- **积分公式**.$\int_{-\infty}^{\infty}exp[ix^2]dx = \sqrt{\pi}exp[i\pi/4]$(Fresnel积分公式); $\int_{-\infty}^{\infty}dxexp[-\alpha x^2+\beta x] = \sqrt{\frac{\pi}{\alpha}}exp[\frac{\beta^2}{4\alpha}]$, $\int_0^{+\infty}x^n exp[-ax^2]dx = \frac{\Gamma(\frac{n+1}{2})}{2a^{\frac{n+1}{2}}}$, $\int_{-\infty}^{+\infty}xexp[-\frac{1}{2}ax^2+bx]dx = \frac{b}{a}\sqrt{\frac{2\pi}{a}}exp[b^2/(2a)]$, $\int_{-\infty}^{+\infty}x^2exp[-\frac{1}{2}ax^2+bx]dx = \frac{1}{a}(1+\frac{b^2}{a})\sqrt{\frac{2\pi}{a}}exp[b^2/(2a)]$; $\int_{-\infty}^{+\infty}x^{2n}exp[-\frac{1}{2}ax^2]dx = \frac{(2n-1)!!}{a^n}\sqrt{\frac{2\pi}{a}}$(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$\epsilon_F$: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$T_F = \epsilon_F/k_B$.$N(U \le \epsilon) = \frac{V}{3\pi^2}(\frac{2m\epsilon}{\hbar^2})^{\frac{3}{2}}, D(\epsilon) = \frac{dN}{d\epsilon} = \frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{\frac{3}{2}}\epsilon^{\frac{1}{2}} = \frac{3N}{2\epsilon}$ (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($k_BT \ll \epsilon$):$\Delta U = \int_0^\infty d\epsilon\epsilon D(\epsilon)f(\epsilon) - \int_0^{\epsilon_F} d\epsilon\epsilon D(\epsilon)$ $= \int_{\epsilon_F}^\infty d\epsilon(\epsilon-\epsilon_F)f(\epsilon)D\epsilon + \int_0^{\epsilon_F} d\epsilon(\epsilon_F-\epsilon)[1-f(\epsilon)]D(\epsilon)$. 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($\tau = k_BT, x = \frac{\epsilon-\epsilon_F}{\tau}$)$\int_{-\infty}^{+\infty} dx x^2\frac{e^x}{(e^x+1)^2} = \frac{\pi^2}{3}, C_e = \frac{1}{3}\pi^2 D(\epsilon_F)k_B^2 T$ ($D(\epsilon_F) = \frac{3N}{2\epsilon_F}$),$C_e = \frac{1}{2}\pi^2 Nk_BT/T_F$. (5)金属比热.$\frac{C}{T} = \gamma + AT^2$($\gamma$索末菲常量). (6)电导率.$\vec{F} = -e(\vec{E} + \frac{1}{c}\vec{v}\times\vec{B})$.若$\vec{F} = -e\vec{E}, \delta\vec{k} = -e\vec{E}t/\hbar, \vec{v} = \delta\vec{k}/m = -e\vec{E}\tau/m$. 电流密度$\vec{j} = nq\vec{v} = ne^2\tau\vec{E}/m, (\vec{j} = \sigma\vec{E})\sigma = \frac{ne^2\tau}{m}, \rho = \sigma^{-1}$. (7)磁场下运动.(CGS制)$\hbar(\frac{d}{dt} + \frac{1}{\tau})\delta\vec{k} = \vec{F} = -e(\vec{E} + \vec{v}\times\vec{E})$.若$\vec{B} \parallel \hat{z}$, $\{v_x = -\frac{e\tau}{m}E_x - \omega_c\tau v_y, v_y = -\frac{e\tau}{m}E_y + \omega_c\tau v_x, v_z = -\frac{e\tau}{m}E_z\}$,回旋频率$\omega_c = \frac{eB}{mc}$ (8)霍尔效应.霍尔系数$R_H = \frac{E_y}{j_xB} = -\frac{1}{nec}$(CGS). (9)金属热导率.$K_e = \frac{1}{3}Cvl = \frac{\pi^2}{3}\frac{nk_B^2T}{mv_F^2}v_Fl = \frac{\pi^2 nk_B^2T\tau}{3m}$

- **近自由电子模型** (0)一维晶体.布拉格衍射条件$(\vec{k}+\vec{G})^2 = \vec{k}^2 \to k = \pm\frac{1}{2}G = \pm\frac{n\pi}{a}$(倒格矢$G = \frac{2\pi n}{a}$) (1)驻波.与时间无关.$\psi(+) = e^{i\pi x/a} + e^{-i\pi x/a} = 2\cos\pi x/a, \psi(-) = e^{i\pi x/a} - e^{-i\pi x/a} = 2i\sin\pi x/a$. $\rho(+) = |\psi(+)|^2 \propto \cos^2\pi x/a, \rho(-) = |\psi(-)|^2 \propto \sin^2\pi x/a$. 大小关系:$\langle\psi(-)|U|psi(-)\rangle < \langle e^{\mp i\pi x/a}|U|e^{\pm i\pi x/a}\rangle < \langle\psi(+)|U|psi(+)\rangle$. 若一维$\psi(x) = \sqrt{2}\cos\pi x/a, \sqrt{2}\sin\pi x/a$,电子势能$U(x) = U\cos 2\pi x/a$,则能隙$E_g = U(+) - U(-) = \int_0^1 dxU(x)[|\psi(+)|^2 - |\psi(-)|^2] = U$. (2)布洛赫函数.若势周期,则$\psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i\vec{k}\cdot\vec{r}}$(其中$u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r}+\vec{T})$). 若非简并,$\psi(x+a) = C\psi(x), C = e^{i2\pi s/N} - > \psi(x) = u_{\vec{k}}(x)e^{i2\pi sx/N}$. (3)克勒尼希-彭尼模型Kölnig-Penney model(周期势阱).$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = \epsilon\psi$. $x \in (0,a) : \psi = Ae^{iKx} + B^{-iKx}, \epsilon = \frac{\hbar^2K^2}{2m}; x \in (-b,0) : \psi = Ce^{Qx} + De^{-Qx}, U_0 - \epsilon = \frac{\hbar^2Q^2}{2m}$. 函数连续+导数连续,有四阶系数行列式为0:$[(Q^2 - K^2)/2QK]\sinh Qb\sin Ka + \cosh Qb\cos Ka = \cos k(a+b)$. 取极限$b = 0, U_0 = \infty(Q \gg K, Qb \ll 1)$,即为周期性$\delta$函数,$P = \frac{Q^2ba}{2}$结论化为$(P/Ka)\sin Ka + \cos Ka = \cos ka$. (4)周期势下的电子波函数.$U(x) = \sum_G U_Ge^{iGx}$,若为实则$U(x) = \sum_{G>0} 2U_G\cos Gx.\psi = \sum_k C(k)e^{ikx}$. 波动方程$\sum_k\frac{\hbar^2}{2m}k^2C(k)e^{ikx} + \sum_G\sum_k U_GC(k)e^{i(k+G)x} = \epsilon\sum_k e^{ikx}$. 中心方程$(\lambda_k - \epsilon)C(k) + \sum_G U_GC(k-G) = 0$(其中$\lambda_k = \frac{\hbar^2k^2}{2m}$) (5)求解行列式

$$\begin{vmatrix} \lambda_{k-g} - \epsilon & U & 0 \\ U & \lambda_k - \epsilon & U \\ 0 & U & \lambda_{k+g} - \epsilon \end{vmatrix}$$

每一个$k$每个$\epsilon$将在不同能带上. (6)中心方程求解K-P方程(周期$\delta$势函数).$U(x) = Aa\sum_s\delta(x-sa), U_G = \int_0^1 dxU(x)cos(Gx) = A$. 中心方程变为$(\lambda_k - \epsilon)C(k) + Af(k) = 0$,其中$f(k) = \sum_n C(k - 2\pi n/a) = f(k \pm 2\pi n/a)$. 从而有$\frac{mAa^2}{2\hbar^2}(Ka)^{-1}\sin Ka + \cos Ka = \cos ka$. (7)布里渊区边界附近的近似解. $k^2 = (\frac{1}{2}G)^2, (k-G)^2 = (\frac{1}{2}G - G)^2 \to k = \pm\frac{1}{2}G$. $(k = \frac{1}{2}G, \lambda = \hbar^2(\frac{1}{2}G)^2/2m)(\lambda - \epsilon)C(\pm\frac{1}{2}G) + UC(\mp\frac{1}{2}G) = 0$. 行列式$|{}^{\lambda-\epsilon, U}_{U, \lambda-\epsilon}| = 0$,解得$\epsilon = \lambda \pm U, E_g = 2U$. 若在$\frac{1}{2}G$附近,则$(\lambda_k - \epsilon)C(k) + UC(k-G) = 0, (\lambda_{k-G})C(k-G) + UC(k) = 0(\lambda_k = \hbar^2k^2/2m)$, 系数行列式$|{}^{\lambda_k-\epsilon, U}_{U, \lambda_{k-G}-\epsilon}| = 0 \to \epsilon = \frac{1}{2}(\lambda_{k-G} + \lambda_k) \pm [\frac{1}{4}(\lambda_{k-G} - \lambda_k)^2 + U^2]^{\frac{1}{2}}$ 用小量$\widetilde{K} = k - \frac{1}{2}G$展开,有$\epsilon_{\widetilde{K}} \approx \frac{\hbar^2}{2m}(\frac{1}{4}G^2 + \widetilde{K}^2) \pm U[1 + 2(\frac{\lambda}{U^2})(\frac{\hbar^2\widetilde{K}^2}{2m})]$. (8)轨道数目.N原胞一维晶体:$k = \pm\frac{2n\pi}{L}$.每个原胞对应一个k+泡利定理$\to$每个能带2N个轨道.