- **积分公式**.$\int_{-\infty}^{\infty}exp[ix^2]dx=\sqrt{\pi}exp[i\pi/4]$(Fresnel积分公式); $\int_{-\infty}^{\infty}dxexp[-\alpha x^2+\beta x]=\sqrt{\frac{\pi}{\alpha}}exp[\frac{\beta^2}{4\alpha}]$, $\int_0^{+\infty}x^nexp[-ax^2]dx=\frac{\Gamma(\frac{n+1}{2})}{2a^{\frac{n+1}{2}}}$, $\int_{-\infty}^{+\infty}xexp[-\frac{1}{2}ax^2+bx]dx=\frac{b}{a}\sqrt{\frac{2\pi}{a}}exp[b^2/(2a)]$, $\int_{-\infty}^{+\infty}x^2exp[-\frac{1}{2}ax^2+bx]dx=\frac{1}{a}(1+\frac{b^2}{a})\sqrt{\frac{2\pi}{a}}exp[b^2/(2a)]$; $\int_{-\infty}^{+\infty}x^{2n}exp[-\frac{1}{2}ax^2]dx=\frac{(2n-1)!!}{a^n}\sqrt{\frac{2\pi}{a}}$(广义Guass积分式); $\int_0^{+\infty}x^{2n+1}exp[-ax^2]dx=\frac{n!}{2a^{n+1}}$; $(\frac{1}{\sqrt{2\pi\hbar}})^3\iiint exp[-\frac{i}{\hbar}\vec{p}'\cdot\vec{r}](p_z\frac{\partial}{\partial p_y}-p_y\frac{\partial}{\partial p_z})exp[\frac{i}{\hbar}\vec{p}\cdot\vec{r}]d\tau=(p_z\frac{\partial}{\partial p_y}-p_y\frac{\partial}{\partial p_z})(\frac{1}{\sqrt{2\pi\hbar}})^3\iiint exp[\frac{i}{\hbar}(\vec{p}-\vec{p}')\cdot\vec{r}]d\tau=(p_z\frac{\partial}{\partial p_y}-p_y\frac{\partial}{\partial p_z})\delta(\vec{p}-\vec{p}')$
- **晶格** (1)三斜(1;$a_1\neq a_2\neq a_3;\alpha\neq\beta\neq\gamma$);单斜(2;$a_1\neq a_2\neq a_3;\alpha=\gamma=\pi/2\neq\beta$); 正交(4;$a_1\neq a_2\neq a_3;\alpha=\beta=\gamma=\pi/2$);四角(2,$a_1=a_2\neq a_3;\alpha=\beta=\gamma=\pi/2$); 立方(3;$a_1=a_2=a_3;\alpha=\beta=\gamma=\pi/2$);三角(1,$a_1=a_2=a_3;\alpha=\beta=\gamma\neq\pi/2$); 六角(1;$a_1=a_2\neq a_3;\alpha=\beta=\pi/2,\gamma=2\pi/3$)(2)sc(简单立方);bcc(体心立方);fcc(面心立方);hcp(六角密堆积) (3)常见结构:NaCl(Cl^-面心&角+Na^+边中&体心);CsCl(Cs^+体心+Cl^-角); 金刚石结构(fcc+000&$\frac{1}{4}\frac{1}{4}\frac{1}{4}$);ZnS结构(Zn000, $0\frac{1}{2}\frac{1}{2},\frac{1}{2}0\frac{1}{2},\frac{1}{2}\frac{1}{2}0$; S$\frac{1}{4}\frac{1}{4}\frac{1}{4},\frac{1}{4}\frac{3}{4}\frac{3}{4},\frac{3}{4}\frac{1}{4}\frac{3}{4},,\frac{3}{4}\frac{3}{4}\frac{1}{4}$)
- **两种指标** 设晶面截距为a_1,a_2,a_3(1)$(a_1^{-1},a_2^{-1},a_2^{-1})$; (2)$[a_1,a_2,a_3]$. 上划线表示负号$[u\bar{v}w]$
- **布拉格条件**$2d\sin\theta=n\lambda;\Delta\vec{k}=\vec{G};2\vec{k}\cdot\vec{G}=\vec{G}^2$;
- **劳厄条件**$\vec{a_1}\cdot\Delta\vec{k}=2\pi v_1;\vec{a_2}\cdot\Delta\vec{k}=2\pi v_2;\vec{a_3}\cdot\Delta\vec{k}=2\pi v_3$;
- **倒格子初基平移矢量**$\vec{b_1}=2\pi\frac{\vec{a_2}\times\vec{a_3}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}},\vec{b_2}=2\pi\frac{\vec{a_3}\times\vec{a_1}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}},\vec{b_3}=2\pi\frac{\vec{a_1}\times\vec{a_2}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}}$
- **倒格矢**$\vec{G}=v_1\vec{b_1}+v_2\vec{b_2}+v_3\vec{b_3},v_i:\mathcal{Z}$
- **几何结构因子** 前提:方向为$\vec{k'}=\vec{k}+\Delta\vec{k}=\vec{k}+\vec{G}$, $S_G=\sum_j f_je^{-i\vec{r_j}\cdot\vec{G}}=\sum_j e^{-i2\pi(x_jv_1+y_jy_2+z_jv_3)}$, 其中$f_j=\int dVn_j(\vec{r})e^{-i\vec{G}\cdot\vec{r}}$
- **第一布里渊区** 倒格子的维格纳-塞茨原胞(1)sc−⟩sc($2\pi/a$);bcc−⟩棱形十二面体($2\pi/a\sqrt{2}$); fcc−⟩截角八面体(八面体的每个角都被切下,使得相邻三个面的正方形的边能围成正六边形)
- **声子-振动** (1)单原子:$u_{s\pm1}=ue^{isKa}exp^{\pm iKa}$色散关系:$w^2=(2C/M)(1-\cos Ka)$; $w^2=(4C/M)\sin^2\frac{1}{2}Ka$;群速:$v_g=\frac{dw}{dK}=\sqrt{\frac{Ca^2}{M}}\cos\frac{1}{2}Ka$; 长波极限($Ka<<1$):$w^2=(C/M)K^2a^2$ (2)双原子:原胞p个原子,3个声学支,3p-3个光学支.$M_1\frac{d^2u_s}{dt^2}=C(v_s+v_{s-1}-2u_s);M_2\frac{d^2v_s}{dt^2}=C(u_{s+1}+u_s-2v_s)$. $u_s=ue^{isKa}e^{-iwt},v_s=ve^{isKa}e^{-iwt}$,行列式系数为0:$M_1M_2w^4-2C(M_1+M_2)w^2+2C^2(1-\cos Ka)=0$;长波极限: 光学支$w^2=2C(\frac{1}{M_1}+\frac{1}{M_2})$,声学支$w^2=\frac{C}{2(M_1+M_2)}K^2a^2$;光学支下原子反向震动即质心固定,由光的电场来激发. (3)波矢选择定则:波矢$\vec{k}$非弹性散射到$\vec{k'}$,同时产生/吸收波矢为$\vec{K}$的声子,那么$\vec{k}=\vec{k'}\pm\vec{K}+\vec{G}$,$\vec{G}$是倒格矢; (4)声子能量:$\epsilon=(n+\frac{1}{2})\hbar\omega$;动能守恒:$\frac{\hbar^2k^2}{2M_n}=\frac{\hbar^2k'^2}{2M_n}\pm\hbar\omega$
- **热学基础** (0)定容热容$C_V=(\frac{\partial U}{\partial T})_V$,声子温度为$\tau=k_BT$,晶格内能$U_{lat}\sum_K\sum_p\langle n_{K,p}\rangle\hbar\omega_{K,p}$ (1)普朗克分布$\langle n\rangle=\frac{1}{e^{\frac{\hbar\omega}{\tau}}-1}$ (2)$U=\sum_K\sum_p\frac{\hbar\omega_{K,p}}{e^{\frac{\hbar\omega_{K,p}}{\tau}}-1}=\sum_p\int d\omega D_p(\omega)\frac{\hbar\omega}{e^{\frac{\hbar\omega}{\tau}}-1}$, $C_{lat}=k_B\sum_p\int d\omega D_p(\omega)\frac{x^2e^x}{(e^x-1)^2}(x=\hbar\omega/\tau=\hbar\omega/k_BT)$,$D(\omega)$即为态密度 (3)一维$D(\omega)$:$L=Na$,每个间隔$\Delta K=\frac{\pi}{L}$内一个模式,每个$K$三个偏振态(两个横向一个纵向)$D(\omega)d\omega=\frac{L}{\pi}\frac{dK}{d\omega}d\omega=\frac{L}{\pi}\frac{d\omega}{d\omega/dK}$(已知色散关系$\omega(K)$) (4)三维$D(\omega)$:$\forall i,K_i=\pm\frac{2n\pi}{L}$,$\vec{K}$的每单位体积内的模式数为$(\frac{L}{2\pi})^3=\frac{V}{8\pi^3}$, 每种偏振模式总数$N=(\frac{L}{2\pi})^3(\frac{4\pi K^3}{3})$,态密度$D(\omega)=\frac{dN}{d\omega}=(\frac{VK^2}{2\pi^2})(\frac{dK}{d\omega})$
- **德拜模型** (1)假设(每种偏振声速恒定,$\omega=vK$)$D(\omega)=\frac{V\omega^2}{2\pi^2v^3}$, 截止频率$\omega_D^3=6\pi^2v^3N/V$,截止波矢$K_D=\omega_D/v=(6\pi^2\frac{N}{V})^{\frac{1}{3}}$, 单偏振态内能$U_i=\int d\omega D(\omega)\langle n(\omega)\rangle\hbar\omega=\int_0^{\omega_D}d\omega(\frac{V\omega^2}{2\pi^2v^3})(\frac{\hbar\omega}{e^{\frac{\hbar\omega}{\tau}}-1})$, 总内能$U=3U_i=\frac{3V\hbar}{2\pi^2v^3}\int_0^{\omega_D}d\omega\frac{\omega^3}{e^{\frac{\hbar\omega}{\tau}}-1}=\frac{3Vk_B^4T^4}{2\pi^2v^3\hbar^3}\int_0^{x_D}dx\frac{x^3}{e^x-1}$(其中$x=\hbar\omega/\tau,x_D=\hbar\omega_D/\tau=\theta/T$), 德拜温度$\theta=\frac{\hbar v}{k_B}(\frac{6\pi^2N}{V})^{\frac{1}{3}}$,$U=9Nk_BT(\frac{T}{\theta})^3\int_0^{x_D}dx\frac{x^3}{e^x-1}$ (2)德拜模型低温极限(T^3率)($\int_0^{\infty}dx\frac{x^3}{e^x-1}=\frac{\pi^4}{15}$):$U\approx3\pi^2Nk_BT^4/5\theta^3$,热容$C_V\approx\frac{12\pi^4}{5}Nk_B(\frac{T}{\theta})^3\approx234Nk_B(\frac{T}{\theta})^3$
- **爱因斯坦模型** 爱因斯坦模型($D(\omega)=N\delta(\omega-\omega_0)$):一维内能$U=n\langle n\rangle\hbar\omega=\frac{N\hbar\omega}{e^{\frac{\hbar\omega}{\tau}}-1}$, 一维比热$C_V=\frac{\partial U}{\partial T}_V=Nk_B(\frac{\hbar\omega}{\tau})^2\frac{e^{\hbar\omega/\tau}}{(e^{\hbar\omega/\tau}-1)^2}$.三维乘系数3.
- **声子热学** (1)态密度$D(\omega)$一般形式:$D(\omega)=\frac{V}{(2\pi)^3}\int_{\text{K空间中}\omega\text{恒定的曲面}}\frac{dS_\omega}{v_g}$ (2)非谐作用($U(x)=cx^2-gx^3-fx^4$):$\langle x\rangle=\frac{\int_{-\infty}^{+\infty}dxxe^{-\beta U(x)}}{\int_{-\infty}^{+\infty}dxe^{-\beta U(x)}}(\beta=\frac{1}{k_BT})$, $\int dxxe^{-\beta U}\approx(\frac{3\pi^{\frac{1}{2}}}{4})(\frac{g}{c^{\frac{5}{2}}})\beta^{-\frac{3}{2}},\int dxe^{-\beta U}\approx(\frac{\pi}{\beta c})^{\frac{1}{2}}$, $\langle x\rangle=\frac{3g}{4c^2}k_BT$ (3)热导.一维下热流量$j_U=-K\frac{dT}{dx}$,热导率$K=\frac{1}{3}Cvl$(C:单位体积比热;v:粒子平均速度;l:平均自由程). (4)过程.$\vec{K_1}+\vec{K_2}=\vec{K_3}+\vec{G}$.正常过程($N$):$\vec{G}=0$;倒逆过程($U$):$\vec{G}\neq0$
- **自由电子** (0)一维无限深井:$\mathcal{H}\psi_n=-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2}=\epsilon_n\psi_n;\epsilon_n=\frac{\hbar^2}{2m}(\frac{n\pi}{L})^2$ (1)费米能ϵ_F:N电子系统基态下的最高能级;e.g.一维无限深井+泡利原理:$2n_F=N,n=n_F,\epsilon_F=\frac{\hbar^2}{2m}(\frac{N\pi}{2L})^2$; (2)温度变量.$f(\epsilon,T,\mu)=\frac{1}{e^{[\epsilon-\mu(T)]/k_BT}+1}$($T=0$时$\mu=\epsilon_F$).取高温极限时成为玻尔兹曼分布或者麦氏分布. (3)三维:$-\frac{\hbar^2}{2m}\nabla^2\psi_k(\vec{r})=\epsilon_{\vec{k}}\psi_k(\vec{r}),\psi_{\vec{k}}(\vec{r})=e^{i\vec{k}\cdot\vec{r}},(\forall i,k_i=\frac{2n\pi}{L})$ $\epsilon_{\vec{k}}=\frac{\hbar^2}{2m}(k_x^2+k_y^2+k_z^2).\hat{p}\psi_{\vec{k}}(\vec{r})=\hbar\vec{k}\psi_{\vec{k}}(\vec{r}),\vec{v}=\frac{\hbar\vec{k}}{m}$. 费米波矢$k_F$,费米能$\epsilon_F=\frac{\hbar^2}{2m}k_F^2$.$k$空间的每个体积元$(\frac{2\pi}{L})^3$存在一个波矢$(k_x,k_y,k_z)$.费米球+泡利定理:$2\cdot\frac{4\pi k_F^3/3}{(2\pi/L)^3}=N$. 费米波矢$k_F=(\frac{3\pi^2N}{V})^{\frac{1}{3}}$,费米能$\epsilon_F=\frac{\hbar^2}{2m}(\frac{3\pi^2N}{V})^{\frac{2}{3}}$,费

米速度$v_F = (\frac{\hbar k_F}{m}) = \frac{\hbar}{m}(\frac{3\pi^2 N}{V})^{\frac{1}{3}}$. 费米温度$T_F = \epsilon_F/k_B$.$N(U \leq \epsilon) = \frac{V}{3\pi^2}(\frac{2m\epsilon}{\hbar^2})^{\frac{3}{2}}$,$D(\epsilon) = \frac{dN}{d\epsilon} = \frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{\frac{3}{2}}\epsilon^{\frac{1}{2}} = \frac{3N}{2\epsilon}$ (4)比热容.总电子内能$U_e \approx \frac{NT}{T_F}k_B T$,电子比热$C_e = \frac{\partial U}{\partial T} \approx Nk_B\frac{T}{T_F}$. 低温极限($k_B T \ll \epsilon$):$\Delta U = \int_0^\infty d\epsilon\epsilon D(\epsilon)f(\epsilon) - \int_0^{\epsilon_F} d\epsilon\epsilon D(\epsilon)$ $= \int_{\epsilon_F}^\infty d\epsilon(\epsilon-\epsilon_F)f(\epsilon)D\epsilon + \int_0^{\epsilon_F} d\epsilon(\epsilon_F-\epsilon)[1-f(\epsilon)]D(\epsilon)$. 电子热容$C_e = \frac{dU}{dT} = \int_0^\infty d\epsilon(\epsilon - \epsilon_F)\frac{df}{dT}D(\epsilon) \approx D(\epsilon_F)\int_0^\infty d\epsilon(\epsilon - \epsilon_F)\frac{df}{dT}$ 低温极限($\tau = k_B T, x = \frac{\epsilon-\epsilon_F}{\tau}$)$\int_{-\infty}^{+\infty} dx x^2 \frac{e^x}{(e^x+1)^2} = \frac{\pi^2}{3}$,$C_e = \frac{1}{3}\pi^2 D(\epsilon_F)k_B^2 T$ ($D(\epsilon_F) = \frac{3N}{2\epsilon_F}$),$C_e = \frac{1}{2}\pi^2 N k_B T/T_F$.