- **积分公式**.$\int_{-\infty}^{\infty} exp[ix^2]dx = \sqrt{\pi}exp[i\pi/4]$(Fresnel积分公式); $\int_{-\infty}^{\infty} dxexp[-\alpha x^2+\beta x] = \sqrt{\frac{\pi}{\alpha}}exp[\frac{\beta^2}{4\alpha}]$, $\int_0^{+\infty} x^n exp[-ax^2]dx = \frac{\Gamma(\frac{n+1}{2})}{2a^{\frac{n+1}{2}}}$, $\int_{-\infty}^{+\infty} xexp[-\frac12 ax^2+bx]dx = \frac{b}{a}\sqrt{\frac{2\pi}{a}}exp[b^2/(2a)]$, $\int_{-\infty}^{+\infty} x^2 exp[-\frac12 ax^2+bx]dx = \frac1a(1+\frac{b^2}{a})\sqrt{\frac{2\pi}{a}}exp[b^2/(2a)]$; $\int_{-\infty}^{+\infty} x^{2n} exp[-\frac12 ax^2]dx = \frac{(2n-1)!!}{a^n}\sqrt{\frac{2\pi}{a}}$(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&$\frac14\frac14\frac14$);ZnS结构(Zn000, $0\frac12\frac12,\frac12 0\frac12,\frac12\frac12 0$; S$\frac14\frac14\frac14,\frac14\frac34\frac34,\frac34\frac14\frac34,,\frac34\frac34\frac14$)
- **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$\vec{k'}=\vec k+\Delta\vec k=\vec k+\vec G$, $S_G=\sum_j f_j e^{-i\vec{r_j}\cdot\vec G}=\sum_j e^{-i2\pi(x_jv_1+y_jy_2+z_jv_3)}$, 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($2\pi/a\sqrt2$); 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:$w^2=(2C/M)(1-\cos Ka)$; $w^2=(4C/M)\sin^2\frac12 Ka$;群速:$v_g=\frac{dw}{dK}=\sqrt{\frac{Ca^2}{M}}\cos\frac12 Ka$; 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$w^2=2C(\frac1{M_1}+\frac1{M_2})$,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:$\epsilon=(n+\frac12)\hbar\omega$;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$K_D=\omega_D/v=(6\pi^2\frac{N}{V})^{\frac13}$, 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$\theta=\frac{\hbar v}{k_B}(\frac{6\pi^2N}{V})^{\frac13}$,$U=9Nk_BT(\frac{T}{\theta})^3\int_0^{x_D}dx\frac{x^3}{e^x-1}$ (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($U(x)=cx^2-gx^3-fx^4$):$\langle x\rangle=\frac{\int_{-\infty}^{+\infty}dxxe^{-\beta U(x)}}{\int_{-\infty}^{+\infty}dxe^{-\beta U(x)}}(\beta=\frac{1}{k_BT})$, $\int dxxe^{-\beta U}\approx(\frac{3\pi^{\frac12}}{4})(\frac{g}{c^{\frac52}})\beta^{-\frac32},\int dxe^{-\beta U}\approx(\frac{\pi}{\beta c})^{\frac12}$, $\langle x\rangle=\frac{3g}{4c^2}k_BT$ (3)热导.一维下热流量$j_U=-K\frac{dT}{dx}$,热导率$K=\frac13 Cvl$(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:$2\cdot\frac{4\pi k_F^2/3}{(2\pi/L)^3}=N$. 费米波矢$k_F=(\frac{3\pi^2N}{V})^{\frac13}$,费米能$\epsilon_F=\frac{\hbar^2}{2m}(\frac{3\pi^2N}{V})^{\frac23}$,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$U_e\approx\frac{NT}{T_F}k_BT$,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($\tau=k_BT, x=\frac{\epsilon-\epsilon_F}{\tau}$)$\int_{-\infty}^{+\infty}dxx^2\frac{e^x}{(e^x+1)^2}=\frac{\pi^2}{3}, C_e=\frac{1}{3}\pi^2 D(\epsilon_F)k_B^2T$ ($D(\epsilon_F)=\frac{3N}{2\epsilon_F}$),$C_e=\frac{1}{2}\pi^2Nk_BT/T_F$. (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.$K_e=\frac{1}{3}Cvl=\frac{\pi^2}{3}\frac{nk_B^2T}{mv_F^2}v_Fl=\frac{\pi^2nk_B^2T\tau}{3m}$

- **近自由电子模型** (0)一维晶体.布拉格衍射条件$(\vec{k}+\vec{G})^2=\vec{k}^2\rightarrow k=\pm\frac{1}{2}G=\pm\frac{n\pi}{a}$(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$U(x)=U\cos2\pi x/a$,则能隙$E_g=U(+)-U(-)=\int_0^1dxU(x)[|\psi(+)|^2-|\psi(-)|^2]=U$. (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$b=0,U_0=\infty(Q\gg K,Qb\ll1)$,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$U(x)=\sum_{G>0}2U_G\cos Gx.\psi=\sum_kC(k)e^{ikx}$. 波动方程$\sum_k\frac{\hbar^2}{2m}k^2C(k)e^{ikx}+\sum_G\sum_kU_GC(k)e^{i(k+G)x}=\epsilon\sum_ke^{ikx}$. 中心方程$(\lambda_k-\epsilon)C(k)+\sum_GU_GC(k-G)=0$(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ϵ将在不同能带上. (6)中心方程求解K-P方程(周期δ势函数).$U(x)=Aa\sum_s\delta(x-sa),U_G=\int_0^1dxU(x)cos(Gx)=A$. 中心方程变为$(\lambda_k-\epsilon)C(k)+Af(k)=0$,其中$f(k)=\sum_nC(k-2\pi n/a)=f(k\pm2\pi n/a)$. 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. $k^2=(\frac{1}{2}G)^2,(k-G)^2=(\frac{1}{2}G-G)^2\rightarrow k=\pm\frac{1}{2}G$. ($k=\frac{1}{2}G,\lambda=\hbar^2(\frac{1}{2}G)^2/2m)(\lambda-\epsilon)C(\pm\frac{1}{2}G)+UC(\mp\frac{1}{2}G)=0$. 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$|{}^{\lambda_k-\epsilon,U}_{U,\lambda_{k-G}-\epsilon}|=0\rightarrow\epsilon=\frac{1}{2}(\lambda_{k-G}+\lambda_k)\pm[\frac{1}{4}(\lambda_{k-G}-\lambda_k)^2+U^2]^{\frac{1}{2}}$ 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$\rightarrow$每个能带2N个轨道.