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）（广泛适用）

$$\Delta S=S_{q+\delta q}(\text{猜想})-S_q(\text{实际})$$
$$=\int_A^B dt\left[L(q+\delta q,\dot{q}+\delta\dot{q})-L(q,\dot{q})\right]$$

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

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

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

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

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

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

$i=1,2,\cdots,n$，$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)-\frac{\partial L}{\partial q_i}=0$（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 $\frac{dp}{dt} = \frac{\partial L}{\partial q_i} = \dot{p}$

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

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

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

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

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

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

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

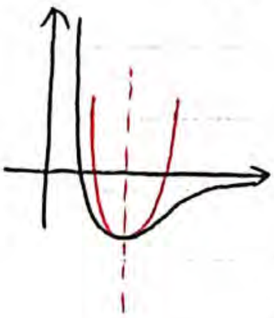
Harmonic oscillation

有宽 $\omega \to \omega_0$ 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)

↓



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

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

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

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

$\left(\omega_0^2 = \frac{k}{m}, \ \bar{\beta} = \frac{\beta}{m}\right)$ 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)

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

$\bar{\beta}^{(0)} \approx 1$

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

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(*)
$$\bar{\beta}^{(0)}\ddot{\xi}^{(0)} + \bar{\beta}\ddot{\xi}^{(1)} + \bar{\beta}^{(2)}\ddot{\xi}^{(2)}$$
$$+ \omega_0^2\left(\bar{\beta}^{(0)}\xi^{(0)} + \bar{\beta}\xi^{(1)} + \bar{\beta}^{(2)}\xi^{(2)}\right)$$
$$+ \frac{1}{2}\bar{\beta}^{(1)}\left(\bar{\beta}^{(0)2}\xi^{(0)2} + \cancel{2\bar{\beta}^{(1)}\xi^{(0)}\xi^{(1)}}\right) = 0$$ 略去二次方项

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

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

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

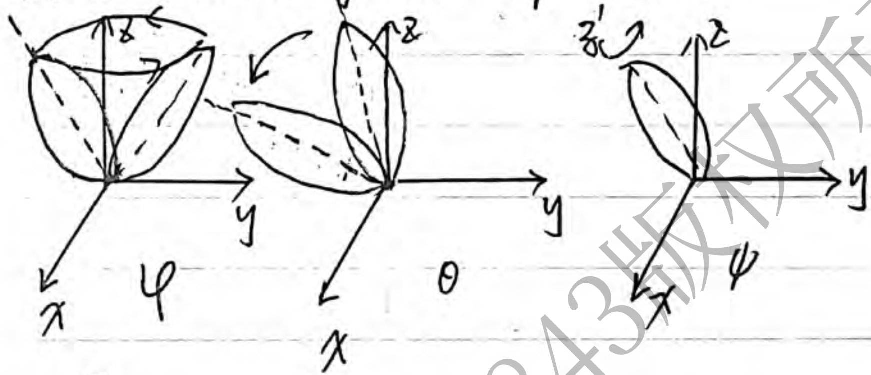
θ小 $\Rightarrow \sin\theta\simeq\theta \Rightarrow \ddot\theta+\frac{2g}{3R}\theta=0$

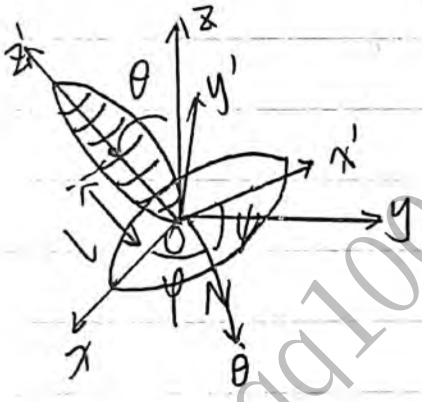
$\omega_0^2=\frac{2g}{3R}$, $\omega_0=\sqrt{\frac{2g}{3R}}$

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

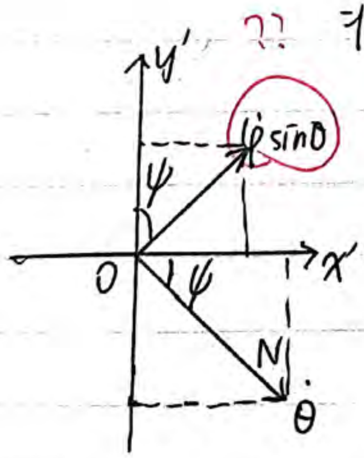
$\Rightarrow ON\perp oz'$, $ON\perp oz$

$\dot\theta$ 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

$$S=\int L(q_i,\dot{q}_i)dt \qquad A \qquad B \qquad L=\frac{dS}{dt}$$

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

假设A固定，B不固定 $\Rightarrow \Delta q_i|_{q=A}=0$

由Lagrange equation知第二项为0

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

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

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

$$\begin{cases}\vec{p}=\nabla S \text{ (梯度)}\\ H=E\text{ (能量)}=-\frac{\partial S}{\partial t}\end{cases}$$

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

做等S线，与线的极值 ⇒ 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

$$-\frac{\partial S}{\partial t}=H=\frac{p_x^2}{2m}+\frac{1}{2}kx^2$$

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

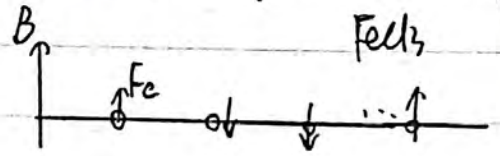
猜测 $S=-E_0t+S_1(x)$；$\frac{\partial S}{\partial t}=E_0$，$\left(\frac{\partial S}{\partial x}\right)^2=\left(\frac{dS_1}{dx}\right)^2$

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

$$\Rightarrow \frac{dS_1}{dx}=\sqrt{(E_0-\frac{1}{2}kx^2)2m}$$

Dilute Magnetism Cooling：稀磁制冷

$FeCl_3$



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
↑↑ ⋯ ↑↑	1	$-N\mu_B B$
↑↓ ⋯ ↑↑	N	$-(N-2)\mu_B B$
↑↓↓ ⋯ ↑↑	$\frac{N(N-1)}{2}$	$-(N-4)\mu_B B$
⋮	⋮	⋮
↓↓ ⋯ ↓↓	1	$N\mu_B B$

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

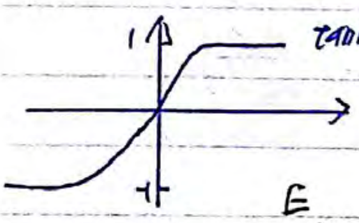
$$= 1\cdot e^{\beta N\mu_B B} + N\cdot e^{\beta(N-2)\mu_B B} + \cdots + 1\, e^{-\beta N\mu_B B}$$

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

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

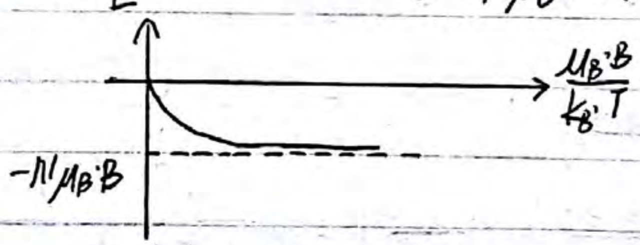
$$dF = -SdT - M\,dB,\quad E = k_B T^2\frac{\partial}{\partial T}(\ln Z)$$

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



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

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



黑体辐射

黑体辐射实验

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:

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

$\nabla\times\vec{H}=\vec{j}+\frac{\partial}{\partial t}\vec{D}$ ② 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 为 size of cavity 那个大小

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

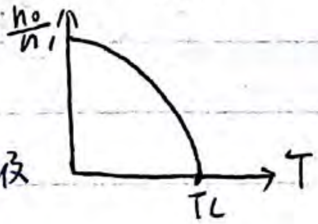
⇒ $\mu<0$

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



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

绝对零度下玻色粒子将全部处在$E=0$的最低能级

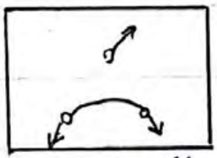
$$U = A + TS + \mu N = A - T\frac{\partial A}{\partial T} - \mu\frac{\partial A}{\partial \mu} = \int_0^{\infty}\frac{D(E)E}{e^{\beta(E-\mu)}+1}dE$$

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

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

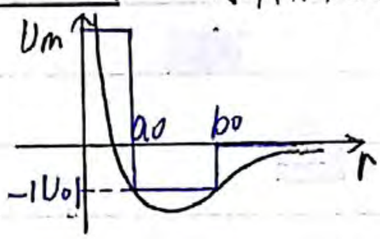
Interaction System 互作用系统

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

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

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

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

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

$$=-k_BT\ln(Z_{ideal})-k_BT\frac{N^2}{2V}I_1$$

$$dF=-SdT-pdV$$

$$p=-\frac{\partial F}{\partial V}=k_BT\frac{\frac{\partial Z_{ideal}}{\partial V}}{Z_{ideal}}+k_BT\frac{-N^2}{2V^2}I_1$$

$$=k_BT\frac{(\ )NV^{N-1}}{(\ )V^N}-\frac{k_BTN^2}{2V^2}I_1=\frac{Nk_BT}{V}-\frac{k_BTN^2}{2V^2}I_1$$

$$=\frac{Nk_BT}{V}-\frac{k_BTN^2}{2V^2}(-V_0+\beta U_0V_I)$$

$$=\frac{Nk_BT}{V}+\frac{k_BTN^2}{2V^2}V_0-\cancel{k_B\beta}\frac{U_0V_IN^2}{2V^2}$$

故 $p+\frac{U_0V_IN^2}{2V^2}=\frac{Nk_BT}{V}+\frac{k_BTN^2V_0}{2V^2}$ $NV_0=V_2$ (分子体积)

$$=\frac{Nk_BT}{V}\left(1+\frac{NV_0}{2V}\right)=\frac{Nk_BT}{V}\left(1+\frac{V_2}{2V}\right).$$

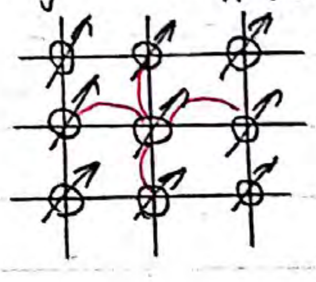
$x\to0$ 时, $1+x=\frac{1}{1-x}$, $p+\frac{U_0V_IN^2}{2V^2}=\frac{Nk_BT}{V}\left(\frac{1}{1-\frac{V_2}{2V}}\right)$

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

$$H=-J\sum_{i,j}\vec{S_i}\cdot\vec{S_j}-\vec{B}\cdot\mu_B\sum_i\vec{S_i}$$

μ_B 玻尔磁子

$J>0$ 铁磁性 $J<0$ 反铁磁性