- **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,$2r = a$); bcc(体心立方,,$4r = \sqrt{3}a$,$\rho = 2m_0/a^3, a = \sqrt[3]{2m_0/\rho}$); fcc(面心立方,$4r = \sqrt{2}a$); 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(金刚石结构基础上的部分替换)(Zn000, $0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0$; S$\frac{1}{4}\frac{1}{4}\frac{1}{4}, \frac{1}{4}\frac{3}{4}\frac{3}{4}, \frac{3}{4}\frac{1}{4}\frac{3}{4}, \frac{3}{4}\frac{3}{4}\frac{1}{4}$) eg1.$r_{Cs} = 1.7, r_{Cl} = 1.81.a = 2(r_{Cs} + r_{Cl})/\sqrt{3}, PF = \frac{4\pi(r_{Cs}^3 + r_{Cl}^3)}{3a^3} \approx 0.682, \rho = \frac{m_{Cs}+m_{Cl}}{a^3} = 4.2$ eg2.NaCl下的CsCl:$a = 2(r_{Cs} + r_{Cl}), PF = \frac{4\pi(r_{Cs}^3 + r_{Cl}^3)\cdot 4}{3a^3} \approx 0.525$

- **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** $\vec{b_1} = 2\pi\frac{\vec{a_2}\times\vec{a_3}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}}$, $\vec{b_2} = 2\pi\frac{\vec{a_3}\times\vec{a_1}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}}, \vec{b_3} = 2\pi\frac{\vec{a_1}\times\vec{a_2}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}}$. $\vec{b_i}\cdot\vec{a_j} = 2\pi\delta_{ij}$

- **倒格矢** $\vec{G} = v_1\vec{b_1} + v_2\vec{b_2} + v_3\vec{b_3}, v_i:\mathcal{Z}$. 倒格矢$\vec{G}_{h_1h_2h_3}$垂直于实空间晶面$(h_1h_2h_3)$. 面间距$d = \frac{2\pi}{|\vec{G_{\vec{h}}}|}$

- **几何结构因子**前提:方向为$\vec{k'} = \vec{k} + \Delta\vec{k} = \vec{k} + \vec{G}$, $S_G = \sum_j f_j e^{-i\vec{r_j}\cdot\vec{G}} = \sum_j f(j)e^{-i2\pi(x_jv_1+y_jy_2+z_jv_3)}$, 其中$f_j = \int dVn_j(\vec{r})e^{-i\vec{G}\cdot\vec{r}}$. eg1.bcc&$(0,0,0) + (\frac{1}{2},\frac{1}{2},\frac{1}{2}), S(v_1,v_2,v_3) = f(1 + e^{-i\pi(v_1+v_2+v_3)})$; eg2.fcc&$(0,0,0) + (0,\frac{1}{2},\frac{1}{2}) + (\frac{1}{2},0,\frac{1}{2}) + (\frac{1}{2},\frac{1}{2},0)$, $S(v_1,v_2,v_3) = f\{1 + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_1+v_3)} + e^{-i\pi(v_1+v_2)}\}$

- **原子形状因子**$f_j = \int dVn_j(\vec{r})e^{-i\vec{G}\cdot\vec{r}}$,球对称极限$f_j = 4\pi\int drn_j(r)r^2\frac{\sin Gr}{Gr}$

- **第一布里渊区**倒格子的维格纳-塞茨原胞.晶格常数a (1)sc→sc($2\pi/a$); bcc→棱形十二面体(长对角线为$2\cdot\frac{\sqrt{2}\pi}{a}$,短对角线为$2\cdot\frac{\pi}{a}$); fcc→截角八面体(八面体每个角被切,使得相邻三个面的正方形边能围成正六边形.小正方形和六边形的边长$l = \frac{\sqrt{2}\pi}{2a}$)

- **声子-振动** (1)无阻尼单原子链:$u_{s\pm1} = ue^{isKa}exp^{\pm iKa}$ 色散关系:$w^2 = (2C/M)(1 - \cos Ka); w^2 = (4C/M)\sin^2\frac{1}{2}Ka$; 群速:$v_g = \frac{dw}{dK} = \sqrt{\frac{Ca^2}{M}}\cos\frac{Ka}{2}$; 长波极限($Ka \ll 1$):$w^2 = (C/M)K^2a^2, v = w/K$ (2)无阻尼双原子链:原胞p个原子,3个声学支,3p-3个光学支.$M_1\frac{d^2u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s); M_2\frac{d^2v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s)$. 试探解$u_s = ue^{isKa}e^{-iwt}, v_s = ve^{isKa}e^{-iwt}$,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($Ka \ll 1$): 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:$\vec{k} = \vec{k'} \pm \vec{K} + \vec{G}$, $\vec{G}$是倒格矢; (4)声子能量:$\epsilon = (n + \frac{1}{2})\hbar\omega$.若$u = u_0\cos Kx\cos\omega t$ $E_k = \int\frac{1}{2}\rho(\frac{\partial u}{\partial t})^2 = \frac{1}{4}\rho V\omega^2u_0^2\langle\sin^2\omega t\rangle = \frac{1}{8}\rho V\omega^2u_0^2 = \frac{1}{2}(n + \frac{1}{2})\hbar\omega$; 动能守恒:$\frac{\hbar^2k^2}{2M_n} = \frac{\hbar^2k'^2}{2M_n} \pm \hbar\omega$ (5)有阻尼单原子链:$m\partial_t^2u_j = C(u_{j+1} + u_{j-1} - 2u_j) - \Gamma\partial_tu_j$. 色散关系:$\omega(k) = \sqrt{\omega_{k_0}^2 - (\frac{\Gamma}{2m})^2} - \frac{i\Gamma}{2m}(\omega_{k_0} = \sqrt{\frac{4C}{m}}|\sin\frac{ka}{2}|)$ 弛豫时间(a)$\omega_{k_0} \geq \Gamma/2m : \tau_k = 2m/\Gamma$; (b)$\omega_{k_D} < \Gamma/2m : \tau_k = \frac{\Gamma}{2m\omega_{k_0}^2}(1 + \sqrt{1 - (\frac{2m\omega_{k_0}}{\Gamma})^2})$

- **热学基础** (0)定容热容$C_V = (\frac{\partial U}{\partial T})_V$, 声子温度$\tau = k_BT$, 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(两横一纵)$D(\omega)d\omega = \frac{L}{\pi}\frac{dK}{d\omega}d\omega = \frac{L}{\pi}\frac{d\omega}{d\omega/dK}$(色散关系$\omega(K)$) (4)三维$D(\omega)$:$\forall i, K_i = \pm\frac{2n\pi}{L}$,$\vec{K}$单位体积内模式数$(\frac{L}{2\pi})^3 = \frac{V}{8\pi^3}$, 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** (0)石墨烯模型(2D). C-C距离d,声速v, 晶格常数$a = \sqrt{3}d$, 原胞面积$A = \frac{\sqrt{3}a^2}{2}$, 德拜波矢$\pi k_D^2 = \frac{(2\pi)^2}{A}$, 德拜温度$\theta_D = \frac{\hbar\omega_D}{k_B} = \frac{\hbar vk_D}{k_B}$. $(\theta_D|_{d=1.42\mathring{A}} = 2.13\times10^3K)$ (1)3D下,假设(每种偏振声速恒定,$\omega = vK$) 态密度$D(\omega) = \frac{V\omega^2}{2\pi^2v^3}$, 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$\theta = \frac{\hbar v}{k_B}(\frac{6\pi^2N}{V})^{\frac{1}{3}}, U = 9Nk_BT(\frac{T}{\theta})^3\int_0^{x_D}dx\frac{x^3}{e^x-1}$ e.g.金刚石模型(3D) C-C距离d,声速v, 晶格常数$a = 4d/\sqrt{3}$, 原胞体积$\Omega = \frac{a^3}{4}$, 德拜波矢$\frac{4}{3}\pi k_D^3 = \frac{(2\pi)^3}{\Omega}$, 德拜温度$\theta_D = \frac{\hbar\omega_D}{k_B} = \frac{\hbar vk_D}{k_B}$. $(\theta_D|_{d=1.42\mathring{A}} = 2.13\times10^3K)$ (2)德拜模型低温极限(T^3律)($\int_0^\infty dx\frac{x^3}{e^x-1} = \frac{\pi^4}{15}$):$U \approx 3\pi^2Nk_BT^4/5\theta^3$,热容$C_V \approx \frac{12\pi^4}{5}Nk_B(\frac{T}{\theta})^3 \approx 234Nk_B(\frac{T}{\theta})^3$

- **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$C_V = \frac{\partial U}{\partial T}_V = Nk_B(\frac{\hbar\omega}{\tau})^2\frac{e^{\hbar\omega/\tau}}{(e^{\hbar\omega/\tau}-1)^2}$. 3D乘系数3.

- **声子热学** (1)态密度$D(\omega)$一般形式:$D(\omega) = \frac{V}{(2\pi)^3}\int_{\text{K中}\partial\omega=0}\frac{dS_\omega}{v_g}$ (2)非谐作用($U(x) = cx^2 - gx^3 - fx^4$): 平均位移$\langle x\rangle = \frac{\int_{-\infty}^{+\infty}dxxe^{-\beta U(x)}}{\int_{-\infty}^{+\infty}dxe^{-\beta U(x)}}(\beta = \frac{1}{k_BT})$, $\int dxxe^{-\beta U} \approx (\frac{3\pi^{\frac{1}{2}}}{4})(\frac{g}{c^{\frac{5}{2}}})\beta^{-\frac{3}{2}}, \int dxe^{-\beta U} \approx (\frac{\pi}{\beta c})^{\frac{1}{2}}$,

$\langle x\rangle = \frac{3g}{4c^2}k_BT$ (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($U$):$\vec G\neq 0$

- **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)(a)3D:$-\frac{\hbar^2}{2m}\nabla^2\psi_k(\vec r)=\epsilon_{\vec k}\psi_k(\vec r),\psi_{\vec k}(\vec r)=e^{i\vec k\cdot\vec r},(\forall i,k_i=\frac{2n\pi}{L})$ $\epsilon_{\vec k}=\frac{\hbar^2}{2m}(k_x^2+k_y^2+k_z^2)$. $\hat p\psi_{\vec k}(\vec r)=\hbar\vec k\psi_{\vec k}(\vec r),\vec v=\frac{\hbar\vec k}{m}$. F波矢$k_F$, F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). F球+泡利定理:$2\cdot\frac{4\pi k_F^3/3}{(2\pi/L)^3}=N$. F波矢$k_F=(\frac{3\pi^2N}{V})^{\frac13}$, F能$\epsilon_F=\frac{\hbar^2}{2m}(\frac{3\pi^2N}{V})^{\frac23}$, F速度$v_F=(\frac{\hbar k_F}{m})=\frac{\hbar}{m}(\frac{3\pi^2N}{V})^{\frac13}$. F温度$T_F=\epsilon_F/k_B$. 态密度$N(U\leq\epsilon)=\frac{V}{3\pi^2}(\frac{2m\epsilon}{\hbar^2})^{\frac32},D(\epsilon)=\frac{dN}{d\epsilon}=\frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{\frac32}\epsilon^{\frac12}=\frac{3N}{2\epsilon}$ (b)2D: $\pi k_F^2\cdot\frac{A}{(2\pi)^2}\cdot 2=N,k_F=\sqrt{2\pi N/A}=\sqrt{2\pi n}$. 色散关系:$\epsilon=\hbar^2k^2/2m,d\epsilon=\hbar^2kdk/m$. 态密度$D(\epsilon)d\epsilon=\frac1A\cdot2\pi kdk\cdot\frac{A}{(2\pi)^2}\cdot2=\frac{kdk}{\pi d\epsilon}d\epsilon=\frac{m}{\pi\hbar^2}d\epsilon$ $n=\int_{-\infty}^{+\infty}D(\epsilon)n_F(\epsilon)d\epsilon=\frac{m}{\pi\hbar^2}\int_0^{+\infty}\frac{d\epsilon}{e^{(\epsilon-\mu)/k_BT}+1}=\frac{mk_BT}{\pi\hbar^2}\ln(e^{\mu/k_BT}+1)$. 化学势$\mu(T)=k_BT\ln(e^{\frac{\pi n\hbar^2}{mk_BT}}-1)$ (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($k_BT\ll\epsilon_F$):$\Delta U=\int_0^\infty d\epsilon\epsilon D(\epsilon)f(\epsilon)-\int_0^{\epsilon_F}d\epsilon\epsilon D(\epsilon)$ $=\int_{\epsilon_F}^\infty d\epsilon(\epsilon-\epsilon_F)f(\epsilon)D\epsilon+\int_0^{\epsilon_F}d\epsilon(\epsilon_F-\epsilon)[1-f(\epsilon)]D(\epsilon)$.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($\tau=k_BT,x=\frac{\epsilon-\epsilon_F}{\tau}$)$\int_{-\infty}^{+\infty}dxx^2\frac{e^x}{(e^x+1)^2}=\frac{\pi^2}{3},C_e=\frac13\pi^2D(\epsilon_F)k_B^2T$ ($D(\epsilon_F)=\frac{3N}{2\epsilon_F}$),$C_e=\frac12\pi^2Nk_BT/T_F$. (5)金属比热.$\frac{C}{T}=\gamma+AT^2$($\gamma$索末菲常量). (6)电导率.$\vec F=-e(\vec E+\frac1c\vec v\times\vec B)$. 若$\vec F=-e\vec E,\delta\vec k=-e\vec Et/\hbar,\vec v=\delta\vec k/m=-e\vec E\tau/m$. 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)$\hbar(\frac{d}{dt}+\frac1\tau)\delta\vec k=\vec F=-e(\vec E+\vec v\times\vec E)$. 若$\vec B=B\hat z$, $\{v_x=-\frac{e\tau}{m}E_x-\omega_c\tau v_y,v_y=-\frac{e\tau}{m}E_y+\omega_c\tau v_x,v_z=-\frac{e\tau}{m}E_z\}$, 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.$K_e=\frac13Cvl=\frac{\pi^2}{3}\frac{nk_B^2T}{mv_F^2}v_Fl=\frac{\pi^2nk_B^2T\tau}{3m}$ (10)洛伦兹常量$L=\frac{K}{\sigma T}=\frac{\pi^2}{3}(\frac{k_B}{e})^2=2.45\times10^{-8}(W\cdot\Omega/deg^2)$

- **近自由电子模型** (0)一维晶体布拉格衍射条件$(\vec k+\vec G)^2=\vec k^2\to k=\pm\frac12G=\pm\frac{n\pi}{a}$(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:$\langle\psi(-)|U|\psi(-)\rangle\leq\langle e^{\mp i\pi x/a}|U|e^{\pm i\pi x/a}\rangle\leq\langle\psi(+)|U|\psi(+)\rangle$. 若一维$\psi(x)=\sqrt2\cos\pi x/a,\sqrt2\sin\pi x/a$,电子势能$U(x)=U\cos2\pi x/a$, 则一级近似能隙$E_g=U(+)-U(-)=\int_0^1dxU(x)[|\psi(+)|^2-|\psi(-)|^2]=U$. (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.$U(x)=\sum_GU_Ge^{iGx}$,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. $k^2=(\frac12G)^2,(k-G)^2=(\frac12G-G)^2\to k=\pm\frac12G$. ($k=\frac12G,\lambda=\hbar^2(\frac12G)^2/2m)(\lambda-\epsilon)C(\pm\frac12G)+UC(\mp\frac12G)=0$. 行列式$\left|\begin{smallmatrix}\lambda-\epsilon,U\\U,\lambda-\epsilon\end{smallmatrix}\right|=0$,解得$\epsilon=\lambda\pm U,E_g=2U$. 若在$\frac12G$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$\left|\begin{smallmatrix}\lambda_k-\epsilon,U\\U,\lambda_{k-G}-\epsilon\end{smallmatrix}\right|=0\to\epsilon=\frac12(\lambda_{k-G}+\lambda_k)\pm[\frac14(\lambda_{k-G}-\lambda_k)^2+U^2]^{\frac12}$ 用小量$\widetilde K=k-\frac12G$展开,有$\epsilon_{\widetilde K}\approx\frac{\hbar^2}{2m}(\frac14G^2+\widetilde K^2)\pm U[1+2(\frac{\lambda}{U^2})(\frac{\hbar^2\widetilde K^2}{2m})]$. (8)轨道数目.N原胞一维晶体:$k=\pm\frac{2n\pi}{L}$.每原胞对应一个k+泡利定理→每个能带2N个轨道.

- **金属受力**自由电子模型.($n_{Cu}\approx10^6$) $k_F=(3\pi^2n)^{\frac13}\propto n^{\frac13};\epsilon_F=\hbar^2k_F^2/2m=\hbar^2(3\pi^2n)^{\frac23}\propto n^{\frac23}$ $D(\epsilon)\propto\epsilon^{\frac12}.\langle\epsilon\rangle=\frac{\int_0^{\epsilon_F}\epsilon D(\epsilon)d\epsilon}{\int_0^{\epsilon_F}D(\epsilon)d\epsilon}=\frac35\epsilon_F$ $E=N\langle\epsilon\rangle\propto V^{-\frac23},P=-\frac{dE}{dV}=\frac25n\epsilon_F\propto\epsilon_F^{\frac52}$. $\frac{dP}{d\epsilon_F}=n\to\Delta P\approx n\Delta\epsilon_F$