**晶格(2)**sc(简单,$2r=a$);bcc($4r=\sqrt{3}a,\rho=\frac{2m_0}{a^3},a=\sqrt[3]{\frac{2m_0}{\rho}}$);fcc($4r=\sqrt{2}a$);hcp(六角密)**(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(金刚石替换)(Zn000,$0\frac12\frac12,\frac12 0\frac12,\frac12\frac12 0$;S$\frac14\frac14\frac14,\frac14\frac34\frac34,\frac34\frac14\frac34,\frac34\frac34\frac14$)[例].$r_{\mathrm{Cs}}=1.7,r_{\mathrm{Cl}}$ 1.81.$a=2(r_{\mathrm{Cs}}+r_{\mathrm{Cl}})/\sqrt{3},PF=\frac{4\pi(r_{\mathrm{Cs}}^3+r_{\mathrm{Cl}}^3)}{3a^3}\approx0.682,\rho=\frac{m_{\mathrm{Cs}}+m_{\mathrm{Cl}}}{a^3}=4.2$;[例].NaCl下CsCl:$a=2(r_{\mathrm{Cs}}+r_{\mathrm{Cl}}),PF=\frac{4\pi(r_{\mathrm{Cs}}^3+r_{\mathrm{Cl}}^3)\cdot4}{3a^3}\approx$ 0.525;**两种指标**晶面截距$a_1,a_2,a_3$(1)$(a_1^{-1}a_2^{-1}a_2^{-1})$;(2)$[a_1,a_2,a_3]$.上划线为负$[u\bar{v}w]$.**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**$\forall i,\vec{a_i}\cdot\Delta\vec{k}=2\pi v_i$;**倒格子基** $\vec{b_1}=2\pi\frac{\vec{a_2}\times\vec{a_3}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}}$, $\vec{b_2}=2\pi\frac{\vec{a_3}\times\vec{a_1}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}}$, $\vec{b_3}=2\pi\frac{\vec{a_1}\times\vec{a_2}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}}$. $\vec{b_i}\cdot\vec{a_j}=2\pi\delta_{ij}$;**倒格矢** $\vec{G}=v_1\vec{b_1}+v_2\vec{b_2}+v_3\vec{b_3},v_i\in\mathcal{Z}$.倒格矢$\vec{G}_{h_1h_2h_3}\perp h_1h_2h_3$(实空间晶面).面间距$d=\frac{2\pi}{|\vec{G_{\vec{h}}}|}$**几何结构因子**前提:方向为$\vec{k'}=\vec{k}+\Delta\vec{k}=\vec{k}+\vec{G}$, $S_G=\sum_j f_je^{-i\vec{r_j}\cdot\vec{G}}=\sum_j f(j)e^{-i2\pi(x_jv_1+y_jv_2+z_jv_3)},f_j=\int dVn_j(\vec{r})e^{-i\vec{G}\cdot\vec{r}}$.[例].bcc&$(0,0,0)+(\frac12,\frac12,\frac12),S(v_1,v_2,v_3)=f(1+e^{-i\pi(v_1+v_2+v_3)})$;[例].fcc&$(0,0,0)+(0,\frac12,\frac12)+(\frac12,0,\frac12)+(\frac12,\frac12,0),S(v_1,v_2,v_3)=f\{1+e^{-i\pi(v_2+v_3)}+e^{-i\pi(v_1+v_3)}+e^{-i\pi(v_1+v_2)}\}$;**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12面体(长对角线$2\cdot\frac{\sqrt{2}\pi}{a}$,短对角线$2\cdot\frac{\pi}{a}$);fcc→截角8面体(8面体每个角被切,使相邻3面的正方形边围成正6边形.小正方形和6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$w^2=(\frac{2C}{M})(1-\cos Ka)=\omega_m^2\sin^2\frac12Ka;w^2=(\frac{4C}{M})\sin^2\frac12Ka$;态密度:$D(\omega)=\frac{Na}{\pi}/|\partial_K\omega|,\partial_K\omega=\frac{a}{2}\omega_m\cos\frac12Ka=\frac{a}{2}(\omega_m^2-\omega^2)^{\frac12}$群速:$v_g=\partial_K\omega=\sqrt{\frac{Ca^2}{M}}\cos\frac{Ka}{2}$;[长波($Ka\ll1$):$w^2=(\frac{C}{M})K^2a^2,v=\frac{w}{K}$离散转连续:$M\partial_t^2u_s=\sum_pC_p(u_{s+p}-u_s)=\sum_{p>0}C_p[(u_{s+p}-u_s)+(u_{s-p}-u_s)]=\sum_{p>0}C_p\{[u(x+pa,t)-u(x,t)]+[u(x-pa,t)-u(x,t)]\}=\sum_{p>0}C_pp^2a^2\partial_x^2u(x,t)$,试探解$u_{s+p}=ue^{-i[\omega t-(s+p)Ka]},\omega^2=\frac{2}{M}\sum_{p>0}C_p(1-cospKa)\approx K^2(a^2/M)\sum_{p>0}p^2C_p=v^2K^2\to\partial_t^2u=v^2\partial_x^2u$]**(2)无阻尼双原子链**:原胞p个原子,3个声支,3p-3个光支.$M_1\frac{d^2u_s}{dt^2}=C(v_s+v_{s-1}-2u_s);M_2\frac{d^2v_s}{dt^2}=C(u_{s+1}+u_s-2v_s)$.试解$u_s=ue^{isKa}e^{-iwt},v_s=ve^{isKa}e^{-iwt}$,系数行列式0:$M_1M_2w^4-2C(M_1+M_2)w^2+2C^2(1-\cos Ka)=0$;长波($Ka\ll1$):光支$w^2=2C(\frac{1}{M_1}+\frac{1}{M_2})$,声支$w^2=\frac{C}{2(M_1+M_2)}K^2a^2$;光支下原子反向震动(质心固定),光电场激发.**(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$\vec{K}$的声子:$\vec{k}=\vec{k'}\pm\vec{K}+\vec{G},\vec{G}$是倒格矢;**(4)声子能量:**$\epsilon=(n+\frac12)\hbar\omega$.若$u=u_0\cos Kx\cos\omega t,E_k=\int\frac12\rho(\frac{\partial u}{\partial t})^2=\frac14\rho V\omega^2u_0^2\langle\sin^2\omega t\rangle=\frac18\rho V\omega^2u_0^2=\frac12(n+\frac12)\hbar\omega$;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)$\omega_{k_D}<\Gamma/2m:\tau_k=\frac{\Gamma}{2m\omega_{k_0}^2}(1+\sqrt{1-(\frac{2m\omega_{k_0}}{\Gamma})^2})$**(6)2D正方**:$M\partial_t^2u_{l,m}=C[(u_{l+1,m}+u_{l-1,m}-2u_{l,m})+(u_{l,m+1}+u_{l,m-1}-2u_{l,m})]$.设$u_{l,m}=u_0e^{i(lK_xa+mK_ya-\omega t)}$,色散关系$\omega^2M=2C(2-\cos K_xa-\cos K_ya)$(a)$K=K(1,0),\omega^2=\frac{2C}{M}(1-\cos Ka)$;(b)$K=K(1,1)/\sqrt{2},\omega^2=\frac{4C}{M}(1-\cos\frac{1}{\sqrt{2}}Ka)$,长波($Ka\ll1$)$\omega^2\approx\frac{Ca^2}{M}(K_x^2+K_y^2)$,群速$v=\frac{\partial\omega}{\partial K}=\sqrt{\frac{Ca^2}{M}}$.**(7)变C等M双原子链**.$M\partial_t^2u_s=C(v_{s-1}-u_s)+10C(v_s-u_s),M\partial_t^2v_s=10C(u_s-v_s)+C(u_{s+1}-v_s)$.试$u_s=ue^{isKa}e^{-i\omega t},v_s=ve^{isKa}e^{-i\omega t}$.$\left|\begin{smallmatrix}M\omega^2-11C, & C(10+e^{-iKa})\\ C(e^{iKa}+10), & M\omega^2-11C\end{smallmatrix}\right|=0,\omega_\pm^2=\frac{C}{M}[11\pm\sqrt{121-20(1-\cos Ka)}]$**(8)**$\omega=\omega(K),K=\omega^{-1}(\omega)$,轨道总数$N(\omega)=(\frac{L}{2\pi})^3\frac{4\pi}{3}K^3$,态密度$D(\omega)=|\partial_\omega N|$**热学基础 (0)**$\frac{\Delta a}{a}=\frac{\Delta V}{3V},C_V=(\frac{\partial U}{\partial T})_V$,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**$\langle n\rangle=(e^{\hbar\omega/\tau}-1)^{-1}$**(2)**$U=\sum_K\sum_p\hbar\omega_{K,p}(e^{\hbar\omega_{K,p}/\tau}-1)^{-1}=\sum_p\int d\omega D_p(\omega)\hbar\omega(e^{\hbar\omega/\tau}-1)^{-1}$, $C_{lat}=k_B\sum_p\int d\omega D_p(\omega)\frac{x^2e^x}{(e^x-1)^2}(x=\frac{\hbar\omega}{\tau}=\hbar\omega/k_BT)$,$D(\omega)$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$d$,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$\pi k_D^2=\frac{(2\pi)^2}{A}$,德拜频率$\omega_D=vk_D$,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,每种偏振声速恒定,$\omega=vK$,态密度$D(\omega)=\frac{V\omega^2}{2\pi^2v^3}$,德拜/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$U=3U_i=\frac{3V\hbar}{2\pi^2v^3}\int_0^{\omega_D}d\omega\frac{\omega^3}{e^{\frac{\hbar\omega}{\tau}}-1}=\frac{3Vk_B^4T^4}{2\pi^2v^3\hbar^3}\int_0^{x_D}dx\frac{x^3}{e^x-1}(x=\frac{\hbar\omega}{\tau},x_D=\frac{\hbar\omega_D}{\tau}=\frac{\theta}{T})$,德拜温度$\theta=\frac{\hbar v}{k_B}(\frac{6\pi^2N}{V})^{\frac13}$,$U=9Nk_BT(\frac{T}{\theta})^3\int_0^{x_D}dx\frac{x^3}{e^x-1}$[例]金刚石(3D)C-C距离$d$,声速$v$,晶格常数$a=\frac{4d}{\sqrt{3}}$,原胞体积$\Omega=\frac{a^3}{4}$,德拜波矢$\frac43\pi k_D^3=\frac{(2\pi)^3}{\Omega}$,德拜温度$\theta_D=\frac{\hbar\omega_D}{k_B}=\frac{\hbar vk_D}{k_B}$.$(\theta_D|_{d=1.54\mathring{A}}=2.39\times10^3K)$(2)低温($T^3$)($\int_0^\infty dx\frac{x^3}{e^x-1}=\frac{\pi^4}{15}$):$U\approxeq3\pi^2Nk_BT^4/5\theta^3$,热容$C_V\approxeq\frac{12\pi^4}{5}Nk_B(\frac{T}{\theta})^3\approxeq234Nk_B(\frac{T}{\theta})^3$;**爱因斯坦**$N\omega_0$振子($D(\omega)=N\delta(\omega-\omega_0)$):1D:$U=N\langle n\rangle\hbar\omega=N\frac{\hbar\omega}{e^{\hbar\omega/\tau}-1}$,1D:$C_V=(\frac{\partial U}{\partial T})_V=Nk_B(\frac{\hbar\omega}{\tau})^2\frac{e^{\hbar\omega/\tau}}{(e^{\hbar\omega/\tau}-1)^2}$.3D再乘3. **声子热学(1)态密度**一般:$D(\omega)=\frac{V}{(2\pi)^3}\int_{\mathrm{K中}\partial\omega=0}\frac{dS_\omega}{v_g}$**(2)非谐作用**($U(x)=cx^2-gx^3-fx^4$):平均位移$\langle x\rangle=\frac{\int_{-\infty}^{+\infty}dxxe^{-\beta U(x)}}{\int_{-\infty}^{+\infty}dxe^{-\beta U(x)}}(\beta=\frac{1}{k_BT})$,$\int dxxe^{-\beta U}\approxeq(\frac{3\pi^{\frac12}}{4})(\frac{g}{c^{\frac52}})\beta^{-\frac32}$, $\int dxe^{-\beta U}\approxeq(\frac{\pi}{\beta c})^{\frac12}$,$\langle x\rangle=\frac{3g}{4c^2}k_BT$**(3)热导**.1D下热流量$j_U=-K\frac{dT}{dx}$,热导率$K=\frac13Cvl$($C$: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($N$):$\vec{G}=0$;倒逆($U$):$\vec{G}\neq0$ **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电子系统基态下最高能级;[例]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**.$f(\epsilon,T,\mu)=(e^{[\epsilon-\mu(T)]/k_BT}+1)^{-1}$($T=0$时$\mu=\epsilon_F$).高温极限:玻尔兹曼分布/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$\epsilon_F=\frac{\hbar^2k_F^2}{2m}$.$K$空间体积元$(\frac{2\pi}{L})^3$存在单波矢$(k_x,k_y,k_z)$.F球+泡利定理:$2\cdot\frac{4\pi k_F^2/3}{(2\pi/L)^3}=N$.F波矢$k_F=(\frac{3\pi^2N}{V})^{\frac13}=(3\pi^2n)^{\frac13}$,F能$\epsilon_F=\frac{\hbar^2}{2m}(\frac{3\pi^2N}{V})^{\frac23}=\frac{\hbar^2}{2m}(3\pi^2n)^{\frac23}$,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$N(U\leq\epsilon)=\frac{V}{3\pi^2}(\frac{2m\epsilon}{\hbar^2})^{\frac32},D(\epsilon)=\frac{dN}{d\epsilon}=\frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{\frac32}\epsilon^{\frac12}=\frac{3N}{2\epsilon}$,**0K**:$U_0=2\sum_{k<k_F}\frac{\hbar^2k^2}{2m}$,**K**中状态数体密度为$\frac{V}{8\pi^3}$,$\frac{U_0}{V}=\frac{2}{8\pi^3}\int_{k<k_F}d^3k\frac{\hbar^2k^2}{2m}=\frac{1}{\pi^2}\frac{\hbar^2k_F^5}{10m},N=2\cdot\frac{4\pi k_F^3}{3}\frac{V}{8\pi^3},U_0=\frac35N\epsilon_F$,压强$P=-(\partial_VU_0)_N=-\frac35(\partial_V\epsilon_F)_N=\frac23\frac{U_0}{V}$,体模量$B=-V(\partial_VP)=-V\partial_V[\frac{N\hbar^2}{5m}(\frac{3\pi^2N}{V})^{\frac23}\frac1V]=\frac{10}{9}\frac{U_0}{V}$**(b)2D:**$2\pi k_F^2\frac{A}{(2\pi)^2}=N,k_F=\sqrt{\frac{2\pi N}{A}}=\sqrt{2\pi n}$.色散:$\epsilon=\frac{\hbar^2k^2}{2m},d\epsilon=\frac{\hbar^2kdk}{m}$.态密度$D(\epsilon)d\epsilon=2\frac{2\pi kdk}{A}\cdot\frac{A}{(2\pi)^2}=\frac{kdkd\epsilon}{\pi d\epsilon}=\frac{md\epsilon}{\pi\hbar^2},n=\int_{-\infty}^{+\infty}D(\epsilon)n_F(\epsilon)d\epsilon=\frac{m}{\pi\hbar^2}\int_0^{+\infty}\frac{d\epsilon}{e^{(\epsilon-\mu)/k_BT}+1}=\frac{mk_BT}{\pi\hbar^2}\ln(e^{\mu/k_BT}+1)$.化学势$\mu(T)=k_BT\ln(e^{\frac{\pi n\hbar^2}{mk_BT}}-1)$**(4)比热容**.总e内能$U_e\approx\frac{NT}{T_F}k_BT$,e比热$C_e=\frac{\partial U}{\partial T}\approx Nk_B\frac{T}{T_F}$.低温($k_BT\ll\epsilon_F$):$\Delta U=\int_0^\infty d\epsilon\epsilon D(\epsilon)f(\epsilon)-\int_0^{\epsilon_F}d\epsilon\epsilon D(\epsilon)=\int_{\epsilon_F}^\infty d\epsilon(\epsilon-\epsilon_F)f(\epsilon)D\epsilon+\int_0^{\epsilon_F}d\epsilon(\epsilon_F-\epsilon)[1-f(\epsilon)]D(\epsilon)$.e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($\tau=k_BT,x=\frac{\epsilon-\epsilon_F}{\tau}$)$\int_{-\infty}^{+\infty}dxx^2\frac{e^x}{(e^x+1)^2}=\frac{\pi^2}{3},C_e=\frac13\pi^2D(\epsilon_F)k_B^2T(D(\epsilon_F)=\frac{3N}{2\epsilon_F}),C_e=\frac{\pi^2Nk_BT}{2T_F}$.**(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$\vec{F}=-e\vec{E},\delta\vec{k}=-e\vec{E}t/\hbar,\vec{v}=\delta\vec{k}/m=-e\vec{E}\tau/m$.电流密度$\vec{j}=nq\vec{v}=ne^2\tau\vec{E}/m$,$(\vec{j}=\sigma\vec{E})\sigma=\frac{ne^2\tau}{m},\rho=\sigma^{-1}$.[电子漂移速度v:$m(\partial_tv+v/\tau)=-eE$,试$E=E_0e^{-i\omega t},v=v_0e^{-i\omega t},v=\frac{-(1+i\omega\tau)}{1+(\omega\tau)^2}\frac{e\tau}{m}E,\sigma(\omega)=j/E=-env/E=\frac{e^2\tau n}{m}(\frac{1+i\omega\tau}{1+(\omega\tau)^2})$]**(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$\omega_c=\frac{eB}{mc}$[漂

移速度理论:$m(\partial_t+\tau^{-1})v_x=-e(E_x+\frac{B}{c}v_y), m(\partial_t+\tau^{-1})v_y=-e(E_y-\frac{B}{c}v_x), m(\partial_t+\tau^{-1})v_z=-eE_z, j=-nev, v_x=\frac{1}{1+(\omega_c\tau)^2}(-\frac{e\tau}{m}E_x+\frac{\omega_c\tau^2 e}{m}E_y), v_y=\frac{1}{1+(\omega_c\tau)^2}(-\frac{\omega_c\tau^2 e}{m}E_x-\frac{e\tau}{m}E_y), v_z=-\frac{e\tau}{m}E_z, [j_x,j_y,j_z]^T=\frac{\sigma_0}{1+(\omega_c\tau)^2}[1,-\omega_c\tau,0;\omega_c\tau,1,0;0,0,1+(\omega_c\tau)^2][E_x,E_y,E_z]^T, \sigma_0=\frac{ne^2\tau}{m}, \omega_c=\frac{Be}{mc}$.若$j_y=0, E_y=-\omega_c\tau E_x, j_x=\sigma_0 E_x$:自由e理论too simple] **(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**.$K_e=\frac{1}{3}Cvl=\frac{\pi^2}{3}\frac{nk_B^2T}{mv_F^2}v_Fl=\frac{\pi^2nk_B^2T\tau}{3m}$(10)洛伦兹常量$L=\frac{K}{\sigma T}=\frac{\pi^2}{3}(\frac{k_B}{e})^2=2.45\times10^{-8}(W\Omega/\deg^2)$.**(10)金属受力**自由电子.$(n_{Cu}\approx10^6)k_F=(3\pi^2n)^{\frac{1}{3}}\propto n^{\frac{1}{3}};\epsilon_F=\hbar^2k_F^2/2m=\hbar^2(3\pi^2n)^{\frac{2}{3}}\propto n^{\frac{2}{3}}, D(\epsilon)\propto\epsilon^{\frac{1}{2}}.\langle\epsilon\rangle=\frac{\int_0^{\epsilon_F}\epsilon D(\epsilon)d\epsilon}{\int_0^{\epsilon_F}D(\epsilon)d\epsilon}=\frac{3}{5}\epsilon_F, E=N\langle\epsilon\rangle\propto V^{-\frac{2}{3}}, P=-\frac{dE}{dV}=\frac{2}{5}n\epsilon_F\propto\epsilon_F^{\frac{5}{2}}.\frac{dP}{d\epsilon_F}=n\to\Delta P\approx n\Delta\epsilon_F$.**(11)求第一布里渊区能带**3D$\epsilon(\vec{K})=\frac{\hbar^2}{2m}[(K_x+g_1\frac{2\pi}{a})^2+(K_y+g_2\frac{2\pi}{a})^2+(K_z+g_3\frac{2\pi}{a})^2]$,**近自由电子模型(0)1D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**!$t:\psi(+)=e^{\frac{i\pi x}{a}}+e^{-\frac{i\pi x}{a}}=2\cos\frac{\pi x}{a}, \psi(-)=e^{\frac{i\pi x}{a}}-e^{-\frac{i\pi x}{a}}=2i\sin\frac{\pi x}{a}.\rho(+)=|\psi(+)|^2\propto\cos^2\frac{\pi x}{a}, \rho(-)=|\psi(-)|^2\propto\sin^2\frac{\pi x}{a}$.大小关系:$\langle\psi(-)|U|\psi(-)\rangle\le\langle e^{\mp i\pi x/a}|U|e^{\pm i\pi x/a}\rangle\le\langle\psi(+)|U|\psi(+)\rangle$.若1D:$\psi(x)=\sqrt{2}\cos\frac{\pi x}{a},\sqrt{2}\sin\frac{\pi x}{a}$,e势能$U(x)=U\cos\frac{2\pi x}{a}$,则1级近似能隙$E_g=U(+)-U(-)=\int_0^1 dxU(x)[|\psi(+)|^2-|\psi(-)|^2]=U$.**(2)布洛赫函数**.若周期势,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,$\psi(x+a)=C\psi(x), C=e^{i2\pi s/N}\to\psi(x)=u_{\vec{k}}(x)e^{i2\pi sx/N}$.**(3)KP模型Kölnig-Penney**(周期$\delta$势阱).$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+U(x)\psi=\epsilon\psi.\ x\in(0,a):\psi=Ae^{iKx}+B^{-iKx}, \epsilon=\frac{\hbar^2K^2}{2m};x\in(-b,0):\psi=Ce^{Qx}+De^{-Qx}, U_0-\epsilon=\frac{\hbar^2Q^2}{2m}$.$\psi$连续+$\psi'$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$(P/Ka)\sin Ka+\cos Ka=\cos ka$.带宽:$\frac{P}{\pi+\theta}(-\theta+\frac{\theta^3}{6})+(-1+\frac{\theta^2}{2})=\cos ka(\theta=-\frac{\pi}{P}(1+\cos ka)), \Delta E=\frac{2\pi^2\hbar^4}{m^2a^4V_0}$. **(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)**$\det\{\{\lambda_{k-g}-\epsilon,U,0\},\{U,\lambda_k-\epsilon,U\},\{0,U,\lambda_{k+g}-\epsilon\}\}$.每一个$k$每个$\epsilon$在不同能带.**(6)中心方程求解K-P**(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$f(k)=\sum_n C(k-2\pi n/a)=f(k\pm2\pi n/a)$.从而有$\frac{mAa^2}{2\hbar^2}(Ka)^{-1}\sin Ka+\cos Ka=\cos ka$.极限$P\ll1$, **(7)BZ近边界近似解**.$k^2=(\frac{1}{2}G)^2, (k-G)^2=(\frac{1}{2}G-G)^2, k=\pm\frac{1}{2}G.(k=\frac{1}{2}G, \lambda=\hbar^2(\frac{1}{2}G)^2/2m)(\lambda-\epsilon)C(\pm\frac{1}{2}G)+UC(\mp\frac{1}{2}G)=0$.行列式$|^{\lambda-\epsilon,U}_{U,\lambda-\epsilon}|=0$,得$\epsilon=\lambda\pm U, E_g=2U$.若在$\frac{1}{2}G$附近,则$(\lambda_k-\epsilon)C(k)+UC(k-G)=0, (\lambda_{k-G})C(k-G)+UC(k)=0(\lambda_k=\frac{\hbar^2k^2}{2m}), |^{\lambda_k-\epsilon,U}_{U,\lambda_{k-G}-\epsilon}|=0, \epsilon=\frac{1}{2}(\lambda_{k-G}+\lambda_k)\pm[\frac{1}{4}(\lambda_{k-G}-\lambda_k)^2+U^2]^{\frac{1}{2}}$.以$\widetilde{K}=k-\frac{1}{2}G$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.N原胞一维**:$k=\pm\frac{2n\pi}{L}$.每原胞一个k+泡利定理,每能带2N轨道. **(9)正方晶格**$U(x)=-4U\cos\frac{2\pi x}{a}\cos\frac{2\pi y}{a}, \vec{r}=x\hat{i}+y\hat{j}, \vec{G}=G_1\hat{b_1}+G_2\hat{b_2}=\frac{2\pi}{a}(g_1\hat{b_1}+g_2\hat{b_2}).;U(\vec{r})=-U(e^{i\frac{2\pi}{a}x}+e^{-i\frac{2\pi}{a}x})(e^{i\frac{2\pi}{a}y}+e^{-i\frac{2\pi}{a}y})=-U[e^{i\frac{2\pi}{a}(x+y)}+e^{i\frac{2\pi}{a}(x-y)}+e^{-i\frac{2\pi}{a}(x-y)}+e^{-i\frac{2\pi}{a}(x+y)}]=U_{G(11)}e^{iG(11)\cdot\vec{r}}+U_{G(\bar{1}1)}e^{iG(\bar{1}1)\cdot\vec{r}}+U_{G(1\bar{1})}e^{iG(1\bar{1})\cdot\vec{r}}+U_{G(\bar{1}\bar{1})}e^{iG(\bar{1}\bar{1})\cdot\vec{r}}=\sum_{G(11)}e^{iG(11)\cdot\vec{r}}$.中心方程$(\lambda_k-\epsilon)C(\vec{K})+U_G(11)C(\vec{K}-\vec{G}(11))+U_{\vec{G}}(\bar{1}\bar{1})C(\vec{K}-\vec{G}(\bar{1}1))+U_G(1\bar{1})C(\vec{K}-\vec{G}(1\bar{1}))+U_G(\bar{1}1)C(\vec{K}-\vec{G}(\bar{1}1))$.若$\vec{K}=\vec{G}(\frac{1}{2}\frac{1}{2})=\frac{1}{2}\vec{G}(11), |^{\lambda_{\frac{1}{2}G(11)}-\epsilon,-U}_{-U,\lambda_{-\frac{1}{2}G(11)}-\epsilon}|=0, \epsilon=\frac{\hbar^2\pi^2}{ma^2}\pm U$ **紧束缚(1)**$E(\vec{k})=\epsilon_i-\sum_s J(\vec{R}_s)e^{-i\vec{k}\cdot\vec{R}_s}(\vec{R}_s=\vec{R}_n-\vec{R}_m)$**(2)1D,s**:$E(\vec{k})=\epsilon_s-J_0-J_1e^{-ika}-J_1e^{ika}=\epsilon_s-J_0-2J\cos ka$;**(3)2D,sc**:$E=\epsilon-2t(\cos(k_xa)+\cos(k_ya))$; Honeycomb:$\phi(\vec{r})=c_A\phi_A(\vec{r})+c_B\phi_B(\vec{r})=\frac{1}{\sqrt{N}}\sum_{\vec{R}_m}e^{i\vec{k}\cdot\vec{R}_m}[c_A\varphi(\vec{r}-\vec{R}_m^A)+c_B\varphi(\vec{r}-\vec{R}_m^B)], E(\vec{k})=\epsilon_1\pm J\sqrt{3+2\cos(\sqrt{3}k_ya)+4\cos(\frac{\sqrt{3}k_ya}{2})\cos(\frac{3k_xa}{2})}$(4)3D,(sc):$\epsilon(\vec{k})=\epsilon_s-J_0-2J_1(\cos k_xa+\cos k_ya+\cos k_za)$;(bcc):$\epsilon(\vec{k})=-\alpha-8\gamma\cos(\frac{k_xa}{2})\cos(\frac{k_ya}{2})\cos(\frac{k_za}{2})$;(fcc)$\epsilon(\vec{k})=-\alpha-4\gamma[\cos(\frac{k_ya}{2})\cos(\frac{k_za}{2})+\cos(\frac{k_za}{2})\cos(\frac{k_xa}{2})+\cos(\frac{k_xa}{2})\cos(\frac{k_ya}{2})]$ **(5)简并**:$\phi(\vec{r})=\frac{1}{\sqrt{N}}\sum_{\vec{R}_m}\sum_j e^{i\vec{k}\cdot\vec{R}_m}c_j\varphi_j(\vec{r}-\vec{R}_m)$ **(6)周期δ势**.$V(x)=-aV_0\delta(x), -\frac{\hbar^2}{2m}\psi''=E\psi, \psi=\sqrt{k}e^{-k|x|}(k=\sqrt{\frac{-2mE}{\hbar^2}}), -\frac{\hbar^2}{2m}\nabla^2\psi'(0)-aV_0\psi(0)=0, k=\frac{mV_0a}{\hbar^2}, E=-\frac{mV_0^2a^2}{2\hbar^2}, \psi=\sqrt{\frac{mV_0a}{\hbar^2}}e^{-\frac{mV_0a}{\hbar^2}|x|}$.TB条件:$k\ll a$.通解$E(k)=\epsilon-J(0)-\sum_{nn}J(R_m)e^{ikR_m}, J(R_m)=\sum_{R_m\neq0}aV_0\int\rho^*\delta(r-R_m)\rho(r-a)\mathrm{d}r=\frac{mV_0^2a^2}{\hbar^2}\sum_{n=1}^\infty e^{-\frac{mV_0a}{\hbar^2}(2na-a)}\approx\frac{mV_0^2a^2}{\hbar^2}e^{-\frac{mV_0a^2}{\hbar^2}}.E(k)=\epsilon-2J(R_m)\cos kR_m-J(0)$.能隙$\Delta E=4J=\frac{4mV_0^2a^2}{\hbar^2}e^{-\frac{mV_0a^2}{\hbar^2}}$ **近自由电子(1)非简并**$\varphi_k(x)=\varphi_k^0(x)+\sum_{k'(k'\neq k)}\frac{\langle k'|V(x)|k\rangle}{E_k^0-E_{k'}^0}\varphi_{k'}(x)(\langle k'|V(x)|k\rangle=\frac{1}{L}\int e^{-i(k'-k)x}V(x)\mathrm{d}x=V_G(G=k'-k)), \varphi_k=\varphi_k^0(x)+\sum_{k'(k'\neq k)}\frac{\langle k'|V(x)|k\rangle}{E_k^0-E_{k'}^0}\varphi_{k'}^0(x)=\varphi_k^0(x)+\sum_{k'(k'\neq k)}\frac{V_G}{E_k^0-E_{k'}^0}\varphi_{k'}^0(x)$,1级:$\langle k|V(x)|k\rangle=\frac{1}{L}\int_0^L V(x)\mathrm{d}x=\overline{V}=0$;2级:$E_k^2=\sum_{k'}\frac{|\langle k'|V(x)|k\rangle|^2}{E_k^0-E_{k'}^0}=\sum_G\frac{|V_G|^2}{\frac{\hbar^2}{2m}[k^2-(k+G)^2]}$.(I)if $(k+G)^2\gg k^2$,自由e;(II)$(k+G)^2=k^2$**(2)简并**$\{^{(E_k^0-E)a+V_G^*b=0}_{V_Ga+(E_{k'}^0-E)b=0}$ $|^{(E_k^0-E),V_G^*}_{V_G,(E_{k'}^0-E)}|=0, E_{k\pm}=\frac{1}{2}\{(E_k^0+E_{k'}^0)\pm\sqrt{(E_k^0+E_{k'}^0)^2+4|V_G|^2}\}$.(I)$E_k^0=E_{k'}^0$(BZ边界):$E_{k\pm}=E_k^0\pm|V_G|$;(II)$|E_k^0-E_{k'}^0|\gg|V_G|$(远离BZ):$E_{k\pm}$ $\{^{E_{k'}^0+\frac{|V_G|^2}{E_{k'}^0-E_k^0}}_{E_k^0+\frac{|V_G|^2}{E_{k'}^0-E_k^0}}$ (III)靠近BZ边界($|E_k^0-E_{k'}^0|\ll|V_G|$):$E_{k\pm}=\frac{1}{2}\left\{E_k^0+E_{k'}^0\pm\left[2|V_G|+\frac{(E_{k'}^0-E_k^0)^2}{4|V_G|}\right]\right\}, E_k^0+E_{k'}^0=2E_0+\frac{\hbar^2}{m}\left(k+\frac{G}{2}\right)^2, (E_{k'}^0-E_k^0)^2=4\left(\frac{\hbar^2}{2m}\right)^2G^2\left(k+\frac{G}{2}\right)^2$,即$E_{k\pm}\approx(E_0\pm|V_G|)+\frac{\hbar^2}{2m}\left(k+\frac{G}{2}\right)^2\pm\left(\frac{\hbar^2}{2m}\right)^2\frac{G^2}{2|V_G|}\left(k+\frac{G}{2}\right)^2$.**(3)2D简单正方**:$V(\vec{r})=-\sum_n a^2V_0\delta(\vec{r}-\vec{R}_n)$.近似条件:势能很小,视为微扰($|U_G|=V_0\ll\frac{\hbar^2}{2m}(\frac{\pi^2}{a^2})$),能隙$2|V_{G=G_2}|=|\frac{1}{a^1}\iint Ve^{i\vec{G}_2\cdot\vec{r}}\mathrm{d}\vec{r}|=2V_0$ **半导体**价带顶($\bigcap$),导带底($\bigcup$)**(1)e群速度**:$\vec{v}_g=\nabla_{\vec{k}}\omega(\vec{k})=\frac{1}{\hbar}\nabla_{\vec{k}}E(\vec{k})$**(2)有效质量**.$\frac{1}{m^*}=\frac{1}{\hbar^2}\frac{\mathrm{d}^2E}{\mathrm{d}k^2}$,方向:$(\frac{1}{m*})_{\mu\nu}=\frac{1}{\hbar^2}\frac{\mathrm{d}^2E}{\mathrm{d}k_\mu\mathrm{d}k_\nu}$;另一种定义:$m^*=\hbar^2k\left(\frac{\partial E}{\partial k}\right)^{-1}$,线性色散$E=a(|\vec{k}-\vec{k}_0|)$:$m^*=\frac{\hbar|\vec{k}|}{v_g}=\frac{\hbar}{v_g}|\vec{k}-\vec{k}_0|$.能隙$\Delta=2m_0v_g^2$.**(3)空穴**:$\vec{k}_h=-\vec{k}_e;E_h(\vec{k}_h)=-E_e(\vec{k}_e);\vec{v}_h=-\frac{1}{\hbar}\nabla_{\vec{k}_h}E_h(\vec{k}_h)=\frac{1}{\hbar}\nabla_{\vec{k}_e}E_e(\vec{k}_e)=\vec{v}_e$.**(4)激子**$\frac{1}{\mu^*}=\frac{1}{m_C^*}+\frac{1}{m_{hh}^*}, (m_C^*=0.067m_e, m_{hh}^*=0.45m_e)$,长度$a_0^*=\frac{\epsilon_rm_e}{\mu^*}\cdot a_0(a_0=\frac{\epsilon_0h^2}{\pi m_ee^2}\approx0.53\text{Å})$**(5)粒子浓度**:$\mathrm{d}n=f(E,T)g(E)\mathrm{d}E(f(E,T)=\frac{1}{1+e^{(E-\mu)/k_BT}}).E-\mu\gg k_BT$极限F-D 分布退化为 B 分布:$f(E,T)\approx e^{-(E-\mu)/k_BT}$.导带找到e:$f_C\approx e^{-\frac{(E-\mu)}{k_BT}}$;价带找到h:$f_h=1-f_V=e^{-(\mu-E)/k_BT}$.$g(E)$因近似抛物线色散($E-E_C=\frac{(k-k_C)^2}{2m_C^*}, E-E_V=-\frac{(k-k_V)^2}{2m_h^*}$),即态密度:$g_C(E)=a(m_C^*)^{\frac{3}{2}}(E-E_C)^{\frac{1}{2}};g_V(E)=a(m_h^*)^{\frac{3}{2}}(E_V-E)^{\frac{1}{2}}, n=\int_{E_C}^\infty f_Cg_C\mathrm{d}E\approx a(m_C^*)^{\frac{3}{2}}\int_{E_C}^\infty(E-E_C)^{\frac{1}{2}}e^{-\frac{E-\mu}{k_BT}}\mathrm{d}E=N_ce^{-\frac{E_C-\mu}{k_BT}}(N_C=2(\frac{k_B}{2\pi\hbar^2})^{\frac{3}{2}}(m_C^*T)^{\frac{3}{2}})$,同理$p\approx N_Ve^{-\frac{\mu-E_V}{k_BT}}(N_V=2(\frac{k_B}{2\pi\hbar^2})^{\frac{3}{2}}(m_h^*T)^{\frac{3}{2}})$.**Law of Mass Action:**$np\approx WT^3e^{-\frac{E_g}{k_BT}}$(前提:$|\mu-E|\gg k_BT$)**(6)化学势**本征半导体$n=p$, $\frac{N_V}{N_C}=e^{\frac{2\mu-E_C-E_V}{k_BT}};\mu=\frac{1}{2}(E_C+E_V)+\frac{3}{4}k_BT\ln\frac{m_h^*}{m_C^*}$**(7)电导率**(I)载流子迁移率$(\mu_e,\mu_h)\mu=\frac{|v|}{E}$(电荷 $q$ 漂移速度 $v=\frac{q\tau E}{m}$, $\tau$为碰撞时间)$\mu_{e/h}=\frac{e\tau_{e/h}}{m_{e/h}}$.半导体:$\sigma=ne\mu_e+pe\mu_h$**(7)掺杂**半导体原子价态为$\nu$.$n$型掺杂(杂质为$\nu+1$);p型掺杂(杂质为 $\nu-1$)(I)浅掺杂能级:类H.(i)掺杂e:$E_d=-\frac{m_c^*}{m_e}\frac{1}{\epsilon_r^2\times\frac{13.6\text{eV}}{n^2}}$;(2)掺杂h:$E_a=-\frac{m_V^*}{m_e}\frac{1}{\epsilon_r^2}\times\frac{13.6\text{eV}}{n^2}$.参与导电.**(8)非本征载流子浓度**掺杂较少,$\mu$还在$E_g$中:$np=WT^3e^{-\frac{E_g}{k_BT}}$.全电离:$N-p=N_D-N_A$.半导体pn结.p型:$\mu(E_F)$比$E_i$更近价带顶;n型:$\mu(E_F)$比$E_i$ 更近导带底.e,h扩散,通过$\mu(E_F)$拉平.(I)金-半导体:(i)肖特基:半

导体$\mu(E_F)\uparrow$,e从半导体到金属;内建$\vec{E}$,导带$E\uparrow$,导带底和费米能级距离↑(ii)欧姆:半导体$\mu(E_F)$低于金属,对e无势垒.(II)金-氧化绝缘体-半(MOS)$E_F$独立,类电容.(i)正电压:e从半导体远端到绝缘端.$\mu(E_F)$更近导带底, n型强化;(ii)反电压:e向半导体远端移动.超限后,发生反型($\mu(E_F)$更近价带顶) **(9)布洛赫振荡**运动方程$\hbar\frac{\mathrm{d}k}{\mathrm{d}t}=-eE$,解$k(t)=k(0)-\frac{eE}{\hbar}t$.色散$\epsilon(k)=\epsilon_0[1-\cos(ak)]$,e群速度$v(k)=\frac{1}{\hbar}\frac{\mathrm{d}\epsilon}{\mathrm{d}k}=\frac{\epsilon_0 a}{\sin(ak)}$.$k(0)=x(0)=0$,$x(t)=\int_0^t v[k(t')]\mathrm{d}t'=\frac{\epsilon_0}{eE}[\cos(\frac{eEa}{\hbar}t)-1]$.$\omega_{\mathrm{BO}}=eEa/\hbar$.观测条件$\tau\gg 2\pi/\omega_{\mathrm{BO}}=h/eEa$. **布洛赫电子动力学(1)运动特征**$\frac{\hbar\mathrm{d}\vec{k}}{\mathrm{d}t}=-e\vec{v}\times\vec{B}$.e群速度$\vec{v}=\frac{1}{\hbar}\nabla_k E(\vec{k})$; $\frac{\mathrm{d}E}{\mathrm{d}t}=\nabla_k(\vec{k})\frac{\mathrm{d}\vec{k}}{\mathrm{d}t}=0$.实空间和倒空间运动方向垂直.**(2)回旋频率**($k_z=0$).周期$T=\frac{2\pi K}{\frac{evB}{\hbar}}=\frac{2\pi}{eB}\frac{\hbar K}{v}=\frac{2\pi m}{eB}$;回旋频率$\omega_c=\frac{2\pi}{T}=\frac{eB}{m_c^*}(m_c^*\ncong m^*)$**(3)磁场中分立能**(1.抛物线色散2.忽略自旋)朗道能级$E(k)=\frac{\hbar^2}{2m}k_z^2+\left(n+\frac{1}{2}\right)\hbar\omega_c$.(I)简并度(i)无磁场:$E(\vec{k})=\frac{\hbar^2}{2m}(k_x^2+k_y^2)$(ii)有磁场:相邻朗道环$L_n,L_{n+1}$所围态简并.态数目$n_k=\Delta A\times\frac{S}{4\pi^2}=\pi\left[\Delta(k_x^2+k_y^2)\right]\times\frac{S}{4\pi^2}=\frac{2\pi m\Delta E}{\hbar^2}\times\frac{S}{4\pi^2}=\frac{2\pi m\hbar\omega_c}{\hbar^2}\times\frac{S}{4\pi^2}=\frac{4\pi^2 eB}{h}\times\frac{S}{4\pi^2}=\frac{eBS}{\hbar}$,朗道能级简并度$p=2n_k=\frac{2e}{h}BS=\frac{BS}{\Phi_0}(\Phi_0=\frac{h}{2e}\approx 2.067\times 10^{-15}(\mathrm{Wb}))$.高量子态条件:$\oint\vec{p}\cdot\mathrm{d}\vec{r}=(n+\gamma)\cdot 2\pi\hbar$, $A_r=\frac{2\pi\hbar}{eB}(n+\gamma)$.$\hat{B}\times\frac{\mathrm{d}\vec{k}}{\mathrm{d}t}=-\frac{eB}{\hbar}\frac{\mathrm{d}\vec{r}_\perp}{\mathrm{d}t}$, $\frac{A_k}{A_r}=(\frac{eB}{\hbar})^2$, $A_k=\frac{2\pi eB}{\hbar}(n+\gamma)$.或$\frac{1}{B}=\frac{2\pi e}{\hbar A_k}(n+\gamma)$, $\Delta(\frac{1}{B})=(\frac{1}{B_{n+1}}-\frac{1}{B_n})=\frac{2\pi e}{\hbar}\frac{1}{A_k}$**(II)de Hass-Van Alphen**(i)2D:横轴为磁矩,横轴为磁场.$\Delta(\frac{1}{B})=\frac{2\pi e}{\hbar}\frac{1}{A_{k_F}}$, $A_F$极值轨道;(ii)fcc(Au,Ag,Cu)$n=\frac{4}{a^3}$, $k_F=(3\pi^2 n)^{\frac{1}{3}}=(\frac{12\pi^2}{a^3})^{\frac{1}{3}}\approx 4.90a^{-1}$,跨越BZ最短距离:$\sqrt{3}b=(\frac{2\pi}{a})\approx 10.88a^{-1}$, $\frac{4\pi}{a}\approx 12.57a^{-1}$, Au:$\Delta(\frac{1}{B})=2\times 10^{-9}\mathrm{G}^{-1}$,极值轨道:$S=\frac{2\pi e}{\hbar}[\Delta(\frac{1}{B})]^{-1}\approx 4.8\times 10^{16}\mathrm{cm}^{-2}$**(4)磁场下2D电子**$E=(n+\frac{1}{2})\hbar\omega_c$(I)展宽(i)本征:$\delta E\approx\frac{\hbar}{\tau}$,分辨条件$\omega_c\tau\gg 1$;(ii)$T$:分辨条件$\hbar\omega_c\gg k_BT$(低温)(II)简并度:单位面积内每个朗道能级的e数.单位面积内朗道能级简并度:$n_L=\frac{2eB}{h}$(i)$\sigma$极小(态密度谷):$N_L=n\frac{2eB}{h}$,(ii)$\sigma$极大(态密度峰):$N_L=(n+\frac{1}{2})\frac{2eB}{h}$,$\sigma$周期:$\Delta(\frac{1}{B})=\frac{2e}{hN_L}$(III)霍尔效应.$\overleftrightarrow{\sigma}=\frac{\sigma_0}{1+(\omega_c\tau)^2}\begin{bmatrix}1,-\omega_c\tau\\ \omega_c\tau,1\end{bmatrix}$,系数$R_H=\frac{E_y}{j_xB}=\frac{\sigma_{xy}}{\sigma_{xx}^2+\sigma_{xy}^2}\frac{1}{B}=\frac{-1}{B}\frac{\omega_c\tau}{\sigma_0}=-\frac{1}{ne}$.2D各向同性:$\begin{bmatrix}J_x\\ J_y\end{bmatrix}=\begin{bmatrix}\sigma_{xx},\sigma_{xy}\\ -\sigma_{xy},\sigma_{yy}\end{bmatrix}\begin{bmatrix}E_x\\ E_y\end{bmatrix}$,霍尔效应:$\begin{Bmatrix}\rho_{xx}=\frac{E_x}{J_x}=\frac{\sigma_{xx}}{\sigma_{xx}^2+\sigma_{xy}^2}\\ \rho_{xy}=\frac{E_y}{J_x}=\frac{\sigma_{xy}}{\sigma_{xx}^2+\sigma_{xy}^2}\end{Bmatrix}$.极限$\omega_c\tau\gg 1,\sigma_{xy}\gg\sigma_{xx}$:$\begin{Bmatrix}\rho_{xx}=\frac{\sigma_{xx}}{\sigma_{xy}^2}\\ \rho_{xy}=\frac{1}{\sigma_{xy}}=R_HB\end{Bmatrix}$; $R_H=\frac{E_y}{J_xB}$.**(5)电阻**(I)e-声子散射(准弹性散射)$E_{k'}=E_k\pm\hbar\omega$, $\vec{k}'=\vec{k}\pm\vec{q}+\vec{G}$.弛豫和散射概率:$\frac{1}{\tau}=(\frac{1}{2\pi})^3\int\omega_{\vec{k},\vec{k}'}(1-\cos\theta)\mathrm{d}\vec{k}'$(i)高T($T>\theta_D$):$\rho\propto\frac{1}{\tau}\propto T$(高温)(ii)低T($q\ll k_F$):$N_{声子}\propto T^3$(低温):$1-\cos\theta=2\sin^2\left(\frac{\theta}{2}\right)=\frac{1}{2}(\frac{q}{k_F})^2$($\theta$很小).低温条件:$q\approx E\approx k_BT$, $1-\cos\theta\approx T^2$, $\omega_{\vec{k},\vec{k}'}\propto T^3$:$\rho\propto\frac{1}{\tau}\propto T^5$(II)剩余电阻率(杂质).$\left(\frac{\partial\rho}{\partial T}\right)_{T\to 0}=0$, $\rho_{T\to 0}=const.$ **(6)磁阻**($R$随$B$的变化)(O)理想:一种载流子,完美球形F面,洛伦兹力平衡于电场力,e运动将对是否有磁场不敏感,磁阻为0.(I)真实(i)$E_F$并不是严格球形,$v_F,m^*,\tau$各向异性;(ii)多条能带经过$E_F$,各能带$v_F,m^*,\tau$不同.[例]两能带:$\frac{\Delta\sigma}{\sigma_0}=-\frac{\sigma_{10}\sigma_{20}}{(\sigma_{10}+\sigma_{20})^2}(\omega_{c1}\tau_1-\omega_{c2}\tau_2)^2\Rightarrow\frac{\Delta\rho}{\rho_0}=\frac{\rho(B)-\rho(0)}{\rho(0)}\propto B^2>0$**(7)相位效应**(O)与杂质弹性散射,e相干:$\vec{k}\to\vec{k}'(|\vec{k}|=|\vec{k}'|)$, $\phi\to\phi'$;与声子非弹性散射,e非相干:$\phi=e^{-iEt/h}$.相位相干长度$l_\phi=v_F\tau_2$.(I)从$x'$到$x''$的总概率:$P=|\sum_i A_i|^2=|\sum_i A_i^2|+\sum_{i\neq j}A_iA_j$.(II)WL.环路:$P=|A_+|^2+|A_-|^2+A_+A_-^*+A_+^*A_-=4A^2$,大于经典概率$P'=2A^2$,$\sigma\downarrow$, $R\uparrow$.对2D:$\Delta\sigma=-\sigma_{00}\ln\frac{\tau_2}{\tau_1}=\sigma_{00}p\ln T$.(III)负磁阻:$\vec{B}=\nabla\times\vec{A}$, $\varphi(\vec{r})=\varphi_0(\vec{r})=e^{-\frac{ie}{\hbar}\int\vec{A}(\vec{r}')\cdot\mathrm{d}\vec{r}'}$, $A_+:A_+e^{-\frac{ie}{\hbar}\oint\vec{A}\cdot\mathrm{d}\vec{l}}=A_+e^{-\frac{ie}{\hbar}\iint\vec{B}\cdot\mathrm{d}\vec{S}}=A_+e^{-\frac{ie}{\hbar}\Phi}$, $A_{(-)}:A_{(-)}e^{\frac{ie}{\hbar}\Phi}=A_{(-)}e^{i2\pi\Phi/(2\Phi_0)}(\Phi_0=\frac{h}{2e})$, $P=2A^2[1+\cos^2(\frac{2\pi\Phi}{\Phi_0})]\leq 4A^2$ **输运现象**$\vec{J}_Q=-\kappa\nabla T$;$\vec{J}_Q=-D\nabla n$;$\vec{J}_e=-\sigma\nabla\varphi$ **(1)非平衡分布函数**:$f_n(\vec{r},\vec{k},t)\frac{\mathrm{d}\vec{r}\mathrm{d}\vec{k}}{(2\pi)^3}$($t$的第$n$能带中,在$(\vec{r},\vec{k})$处单位体积$\mathrm{d}\vec{r}\mathrm{d}\vec{k}$某自旋的平均e数)**(2)非平衡电流**$\vec{J}_e=-en(\vec{r},t)\vec{v}_d=-\frac{2}{(2\pi)^3}\int e\vec{v}_{\vec{k}}f(\vec{r},\vec{k},t)\mathrm{d}\vec{k}$**(3)平衡**:$\vec{J}=-\frac{2}{(2\pi)^3}\int e\vec{v}_{\vec{k}}f_0\mathrm{d}\vec{k}=0$**(4)从平衡到非平衡**:$\frac{\mathrm{d}\vec{k}}{\mathrm{d}t}=-\frac{e\vec{E}}{\hbar}$, $\vec{J}=-\frac{2}{(2\pi)^3}\int e\vec{v}_{\vec{k}}f\mathrm{d}\vec{k}\neq 0$**(5)玻尔兹曼方程**$\frac{\partial f}{\partial t}=(\frac{\partial f}{\partial t})_{漂移}+(\frac{\partial f}{\partial t})_{碰撞}$(I)漂移无碰撞:$f(\vec{r},\vec{k},\vec{t})=f(\vec{r}-\dot{\vec{r}}\mathrm{d}t,\vec{k}-\dot{\vec{k}}\mathrm{d}t,t-\mathrm{d}t)$(II)碰撞+漂移:$f(\vec{r},\vec{k},\vec{t})=f(\vec{r}-\dot{\vec{r}}\mathrm{d}t,\vec{k}-\dot{\vec{k}}\mathrm{d}t,t-\mathrm{d}t)+(\frac{\partial f}{\partial t})_{碰撞}\mathrm{d}t$.稳态($\partial_t f=0$)$\dot{\vec{k}}\frac{\partial f}{\partial\vec{k}}+\dot{\vec{r}}\frac{\partial f}{\partial\vec{r}}=(\frac{\partial f}{\partial t})_{碰撞}$.近似条件:$f=f_0+f_1(f_1\ll f_0)$, $(\frac{\partial f}{\partial t})=\frac{f_0-f}{\tau}=-\frac{f_1}{\tau}$.近似玻尔兹曼方程:$\dot{\vec{k}}\frac{\partial f_0}{\partial\vec{k}}+\dot{\vec{r}}\frac{\partial f_0}{\partial\vec{r}}=-\frac{f_1}{\tau}$(III)直流$\sigma$.仅$\vec{E}$下:$-\frac{e\vec{E}}{\hbar}\frac{\partial f_0}{\partial\vec{k}}=-\frac{f_1}{\tau}$, $\vec{J}_e=-\frac{2e}{(2\pi)^3}\int f\vec{v}_{\vec{k}}\mathrm{d}\vec{k}=-\frac{e}{4\pi^3}\int(f_0+f_1)\vec{v}_{\vec{k}}\mathrm{d}\vec{k}=-\frac{e}{4\pi^3}\int f_1\vec{v}_{\vec{k}}\mathrm{d}\vec{k}$.已知$f_1=\frac{e\tau\vec{E}}{\hbar}\frac{\partial f_0}{\partial\vec{k}}$; $\frac{\partial f_0}{\partial\vec{k}}=\frac{\partial f_0}{\partial\epsilon}\frac{\partial\epsilon}{\partial\vec{k}}$; $\vec{k}=\frac{1}{\hbar}\frac{\partial\epsilon}{\partial\vec{k}}$, $\vec{J}_e=\frac{e^2}{4\pi^3}\int\tau\frac{\partial f_0}{\partial\epsilon}\vec{k}_{\vec{k}}(\vec{v}_{\vec{k}}\cdot\vec{E})\mathrm{d}\vec{k}=\frac{e^2}{4\pi^3}\int\tau\frac{\vec{v}_{\vec{k}}(\vec{v}_{\vec{k}}\cdot\vec{E})}{\hbar v_k}(-\frac{\partial f_0}{\partial\epsilon})\mathrm{d}S\mathrm{d}\epsilon=\frac{e^2}{4\pi^3\hbar}\int\tau\frac{\vec{v}_k(\vec{v}_{\vec{k}}\cdot\vec{E})}{v_k}\mathrm{d}S_F$, $\vec{J}_e=[\frac{e^2}{4\pi^3\hbar}\int\tau\frac{\vec{v}_{\vec{k}}\vec{v}_{\vec{k}}}{v_k}\mathrm{d}S_F]\cdot\vec{E}=\overleftrightarrow{\sigma}\cdot\vec{E}$[例]立方晶系:$\sigma=\sigma_{xx}=\sigma_{yy}=\sigma_{zz}=\frac{(\sigma_{xx}+\sigma_{yy}+\sigma_{zz})}{3}=\frac{e^2}{4\pi^3\hbar}\int\tau\frac{v_{k_x}^2}{v_k}\mathrm{d}S_F=\frac{1}{12\pi^3}\frac{e^2}{\hbar}\int\tau v_k\mathrm{d}S_F$.各向同性$m^*,\tau$:$\sigma=\frac{\tau e^2}{12\pi^3 m^*}\int k_F\mathrm{d}S_F$.球面F面:$\sigma=\frac{\tau}{3\pi^2}\frac{e^2k_F^3}{m^*}=\frac{ne^2\tau_{E_F}}{m^*}$**(6)热电势**.$T,\mu$:$\frac{\partial f_0}{\partial T}=-\frac{\partial f_0}{\partial\epsilon}\frac{\epsilon-\mu}{T}$, $\frac{\partial f_0}{\partial\mu}=-\frac{\partial f_0}{\partial\epsilon}$,无$\vec{E}$方程:$-\frac{\partial f_0}{\partial\epsilon}\vec{v}_{\vec{k}}\cdot[\frac{\epsilon_k-\mu}{T}\nabla T+\nabla\mu]=-\frac{f_1}{\tau}$.电流密度:$\vec{J}_e=\frac{e}{4\pi^3}\int\tau\frac{(\vec{v}_{\vec{k}}\vec{v}_{\vec{k}})\cdot\nabla\mu}{\hbar v_k}(-\frac{\partial f_0}{\partial\epsilon})\mathrm{d}S\mathrm{d}\epsilon+\frac{e}{4\pi^3}\int\tau\frac{(\vec{v}_{\vec{k}}\vec{v}_{\vec{k}})\cdot\nabla T}{\hbar v_k}(\frac{\epsilon-\mu}{T})(-\frac{\partial f_0}{\partial\epsilon})\mathrm{d}S\mathrm{d}\epsilon$.$\mu$梯度$\frac{\nabla\mu}{e}$与外$\vec{E}$等价. **(7)热流类比**$\vec{J}_e=\frac{e^2}{4\pi^3}\int\tau\frac{(\vec{v}_{\vec{k}}\vec{v}_{\vec{k}})\cdot(\vec{E}+\frac{\nabla\mu}{e})}{\hbar v_k}(-\frac{\partial f_0}{\partial\epsilon})\mathrm{d}S\mathrm{d}\epsilon+\frac{e}{4\pi^3}\int\tau\frac{(\vec{v}_{\vec{k}}\vec{v}_{\vec{k}})\cdot\nabla T}{\hbar v_k}(\frac{\epsilon-\mu}{T})(-\frac{\partial f_0}{\partial\epsilon})\mathrm{d}S\mathrm{d}\epsilon$,定义热流:$\vec{J}_Q=\frac{1}{4\pi^3}\int(\epsilon_k-\mu)\vec{v}_kf_1\mathrm{d}\vec{k}=-\frac{e}{4\pi^3}\int\vec{E}\cdot[\tau\frac{(\vec{v}_{\vec{k}}\vec{v}_{\vec{k}})(\epsilon_k-\mu)}{\hbar v_k}(-\frac{\partial f_0}{\partial\epsilon})\mathrm{d}S\mathrm{d}\epsilon]-\frac{1}{4\pi^3}\int\nabla T\cdot[\tau\frac{(\vec{v}_{\vec{k}}\vec{v}_{\vec{k}})}{\hbar v_k}\frac{(\epsilon-\mu)^2}{T}(-\frac{\partial f_0}{\partial\epsilon})\mathrm{d}S\mathrm{d}\epsilon]$.设$\zeta_n=\frac{\tau}{12\pi^3\hbar}\int v_k(\epsilon_k-\mu)^n\left(-\frac{\partial f_0}{\partial\epsilon}\right)\mathrm{d}S\mathrm{d}\epsilon$, $\vec{J}_e=e^2\zeta_0\vec{E}-\frac{e}{T}\zeta_1(-\nabla T)$, $\vec{J}_Q=-e\zeta_1\vec{E}+\frac{1}{T}\zeta_2(-\nabla T)$.无外$\vec{E}$:$\vec{J}_e=0\Rightarrow e^2\zeta_0\vec{E}-\frac{e}{T}\zeta_1(-\nabla T)=0$, $\vec{E}=\frac{1}{eT}\frac{\zeta_1}{\zeta_0}(-\nabla T)$,热流密度:$\vec{J}_Q=\frac{1}{T}\left(\zeta_2-\frac{\zeta_1^2}{\zeta_0}\right)(-\nabla T)$,热导率:$\kappa=\frac{1}{T}\left(\zeta_2-\frac{\zeta_1^2}{\zeta_0}\right)$, $\sigma=e^2\zeta_0$.**(8)补充:热电势**热电场:$\vec{E}=\frac{1}{eT}\frac{\zeta_1}{\zeta_0}(-\nabla T)$,热电系数(单位$T$差下材料中$\phi$的变化量):$S=-\frac{1}{eT}\frac{\zeta_1}{\zeta_0}=-\frac{\pi^3}{3}\frac{k_B^2T}{e}\left[\frac{\partial\ln\sigma}{\partial\epsilon}\right]_{E_F}T\left(\frac{\partial\ln\langle\tau\rangle}{\partial\epsilon}+\frac{\partial\ln\langle v_k\rangle}{\partial\epsilon}+\frac{\partial\ln S}{\partial\epsilon}\right)_{E_F}$ **多e(0)原始**:$\hat{H}_T=\sum_i\frac{|\vec{p_i}|^2}{2m}+\sum_n\frac{|\vec{p}_n|^2}{2M_n}+\frac{1}{2}\sum'_{ij}\frac{e^2}{|\vec{r_i}-\vec{r_j}|}+\frac{1}{2}\sum'_{nn'}\frac{Z_nZ_{n'}e^2}{|\vec{R}_n-\vec{R}_{n'}|}+\sum_{n,i}V_n(\vec{r}_i-\vec{R}_n)+\hat{H}_R$(价e动,原子实动,e间库伦,原子实间库伦,e和原子实之间,s-L修正)**(1)B-O绝热**.(I)e:$\hat{H}_e=\sum_i[\frac{|\vec{p_i}|^2}{2m}+\sum_n V_n(\vec{r_i}-\vec{R_n})]+\frac{1}{2}\sum'_{ij}\frac{e^2}{|\vec{r_i}-\vec{r_j}|}+\hat{H}_R$,原子实:$\hat{H}_c=\sum_n\frac{|\vec{p_n}|^2}{2M_n}+\frac{1}{2}\sum'_{nn'}\frac{Z_nZ_{n'}e^2}{|\vec{R_n}-\vec{R_{n'}}|}+V_{\mathrm{ec}}(\{\vec{R_n}\})$(II)$\{-\frac{\hbar^2}{2m}\sum_j\nabla_j^2-\sum_{j,l}\frac{Z_le^2}{|r_j-R_l|}+\frac{1}{2}\sum_{j\neq j'}\frac{e^2}{|r_j-r_{j'}|}-E\}\Psi(\{r_N\})=0$, $\hat{P}_{jj'}\Psi=-\Psi$, $.n(r)=n(r;\{R_N\})$, $E=E(\{R_N\})$.**(2)$H_2$Model**:(I)HL:$\Psi_{HL}=A[\varphi_H(r_1-R_1)\varphi_H(r_2-R_2)+\varphi_H(r_1-R_2)\varphi_H(r_2-R_1)]\chi_0$(HL=Heitler-London).$\varphi_H(r)$ 是e轨道在基态; $\chi_0$ 代表自旋单子态.(II)Mullikan Ansatz:$\Psi_{\mathrm{HF}}=\frac{1}{\sqrt{2}}\mathrm{Det}[\varphi_m(r_1)\alpha(1)\varphi_m(r_2)\beta(2)]$.(III)JC:$\Psi_{JC}=\Psi(r_1,r_2)\chi_0$**(III)Hartree-Fock**对e:$\hat{H}=-\sum_i\frac{\hbar^2}{2m_e}\nabla_{\vec{r_i}}^2+\sum_i V_{\mathrm{ion}}(\vec{r_i})+\frac{e^2}{2}\sum_{(i\neq j)}\frac{1}{|\vec{r_i}-\vec{r_j}|}$,多体态:$\Psi^H(\{\vec{r_i}\})=\phi_1(\vec{r_1})\ldots\phi_N(\vec{r}_N)$, $E^H=\langle\Psi^H|\hat{H}|\Psi^H\rangle=\sum_i\langle\phi_i|\frac{-\hbar^2\nabla_{\vec{r}}^2}{2m_e}+V_{\mathrm{ion}}(\vec{r})|\phi_i\rangle+\frac{e^2}{2}\sum_{ij(i\neq j)}\langle\phi_i\phi_j|\frac{1}{|\vec{r}-\vec{r}'|}|\phi_i\phi_j\rangle$, $\delta[E^H-\sum_i\epsilon_i(\langle\phi_i|\phi_i\rangle-1)]=0$, $\langle\delta\phi_i|-\frac{\hbar^2\nabla_{\vec{r}}^2}{2m_e}+V_{\mathrm{ion}}(\vec{r})|\phi_i\rangle+e^2\sum_{i\neq j}\langle\delta\phi_i\phi_j|\frac{1}{|\vec{r}-\vec{r}'|}|\phi_i\phi_j\rangle-\epsilon_i\langle\delta\phi_i|\phi_i\rangle=\langle\delta\phi_i|[-\frac{\hbar^2\nabla_{\vec{r}}^2}{2m_e}+V_{\mathrm{ion}}+e^2\sum_{i\neq j}\langle\phi_j|\frac{1}{|\vec{r}-\vec{r}'|}|\phi_j\rangle-\epsilon]|\phi_i\rangle=0$.Hatree:$[-\frac{\hbar^2\nabla\vec{r}^2}{2m_e}+V_{\mathrm{ion}}(\vec{r})+e^2\sum_{j\neq i}\langle\phi_j|\frac{1}{|\vec{r}-\vec{r}'|}$ $\epsilon_i\phi_i(\vec{r})$,Hatree势:$V_i^H(\vec{r})=e^2\sum_{i\neq j}\langle\phi_j|\frac{1}{|\vec{r}-\vec{r}'|}|\phi_j\rangle$.平均场近似:Hatree-Fock多体态:$\Psi^{\mathrm{HF}}(\{\vec{r_i}\})=\frac{1}{\sqrt{N!}}\begin{vmatrix}\phi_1(\vec{r_1}) & \phi_1(\vec{r_N})\\ \phi_N(\vec{r_1}) & \phi_N(\vec{r_N})\end{vmatrix}$.$(\phi_i(\vec{r})\approx\psi_i(\vec{r})\chi_i($ 能量:$E^{\mathrm{HF}}=\langle\Psi^{\mathrm{HF}}|\hat{H}|\Psi^{\mathrm{HF}}\rangle=\sum_i\langle\phi_i|\frac{-\hbar^2\nabla_{\vec{r}}^2}{2m_e}+V_{\mathrm{ion}}(\vec{r})|\phi_i\rangle+\frac{e^2}{2}\sum_{ij(i\neq j)}\langle\phi_i\phi_j|\frac{1}{|\vec{r}-\vec{r}'|}|\phi_i\phi_j\rangle-\frac{e^2}{2}\sum_{ij(i\neq j)}\langle\phi_i\phi_j|\frac{1}{|\vec{r}-\vec{r}'|}|\phi_j\phi_i\rangle$,$[\frac{-\hbar^2\nabla_{\vec{r}}^2}{2m_e}+V_{\mathrm{ion}}+V_i^H(\vec{r})]\phi_i(\vec{r})-e^2\sum_{j\neq i}\langle\phi_j|\frac{1}{|\vec{r}-\vec{r}'|}|\phi_i\rangle\phi_j(\vec{r})=\epsilon_i\phi_i(\vec{r})$.密度:$\rho_i(\vec{r})=|\phi_i(\vec{r})|^2$, $\rho(\vec{r})=\sum_i\rho_i(\vec{r})$; $V_i^H(\vec{r})=e^2\sum_{j\neq i}\int\frac{\rho_j(\vec{r}')}{|\vec{r}-\vec{r}'|}\mathrm{d}\vec{r}'=e^2\int\frac{\rho(\vec{r}')-\rho_i(\vec{r}')}{|\vec{r}-\vec{r}'|}\mathrm{d}\vec{r}'$ **粒子交换**:$\rho_i^X(\vec{r},\vec{r}')=\sum_{j\neq i}\frac{\phi_i(\vec{r}')\phi_i^*(\vec{r})\phi_j(\vec{r})\phi_j^*(\vec{r}')}{\phi_i(\vec{r})\phi_i^*(\vec{r})}$;HF势:$V_i^{HF}(\vec{r})=e^2\int\frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}\mathrm{d}\vec{r}'-e^2\int\frac{\rho_i(\vec{r}')+\rho_i^X(\vec{r},\vec{r}')}{|\vec{r}-\vec{r}'|}\mathrm{d}\vec{r}'$,单HF:$[\frac{-\hbar^2\nabla_{\vec{r}}^2}{2m_e}+V_{ion}(\vec{r})+V_i^{HF}(\vec{r})]\phi_i($ $\epsilon_i\phi_i(\vec{r})$.**(IV)Jellium Model(均匀电子气)**$\phi_i(\vec{r})=\frac{e^{i\vec{k}_i\cdot\vec{r}}}{\sqrt{\Omega}}$($\Omega$为晶胞体积.均匀电子气的波矢的数值范围为$k\in[0,k_F]$).$\frac{4\pi}{3}r_s=\frac{\Omega}{N}=n^{-1}=$

$\frac{3\pi^2}{k_F^3}$, $\frac{\hbar^2}{2m_e a_0^2}=\frac{e^2}{2a_0}=1$Ry.态方程$[-\frac{\hbar^2\nabla_{\vec r}^2}{2m_e}-e^2\int\frac{\rho_{\vec k}^{HF}(\vec r,\vec r')}{|\vec r-\vec r'|}\mathrm{d}\vec r']\phi_{\vec k}(\vec r)=\epsilon_{\vec k}\phi_{\vec k}(\vec r)$.平面波证明:$-\frac{\hbar^2\nabla^2}{2m_e}\frac{e^{i\vec k\cdot\vec r}}{\sqrt\Omega}=\frac{\hbar^2\hat k^2}{2m_e}\frac{e^{i\vec k\cdot\vec r}}{\sqrt\Omega}$,$e^2[\int\frac{\rho_{\vec k}^{HF}(\vec r,\vec r')}{|\vec r-\vec r'|}\mathrm{d}\vec r']\phi_{\vec k}(\vec r)=\frac{-e^2}{\sqrt\Omega}\int\frac{\rho_{\vec k}^{HF}(\vec r,\vec r')}{|\vec r-\vec r'|}\mathrm{d}\vec r' e^{i\vec k\cdot\vec r}=\frac{-e^2}{\sqrt\Omega}\sum_{\vec k'}\int\frac{\phi_{\vec k}(\vec r')\phi_{\vec k}^*(\vec r)\phi_{\vec k'}(\vec r)\phi_{\vec k'}^*(\vec r')}{\phi_{\vec k}(\vec r)\phi_{\vec k}^*(\vec r)}\frac{1}{|\vec r-\vec r'|}\mathrm{d}\vec r' e^{i\vec k\cdot\vec r}=\frac{-e^2}{\sqrt\Omega}\sum_{\vec k'}\int\frac{e^{-i(\vec k-\vec k')\cdot(\vec r-\vec r')}}{\Omega}\frac{\mathrm{d}\vec r' e^{i\vec k\cdot\vec r}}{|\vec r-\vec r'|}$,$(\int\frac1r e^{i\vec k\cdot\vec r}\mathrm{d}\vec r=\frac{4\pi^2}{k^2}$,$\sum_{\vec k}f(\vec k)=\frac{\Omega}{(2\pi)^3}\int f(\vec k)\mathrm{d}\vec k)$,$\frac{-4\pi^2}{\sqrt\Omega}[\int_{k'<k_F}\frac{\mathrm{d}\vec k'}{(2\pi)^3}\frac{1}{|\vec k-\vec k'|^2}]e^{i\vec k\cdot\vec r}=-\frac{e^2}{\pi}k_F F(\frac{k}{k_F})\frac{e^{i\vec k\cdot\vec r}}{\sqrt\Omega}$.$(F(x)=1+\frac{1-x^2}{2x}\ln|\frac{1+x}{1-x}|)$.(II)$\phi_{\vec k}(\vec r)$能量:$\epsilon_{\vec k}=\frac{\hbar^2k^2}{2m_e}-\frac{e^2}{\pi}k_F F(\frac{k}{k_F})$,总能量$E^{HF}=2\sum_{k<k_F}\frac{\hbar^2|\vec k|^2}{2m_e}-\frac{e^2k_F}{\pi}\sum_{k<k_F}[1+\frac{k_F^2-k^2}{2kk_F}\ln|\frac{k_F+k}{k_F-k}|]$.平均能:$\frac{E^{HF}}{N}=\frac35\epsilon_F-\frac34\frac{e^2k_F}{\pi}=[\frac{2.21}{(r_s/a_0)^2}-\frac{0.916}{(r_s/a_0)}]$Ry.交换能:$\frac{E^X}{N}=-\frac{3e^2}{4}(\frac3\pi)^{\frac13}n^{\frac13}=-1.447(a_0^3n)^{\frac13}$Ry;高$n$:$\frac EN=[\frac{2.21}{(r_s/a_0)^2}-\frac{0.916}{(r_s/a_0)}+0.0622\ln\frac{r_s}{a_0}-0.096+\mathcal O(\frac{r_s}{a_0})]$**DFT**(1)$\mathcal H=T+W+V=-\sum_i\frac{\hbar^2}{2m_e}\nabla_{\vec r_i}^2+\sum_i V_{\rm ion}(\vec r_i)+\frac{e^2}{2}\sum_{ij(j\neq i)}\frac{1}{|\vec r_i-\vec r_j|}$.DF:$F[n(r)]=\langle\Psi|T+W|\Psi\rangle=F[n(\vec r)]=T^S[n(\vec r)]+\frac{e^2}{2}\iint\frac{n(\vec r)n(\vec r')}{|\vec r-\vec r'|}\mathrm{d}\vec r\mathrm{d}\vec r'+E^{XC}[n(\vec r)]$,$E[n(\vec r)]=\langle\Psi|\mathcal H|\Psi\rangle=F[n(\vec r)]+\int V(\vec r)n(\vec r)\mathrm{d}\vec r$,变分:$\delta n(\vec r)=\delta\phi_i(\vec r)\phi_i(\vec r)$,约束$\int\delta n(\vec r)\mathrm{d}\vec r=\int\delta\phi_i(\vec r)\phi_i(\vec r)\mathrm{d}\tilde r=0$,Kohn-Sham:$[-\frac{\hbar^2}{2m_e}\nabla_{\vec r}^2+V^{\rm eff}(\vec r,n(\vec r))]\phi_i(\vec r)=\epsilon_i\phi_i(\vec r)(V^{\rm eff}(\vec r,n(\vec r))=V(\vec r)+e^2\int\frac{n(\vec r')}{|\vec r-\vec r'|}\mathrm{d}\vec r'+\frac{\delta E^{XC}[n(\vec r)]}{\delta n(\vec r)})$.$E^{XC}[n(\vec r)]=\int n(\vec r)\epsilon^{XC}([n],\vec r)\mathrm{d}\vec r$.LDA:$E_{\rm LDA}^{XC}=\int\epsilon^{XC}[n(\vec r)]n(\vec r)\mathrm{d}\vec r$;GGA:$E_{\rm GGA}^{XC}=\int\epsilon^{XC}[n(\vec r),|\nabla n(\vec r)|]n(\vec r)\mathrm{d}\vec r$. **Kittle(1)Wannier**正交:$\Psi_k=N^{-\frac12}e^{ik\cdot r}u_k(\vec r)$,$\int\mathrm{d}\tau w^*(\vec r-\vec r_n)w(\vec r-\vec r_n)=\frac1N\sum_{kk'}e^{ikr_n}e^{-ik'r_m}\delta_{kk'}=\delta_{nm}$.线晶格:$\psi_k=N^{-\frac12}e^{ikx}u_0(x)$,$w(x-x_n)=N^{-1}u_0(x)\sum e^{ik(x-x_n)}=u_0(x)\frac1N\frac{L}{2\pi}\int_{-\pi/a}^{\pi/a}e^{ik(x-x_m)}\mathrm{d}k=u_0(x)\frac{\sin\frac\pi a(x-x_n)}{\frac\pi a(x-x_n)}$.**(2)2D矩形**$\vec a=2A\hat x$,$\vec b=4A\hat y$.$\vec A=\frac\pi a\hat x$,$\vec B=\frac{\pi}{2A}\hat y$.$\vec G=\frac{2\pi}{4A}(2g_1\hat x+g_2\hat y)$.$2\frac{\pi k_F^2}{\frac{(2\pi)^2}{ab}}=Z$,$k_F=\sqrt{\frac{\pi}{4A^2}}$**(3)3D六角密**$a,c$.$U(\vec r)=\sum_{n=1}^m U(\vec r-\vec R_n)=\sum_{n=1}^m\sum_G U(G)e^{iG(r-R_n)}=\sum_G S(\vec G)e^{iGr}$.$G=m_1\vec b_1+m_2\vec b_2+m_3\vec b_3$.$a_1=a(1,0,0)$,$a_2=a(-\frac12,\frac{\sqrt3}{2},0)$,$a_3=c(0,0,1)$;$b_1=\frac{2\pi}{a}(1,\frac{1}{\sqrt3},0)$,$b_2=\frac{2\pi}{a}(0,\frac{2}{\sqrt3},0)$,$b_3=\frac{2\pi}{c}(0,0,1)$.$\vec G=2\pi[\frac{m_1}{a}\hat x+(-\frac{m_1}{\sqrt3a}+\frac{m_2}{\sqrt3a})\hat y+\frac{m_3}{c}\hat z]$.$S(\vec G)=1+e^{-i2\pi(\frac{2m_1}{3}+\frac{m_2}{3}+\frac{m_3}{2})}$(i)$\vec G_c(m_1,m_2=0,m_3=\pm1)S(G)=0$,$U(\pm\vec G_c=0)$(ii)$\vec G=\pm2\vec G_cS(\pm2\vec G_c)=2$,$U(\pm2\vec G_c\neq0)$.$U(\pm\vec G_c)=0$,能区↑,容$4N$e.**(4)开轨道**$d_{\rm BZ}=G$,$B\perp\partial$BZ.$\frac{\hbar\mathrm{d}\mathbf k}{\mathrm{d}t}=\frac{-e\mathbf v\times\mathbf B}{c}$.$T=\int\mathrm{d}t=\int_0^G\frac{c\hbar}{evB}\mathrm{d}k=\frac{c\hbar G}{evB}$.if $\vec B=B\hat z$,$\frac{\mathrm{d}U_x}{\mathrm{d}t}=\frac{-ev_yB}{mc}$,$\frac{\mathrm{d}U_y}{\mathrm{d}t}=\frac{ev_xB}{mc}$,$\frac{\mathrm{d}U_z}{\mathrm{d}t}=0$.**(5)K的De Hass-van Alphen**$\Delta(\frac1B)=\frac{2\pi e}{\hbar cS}$,$S=\pi k_F^2$,$k_F=(\frac{3\pi^2N}{V})$.$n=\frac{2}{a^3}$,$\Delta(\frac1B)=5.46\times10^{-9}\mathrm{G}^{-1}$.极值轨道$A_n=(\frac{\hbar c}{eB})^2S_n(S_n=\pi k_F^2)$**(6)开轨道磁致R**.$\sigma_{yy}=S\sigma_0$.if $\omega_c\tau\ll1$.$\overleftrightarrow{\sigma}=[Q^{-2},Q^{-1},0,Q^{-1},S,0,0,0,1](Q=\omega_c\tau)$.霍尔:$j_y=\sigma_{yx}E_x+\sigma_{yy}E_y=0$,$E_y=\frac{-\sigma_{yx}E_x}{\sigma_{yy}}=\frac{-E_x}{SQ}$.$j_x=\sigma_{xx}E_x+\sigma_{xy}E_y=\frac{\sigma_0(S+1)E_x}{SQ^2}$,$\rho=\frac{E_x}{j_x}=\frac{SQ^2}{\sigma_0(S+1)}$**Yan(1)周期势**$V(x)=\{\frac{m\omega^2}{2}[b^2-(x-na)^2],[na-b,na+b]; 0,[(n-1)a+b,na-b]$.$\overline V=\frac{1}{4b}\int_{-b}^b\frac{m\omega^2}{2}(b^2-x^2)\mathrm{d}x=\frac{b^2m\omega^2}{6}$.$V_n=\frac1a\int_{-b}^b e^{\frac{-i2\pi nt}{a}}V(t$ $\frac1a\int_{-b}^b\frac{m\omega^2}{2}(b^2-t^2)e^{\frac{-i2\pi nt}{a}}\mathrm{d}t=\frac{m\omega^2b^2}{2\pi^3n^3}(8\sin\frac{n\pi}{2}-4n\pi\cos\frac{n\pi}{2})$.$|2V_1|=\frac{8m\omega^2b^2}{\pi^3}$,$|2V_2|=\frac{m\omega^2b^2}{\pi^2}$.**(2)紧束缚**.$(bcc):a(\frac{\pm1}{2},\frac{\pm1}{2},\frac{\pm1}{2})$;$(fcc)a(\frac{\pm1}{2},\frac{\pm1}{2},0$ **式晶格**.原胞长$a$,内相对距$b$.s:$\phi(r)=\frac{1}{\sqrt N}\sum_{R_m}[eikR_m^A\rho(r-R_m^A)+C_Be^{ikR_m^B}\rho(r-R_m^B)]$.$E(k)=E-J_0-\sum e^{-ikR_m}J(R_m)=E-J_0-(J_1+e^{-ika}J_2)e^{-ik[(n-1)a+b]}=E-J_0-2J_1\cos\frac{ka}{2}e^{-ik[(n-\frac12)a+b]}$.**Cu中Zn**.F球相切$\partial$BZ:$N=\frac{Vk_F^3}{3\pi2}=\frac{V\sqrt{\mathbf{3}}\pi}{a^3}$;$\frac{2x+1}{1+x}=\frac{\sqrt3\pi}{4}(x=n(Zn):n(Cu))$**(4)椭色散**$\epsilon(\vec k)=\hbar^2\sum_i^3\frac{k_i^2}{2m_i}$.$N=2(\frac{L}{2\pi})^3\frac43(\frac{\epsilon}{\hbar^2})^{\frac32}(m_xm_ym_z)^{\frac12}$.$D(\epsilon)=\frac{\mathrm{d}N}{\mathrm{d}\epsilon}=\frac{V}{2\pi^2}(\frac{2}{\hbar^2})^{\frac32}(m_xm_ym_z)^{\frac12}\epsilon^{\frac12}$.$U-U_0=\frac{\pi^2}{6}g(\epsilon)(k_BT)^2$,$\frac{\partial U}{\partial T}=\frac{\pi^2}{3}g(\epsilon)k_BT^2$,自由:$C_V=\frac{\pi^2k_B^2T}{3}\frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{\frac32}\epsilon_F^{\frac12}$;椭球:$C_V=\frac{\pi^2k_B^2T}{3}\frac{V}{2\pi^2}(\frac{2}{\hbar^2})^{\frac32}(m_xm_ym_z)^{\frac12}\epsilon_F^{\frac12}$.**(4)1D导体**$\epsilon(k)=\epsilon_0-\frac\Delta2\cos ka$.$T=0$,$k_F$.$v=\frac{\mathrm{d}\epsilon}{\mathrm{d}k}=\frac{a\Delta}{2\hbar}\sin ka$.$z=\int v\mathrm{d}t=\frac{\Delta}{2eE}(\cos ka-1)$,$k=k_0-\frac{eEt}{\hbar}$,$v=\frac{\mathrm{d}Z}{\mathrm{d}t}=\frac{\Delta a}{2\hbar}\sin k_0a-\frac{eEat}{\hbar}$.$v_{max}=\frac{\Delta a}{2\hbar}$,$\omega_{\rm BO}=\frac{eEa}{\hbar}$.$E_F$以下均占,以上均空:$j=\frac{-e}{L}\int_{-k_F}^{k_F}v(t)\frac{2\mathrm{d}k}{\frac{2\pi}{L}}=\frac{e\Delta}{\pi\hbar}\sin k_Fa\sin\frac{eEat}{\hbar}$.$N=\frac{2k_F}{\frac{2\pi}{L}}2$,$j_{max}=\frac{e\Delta}{\pi\hbar}\sin k_Fa=\frac{\Delta e}{\pi\hbar}\sin\frac{\pi na}{2}$.**(5)非抛(i)**$\frac{\hbar^2k^2}{2m_e}=\epsilon(1+\alpha\epsilon)$.$g(\epsilon)=\frac{2}{(2\pi)^3}\int\frac{\mathrm{d}S_\epsilon}{|\nabla_kE(k)|}$.$\frac{\hbar^2|k|}{m}=\nabla_k\epsilon(1+2\alpha\epsilon)$,$g(\epsilon)=\frac{2}{(w\pi^3)}\int\frac{\mathrm{d}S}{\hbar^2|k|}m(1+2\alpha\epsilon)=\frac{4\pi k^22}{(2\pi)^3}\frac{m(1+2\alpha\epsilon)}{\hbar^2k}$,$k=\frac{\sqrt{2m\epsilon(1+\alpha\epsilon)}}{\hbar}$,$g(\epsilon)=\frac{m(1+2\alpha\epsilon)}{\pi^2\hbar^3}\sqrt{2m\epsilon(1+\alpha\epsilon)}$.**(5)**$\mu$ 0.5eV.$m_h^*=2m_e^*$,$\mu=\frac{E_c+E_V}{2}+\frac{3k_BT}{4}\ln\frac{m_h^*}{m_e^*}$.设价带顶0,$\mu=0.25\mathrm{eV}+\frac{3k_BT_1}{4}\ln\frac{2m_e}{m_e}$,$\Delta\mu=\frac{3k_B\Delta T}{4}\ln2$.**(6)测带隙**$n=p\propto T^{\frac32}e^{\frac{-E_g}{2k_BT}}$,$\sigma\propto\frac1U$,$\ln U=C+\frac{E_g}{2k_BT}$**(7)有效质量**$E_{1,2}(\vec k)=E_V-\frac{\hbar^2}{2m}\{AK^2\pm[B^2k^4+C^2(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)]\}$.(i)$[1,0,0]:k_x=k,k_y=k_z=0$.$E(\vec k)=E_V-\frac{\hbar^2}{2m}(A\pm B)k_x^2$,$\frac{1}{m^*}=\frac{-\mathrm{d}^2E}{\hbar^2\mathrm{d}k^2}=\frac{A\pm B}{m}$;(ii)$\forall i,k_i=\frac{k}{\sqrt3}$.$E=E_V-\frac{\hbar^2}{2m}\{k^2(A^2\pm(B^2+\frac{C^2}{3})^{\frac12})\}$,$m^*=\frac{m}{A^2\pm(B^2+\frac{C^2}{3})^{\frac13}}$**(8)杂质轨道**$E_g=0.23$eV,$\epsilon=18$,$m_e^*=0.015m$.电离$E_d=\frac{e^4m_e}{2\epsilon^2\hbar^2}$.基态半径$a_d=\frac{\epsilon\hbar^2}{mne^2}$.杂质重叠临界浓度(fcc):$V=Na^3$,$N_0=\frac{3V}{4\pi a_d^3}$,$C_{\rm min}=\frac{N_0}{4N}$.**(9)**$\sigma_{\rm min}$.$\sigma=ne\mu_n+pe\mu_p$,$np=n_i^2$,$\sigma=\frac{n_i^2e\mu_n}{p}+pe\mu_p$.Min:$p=\sqrt{\frac{\mu_n}{\mu_p}}n_i$,$n=\sqrt{\frac{\mu_p}{\mu_n}}n_i$.$\sigma=2n_ie\sqrt{\mu_n+\mu_p}$,$\sigma_i=n_ie(\mu_n+\mu_p)$,$\sigma=\frac{2\sigma_i\sqrt{\mu_n\mu_p}}{\mu_n+\mu_p}$.**(10)施主电离**.施主密度$n=10^{13}\mathrm{cm}^{-3}$,电离$E_d=1$meV,$m^*=0.01m$.低温$(k_BT\ll E_g)$,$n\approx(n_0N_d)^{\frac21}e^{\frac{-E_d}{k_BT}}(n_0=2(\frac{m_ek_BT}{2\pi\hbar^2})^{\frac32})$.霍尔系数$R_H=\frac{-1}{nec}$**(11)双载流(i)霍尔**迁移率$\mu_h=\frac{e\tau_h}{m_hc}$,$\mu_e=\frac{e\tau_e}{m_ec}$.$\vec E=E_x\hat x$,$\vec B=B_z\hat z$.$(E_y)_h=\frac{e\tau_hB_zE_x}{m_hc}=\frac{\mu_hB_zE_x}{c}$,$(E_y)_h=\frac{-e\tau_eB_zE_x}{m_ec}=\frac{-\mu_eB_zE_x}{c}$.$\hat y$:$(j_y)_h=\sigma_h(E_y)_h=-pe\mu_h\frac{\mu_hB_zE_x}{c}$,$(j_y)_e=\sigma_e(E_y)_e=ne\mu_e\frac{\mu_eB_zE_x}{c}$.$j_y=(j_y)_h+(j_y)_e=\frac ec(n\mu_e^2-p\mu_h^2)B_zE_x$.霍尔电场$\sigma E_y+j_y=0$,$E_y=\frac{(p\mu_h^2-n\mu_e^2)B_zE_x}{c(p\mu_h+n\mu_e)}$.$j_x=(pe\mu_h+ne\mu_e)E_x$,$E_y=\frac{(p-nb^2)B_zj_x}{(p+nb)^2ec}(b=\frac{\mu_e}{\mu_h})$.$R_H=\frac{E_y}{j_xB_z}$.**(ii)磁致R**.强$\vec B(\omega_c\tau\gg1)$.$m_e(\frac{\mathrm{d}}{\mathrm{d}t}+\frac{1}{\tau_e})v_e=-e(\vec E+\frac{\vec v_e}{c}\times\vec B)$,$m_h(\frac{\mathrm{d}}{\mathrm{d}t}+\frac{1}{\tau_h})v_h=e(\vec E+\frac{\vec v_h}{c}\times\vec B)$.$\vec B=B\hat z$.稳定:$\frac{\mathrm{d}v_e}{\mathrm{d}t}=\frac{\mathrm{d}v_h}{\mathrm{d}t}=0$.$v_{ex}=-\frac{e\tau_eE_x}{m_e}-\frac{e\tau_eBv_{ey}}{cm_e}=-\frac{e\tau_eE_x}{m_e}-\omega_e\tau_ev_{ey}$;$v_{ey}=-\frac{e\tau_eE_y}{m_e}+\omega_e\tau_ev_{ex}$;$v_{ez}=\frac{-e\tau_eE_x}{m_e}(\omega_e=\frac{eB}{m_ec})$.解$v_{ex}=\frac{-e\tau_e(B_x-\omega_e\tau_eB_y)}{m_e[1+(\omega_e\tau_e)^2]}$,$v_{ey}=\frac{-e\tau_e(E_y+\omega_e\tau_eE_x)}{m_e[1+(\omega_e\tau_e)^2]}$,$v_e=\frac{-e\tau_eE_x}{m_e}$.空穴:变e,换h.设$a=\frac{e\tau_e}{m_e[1+(\omega_e\tau_e)^2]}$,$b=\frac{e\tau_h}{m_h[1+(\omega_h\tau_h)^2]}$.$j=e(pv_h-nv_e)$,$j_x=e[(pb+na)E_x+(pb\omega_h\tau_h-na\omega_e\tau_e)E_y]$;$j_y=e[(na\omega_e\tau_e-pb\omega_h\tau_h)E_x+(pb+na)E_y]$;$j_z=e^2[\frac{\tau_hp}{m_h}+\frac{\tau_en}{m_E}]E_z$.$j_y=\sigma_{yx}E_x+\sigma_{yy}E_y+\sigma_{yz}E_z$,$\sigma_{yx}=e(na\omega_e\tau_e-pb\omega_h\tau_h)=e[\frac{ne\tau_e\omega_e\tau_e}{m_e[1+(\omega_e\tau_e)^2]}-\frac{pe\tau_h\omega_h\tau_h}{m_h[1+(\omega_h\tau_h)^2]}]\approx e[\frac{ne}{m_e\omega_e}-\frac{pe}{m_h\omega_k}]\approx\frac{ec(n-p)}{B}$.霍尔电场:$j_y=0$,$E_y=\frac{(pb\omega_h\tau_h-na\omega_e\tau_e)E_x}{pb+na}$,$Q_i=\omega_i\tau_e\ll1$,$E_y\approx(\frac{pe\tau_h}{m_hQ_h^2}+\frac{ne\tau_e}{m_eQ_e^2})^{-1}(\frac{pe\tau_h}{m_hQ_h}-\frac{ne\tau_e}{m_eQ_e})E_x=-(n-p)(\frac{p}{Q_h}+\frac{n}{Q_e})^{-1}E_x$.有效$\sigma$.$j_x=\sigma_{\rm eff}E_x=e[(pb+na)E_x+(pbQ_h-naQ_e)E_y]\approx e[(\frac{pe\tau_h}{m_hQ_h^2}+\frac{ne\tau_e}{m_eQ_e^2})E_x+(\frac{pe\tau_h}{m_hQ_h}-\frac{ne\tau}{m_eQ_e})E_y]$,$Q=\omega\tau=\frac{eB\tau}{mc}$,$j_x\approx\frac{ec}{B}[(\frac{p}{Q_h}+\frac{n}{Q_e})E_x+(p-n)E_y]=\frac{ec}{B}[(\frac{p}{Q_h}+\frac{n}{Q_e})E_x+(p-n)^2(\frac{p}{Q_h}+\frac{n}{Q_e})^{-1}E_x]=\sigma_{\rm eff}E_x$.**(12)椭色散与斜H**.$\epsilon=\sum_i^3\frac{\hbar^2k_i^2}{2m_i}$,$\vec H:\alpha,\beta,\gamma$(方向余弦).$\vec v(k)=\frac{\nabla_kE}{\hbar}=\sum_i\frac{\hbar k_i}{m_i}\hat x_i$,$B=B(\alpha\hat x+\beta\hat y+\gamma\hat z)$.$\frac{\hbar\mathrm{d}\vec k}{\mathrm{d}t}=-\hbar eB[(\frac{k_1\hat x}{m_1}+\frac{k_2\hat y}{m_2}+\frac{k_3\hat z}{m_3})\times(\alpha\hat x+\beta\hat y+\gamma\hat z)]$.方程组$\frac{\mathrm{d}k_1}{\mathrm{d}t}=-eB(\frac{k_2\alpha}{m_2}-\frac{k_3\beta}{m_3})$;$\frac{\mathrm{d}\vec k_2}{\mathrm{d}t}=-eB(\frac{k_3\alpha}{m_3}-\frac{k_1\alpha}{m_1})$,$\frac{\mathrm{d}k_3}{\mathrm{d}t}-eB(\frac{k_1\beta}{m_1}-\frac{k_2\alpha}{m_2})$.试解$k_i=k_{i0}e^{i\omega t}$,系数行列式:**Det**$[i\omega,\frac{eB\alpha}{m_2},\frac{-eB\beta}{m_3},\frac{-eB\alpha}{m_1},i\omega,\frac{eB\alpha}{m_3},\frac{eB\beta}{m_1},\frac{-eB\alpha}{m_2},i\omega]=0$,$\omega=eB\sqrt{\frac{\alpha^2}{m_2m_3}+\frac{\gamma^2}{m_1m_2}+\frac{\beta^2}{m_1m_3}}=\frac{Be}{m^*}$**(13)圆筒F面**$S=\frac{\pi r^2}{\cos\alpha}$,$\Delta(\frac1B)=\frac{2\pi e}{\hbar S}=\frac{2e\cos\alpha}{\hbar r^2}$.回旋质量:$\vec B=B\sin\alpha\hat x+B\cos\alpha\hat z$.$E=\frac{\hbar^2}{2m}(k_x^2+k_y^2)$.$\vec v_k=\frac{\nabla E}{\hbar}=\frac{\hbar}{m}(k_x\hat x+k_y\hat y)$.方程组$\frac{\mathrm{d}k_x}{\mathrm{d}t}=-\frac{eB\cos\alpha k_y}{m}$;$\frac{\mathrm{d}k_y}{\mathrm{d}t}=\frac{eB\cos\alpha k_x}{m}$;$\frac{\mathrm{d}k_z}{\mathrm{d}t}=\frac{eBk_0\sin\alpha}{m}$,$k_y(t)=k_y(0)e^{\frac{ieB\cos\alpha t}{m}}$.**(14)非抛(ii)**色散:$\frac{\hbar^2|k|^2}{2m}=E(1+\alpha E)$.$\frac{\hbar^2|k|}{m}=\nabla_kE(1+2\alpha E)$,$\vec v=\frac{\nabla_kE}{\hbar}$,$\hbar\frac{\mathrm{d}k}{\mathrm{d}t}=-e\vec v\times\vec B=\frac{-e\hbar lB}{m(1+2\alpha E)}$,$T=\frac{\oint\mathrm{d}k}{|\frac{\mathrm{d}k}{\mathrm{d}t}|}=\frac{2\pi k}{\frac{eBk}{m(1+2\alpha E)}}=\frac{2\pi m(1+2\alpha E)}{eB}$,$\omega=\frac{eB}{m(1+2\alpha E)}$,$m_c^*=m(1+2\alpha E)$.**(15)铁磁态(Jellium)**完全极化:$V'=2V$,$k_F'=2^{\frac13}k_F$,$\frac{3\epsilon_F}{5}\propto k_F^2$,$\frac{3e^2k_F}{\pi}\propto k_F$,$(2^{\frac23}-1)\frac{2.21}{(\frac{r_s}{a_0})^2}-(2^{\frac13}-1)\frac{0.916}{(\frac{r_s}{a_0})}<0$,$\frac{r_s}{a_0}>5.45$**(16)Jellium发散**$\phi_i=\frac{e^{ik_ir}}{\sqrt\Omega}$,$E_2=\frac{-e^2}{2}\sum_{ij}\langle\phi_i\phi_j|\frac{1}{|\vec r-\vec r'|}|\phi_i\phi_j\rangle=\frac{-e^2N^2}{2\Omega^2}\int\frac{e^{-ik_ir}e^{-ik_jr'}e^{ik_ir}e^{ik_jr'}}{|\vec r-\vec r'|}\mathrm{d}\vec r\mathrm{d}\vec r'=\frac{-e^2N^2}{2\Omega^2}\int\frac{\mathrm{d}\vec r\mathrm{d}\vec r'}{|\vec r-\vec r'|}$.Avg.$\frac{E_2}{N}=-\frac{e^2N}{2\Omega^2}\int\frac{\mathrm{d}\vec r\mathrm{d}\vec r'}{|\vec r-\vec r'|}\propto\frac{N}{\Omega^2}\int\frac{\mathrm{d}(\vec r-\vec r')\mathrm{d}(\vec r+\vec r)}{|\vec r-\vec r'|}\propto N^{\frac32}$.