\cdot M\to 0$ 平均粒子数不可能为0

当$\mu=0$时，$f^{B\cdot E}(E=0)=\frac{1}{e^{\beta\cdot 0}-1}=$"$\frac{1}{0}$型"　$n_0(T)=n[1-(\frac{T}{T_c})^{\frac{3}{2}}]$



$N=N_0+(k_BT)^{\frac{3}{2}}M=\frac{1}{e^{-\beta\mu}-1}+(k_BT)^{\frac{3}{2}}M$

绝对零度下玻色粒子将全部处在$E=0$的最低能级

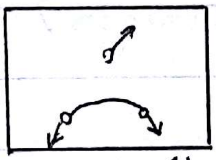
$$U = A + TS + \mu N = A - T\frac{\partial A}{\partial T} - \mu\frac{\partial A}{\partial \mu} = \int_0^\infty \frac{D(E)E}{e^{\beta(E-\mu)}+1}\,dE$$

$$\Rightarrow PV = \frac{2}{3}U$$

当$T \to 0$时，$U \to E_F \cdot N$，$PV = \frac{2}{3}E_F N$

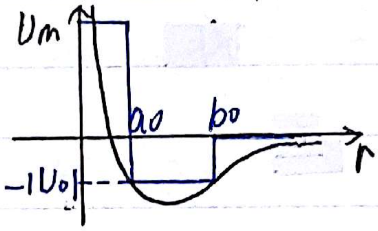
Interaction System 互作用系统

Van der waal gas 范德华气体



具有二体互作用的有限大体积的气体

将实际的分子势能曲线简化



$$U_m = \begin{cases} +\infty & (r < a_0) \\ -|U_0| & (a_0 \le r < b_0) \\ 0 & (r \ge b_0) \end{cases}$$

近似：$U_0 \approx 10\,meV$，$a_0 = r_0\,(10^{-10}m)$，$b_0 = 10a_0$

哈密顿量 $H = \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i,j}{}' U_m(|\vec{r}_i - \vec{r}_j|)$

正则系综

$$Z = \sum_{\varepsilon_i}\Omega(\varepsilon_i)e^{-\beta\varepsilon_i} = \frac{\int\cdots\int d\vec{r}_1\cdots d\vec{r}_N\,d\vec{p}_1\cdots d\vec{p}_N\,e^{-\beta\left(\sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum'_{i,j} U_m(|\vec{r}_i - \vec{r}_j|)\right)}}{h^{3N}\cdot N!}$$

$$= \frac{1}{h^{3N}\cdot N!}\left(\frac{2\pi m}{\beta}\right)^{\frac{3}{2}N} Z_C$$

$$Z_C = \int\cdots\int d\vec{r}_1\cdots d\vec{r}_N\,e^{-\beta\left(\sum'_{i,j} U_m(|\vec{r}_i - \vec{r}_j|)\right)}$$

$$= \int\cdots\int d\vec{r}_1\cdots d\vec{r}_N \prod_{i<j} e^{-\beta U_m(|\vec{r}_i - \vec{r}_j|)}$$

令 $f_{ij} = e^{-\beta U_m(|\vec{r}_i - \vec{r}_j|)} - 1$

$$Z_C = \int\cdots\int d\vec{r}_1\cdots d\vec{r}_N \prod_{i<j}(1+f_{ij})$$

$$\prod_{i<j}(1+f_{ij}) = (1+f_{12})(1+f_{13})\cdots(1+f_{1N})$$
$$\times(1+f_{23})\cdots(1+f_{2N})$$
$$\vdots$$
$$\times(1+f_{N-1,N})$$

$$F=-k_BT\ln Z=-k_BT\ln\left[Z_{ideal}\cdot\left(1+\frac{N^2}{2V}I_1\right)\right]$$
$$=-k_BT\ln(Z_{ideal})-k_BT\ln\left(1+\frac{N^2}{2V}I_1\right)$$
$$=-k_BT\ln(Z_{ideal})-k_BT\frac{N^2}{2V}I_1$$

$$dF=-SdT-pdV$$
$$p=-\frac{\partial F}{\partial V}=k_BT\frac{\frac{\partial Z_{ideal}}{\partial V}}{Z_{ideal}}+k_BT\frac{-N^2}{2V^2}I_1$$
$$=k_BT\frac{(\ )NV^{N-1}}{(\ )V^N}-\frac{k_BTN^2}{2V^2}I_1=\frac{Nk_BT}{V}-\frac{k_BTN^2}{2V^2}I_1$$
$$=\frac{Nk_BT}{V}-\frac{k_BTN^2}{2V^2}(-V_0+\beta U_0V_I)$$
$$=\frac{Nk_BT}{V}+\frac{k_BTN^2}{2V^2}V_0-\cancel{k_BT\beta}\frac{U_0V_IN^2}{2V^2}$$

故 $p+\frac{U_0V_IN^2}{2V^2}=\frac{Nk_BT}{V}+\frac{k_BTN^2V_0}{2V^2}$ $NV_0=V_2$（气体体积）
$$=\frac{Nk_BT}{V}\left(1+\frac{NV_0}{2V}\right)=\frac{Nk_BT}{V}\left(1+\frac{V_2}{2V}\right).$$

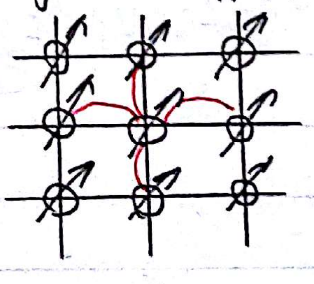
$x\to0$时，$1+x=\frac{1}{1-x}$，$p+\frac{U_0V_IN^2}{2V^2}=\frac{Nk_BT}{V}\left(\frac{1}{1-\frac{V_2}{2V}}\right)$

即 $p+\frac{N^2}{V^2}\frac{U_0V_I}{2}=\frac{Nk_BT}{V-\frac{V_2}{2}}$ 即 $\left(p+\frac{N^2}{V^2}\frac{V_I}{2}U_0\right)\left(V-\frac{V_2}{2}\right)=Nk_BT$

$$\Rightarrow (p+p')\left(V-\frac{V_2}{2}\right)=Nk_BT$$

$$\left(p+\frac{m^2a}{M^2V^2}\right)\left(V-\frac{m}{M}b\right)=\frac{m}{M}RT$$（范德瓦尔斯气态方程）

Ising Model 伊辛模型



(1) 只有两种自旋状态 ↑↓ $S_i\{\uparrow,\downarrow\}$

(2) 每个粒子只与最近的4个粒子有相互作用

$$H=-J\sum_{<ij>}\vec{S_i}\cdot\vec{S_j}-\vec{B}\cdot\mu_B\sum_i\vec{S_i}$$

μ_B 玻尔磁子

$J>0$ 铁磁性 $J<0$ 反铁磁性