③ 3D 情况

$$\vec{a} = \frac{1}{\hbar^2}\nabla_k[\nabla_k \varepsilon_n(k)]\cdot\vec{F}$$

$$\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \frac{1}{m^*}\begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix}, \quad \frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon_n(k)}{\partial k_\alpha \partial k_\beta}, \ (\alpha,\beta = x,y,z).$$

矩阵形式.

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\begin{pmatrix} \frac{\partial^2\varepsilon}{\partial k_x^2} & \frac{\partial^2\varepsilon}{\partial k_x\partial k_y} & \frac{\partial^2\varepsilon}{\partial k_x\partial k_z} \\ \frac{\partial^2\varepsilon}{\partial k_y\partial k_x} & \frac{\partial^2\varepsilon}{\partial k_y^2} & \frac{\partial^2\varepsilon}{\partial k_y\partial k_z} \\ \frac{\partial^2\varepsilon}{\partial k_z\partial k_x} & \frac{\partial^2\varepsilon}{\partial k_z\partial k_y} & \frac{\partial^2\varepsilon}{\partial k_z^2} \end{pmatrix}$$

✓ (对角化 $\frac{1}{m^*}$ 矩阵 找主轴方向)

✓ 对于不平行主轴的作用力，产生不平行于主轴的加速度。
(晶格电子不仅仅感受外力，还有晶格周期势)

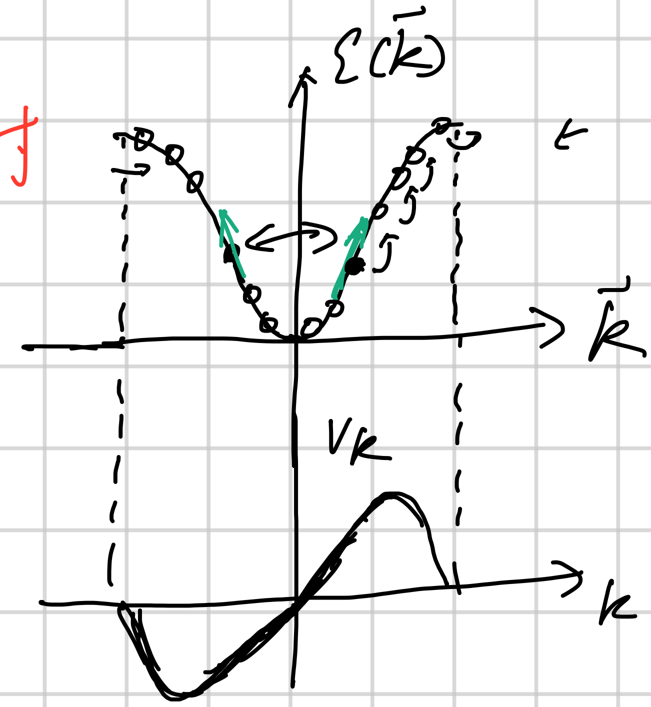
## III. 稳恒电场中的电子运动(能带电子)

① 运动方程 $\hbar\frac{d\vec{k}}{dt} = -e\vec{E}$ ← 不含时

$\hbar\vec{k}(t) - \hbar\vec{k}(0) = -e\vec{E}\cdot t$

→ $\vec{k}(t) = \vec{k}(0) - e\vec{E}\cdot t/\hbar$ ✓

稳恒电场下，电子波矢匀速移动.




($\vec{k}$ 描述布洛赫电子)

② 运动速度分析 (半正，半负)

$\varepsilon(k) = \varepsilon(-k) \Rightarrow v(k) = -v(-k)$

($\vec{k}$ 和 $-\vec{k}$ 处运动速度相反)

✓ 无外场(对称填充) ⇒ 无电流
(满或不满)

能带 $\underbrace{\varepsilon(k)=\varepsilon(-k)} \Rightarrow V(k)=-V(-k)$

$$\left[-\frac{\hbar^2}{2m}(\nabla+ik)^2+V(r)\right]u_k(r)=\varepsilon_k u_k(r)$$

$*$ $$\left[-\frac{\hbar^2}{2m}(\nabla-ik)^2+V(r)\right]u_k^*(r)=\varepsilon_k u_k^*(r)$$

$k\to -k$ $$\left[-\frac{\hbar^2}{2m}(\nabla-ik)^2+V(r)\right]u_{-k}(r)=\varepsilon_{-k} u_{-k}(r)$$

$$\Rightarrow \quad \varepsilon(-k)=\varepsilon(k), \quad u_{-k}(r)=u_k^*(r)$$

✓ $\nabla_k\varepsilon_k=\nabla_{-k}\varepsilon(-k)=-\nabla_k\varepsilon(-k)\Rightarrow V(k)=-V(-k)$

② 有外场能带导电分析

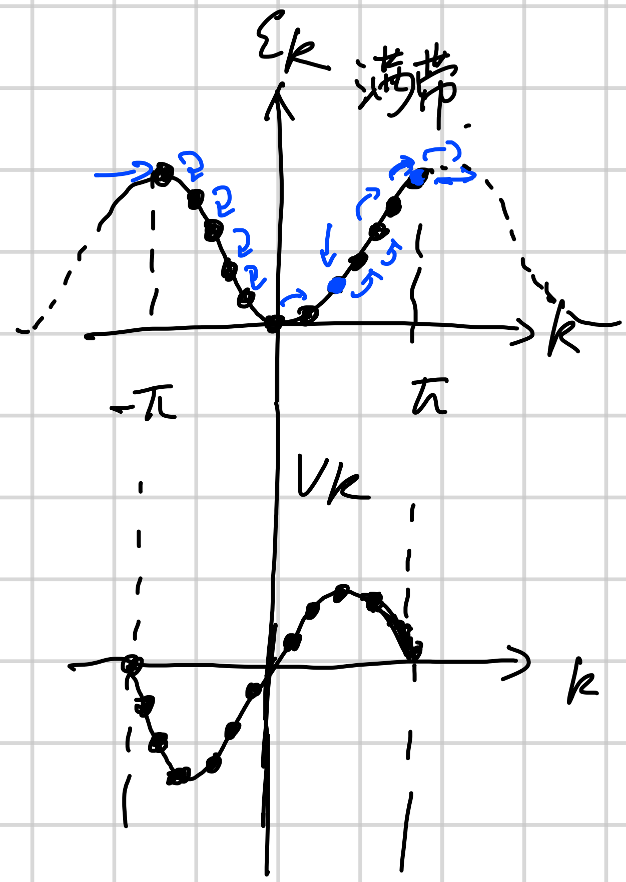
(i) 满带. $\sum_k V(k)n_k=0$, 无净电流

✓ $\dfrac{d\vec{k}}{dt}=-e\vec{E}/\hbar$. 匀 $\vec{k}$ 移动.

✓ $\vec{k}$空间中电子“均匀流动”，但第一布里渊区永远满填充.

✓ 实空间，净电流为零.

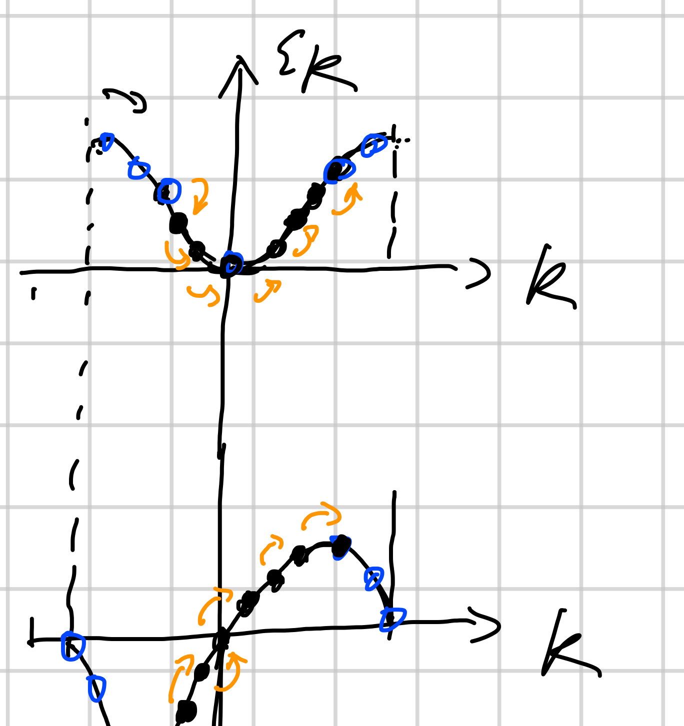
☆ 满带不导电




(ii) 部分填充，Sommerfeld 模型

✓ 在外场下，能带分布可能呈现非对称情况. ⇒ 实空间电流不抵消.

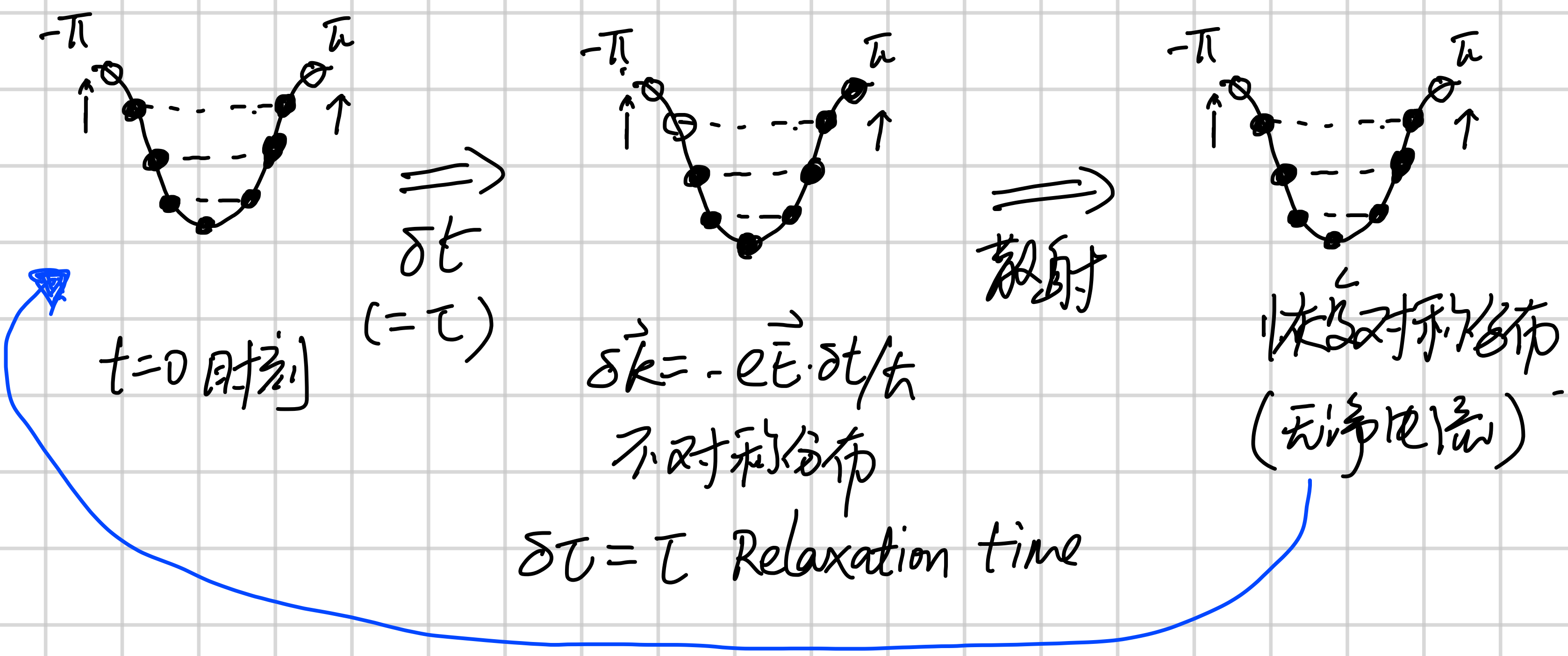
⇒ 产生净电流




$\sum_k V(k)\cdot n_k \neq 0$

✓ Sommerfeld model

# 电子气的导电状态+半经典处理 (Revisit of Drude-Sommerfeld The.)




$\delta \vec{k} = -e\vec{E}\cdot\tau/\hbar$.

✓ 漂移速度 (drifting velocity) $\vec{v}_d = \frac{-e\vec{E}\cdot\tau}{m^*}$.

✓ 电流 (electric current) $\vec{J} = -ne\vec{v}_d = -ne\cdot\frac{-e\vec{E}\cdot\tau}{m}$

✓ 欧姆定律 $\vec{J} = \sigma\vec{E}$ $\quad = (ne^2\tau/m)\cdot\vec{E}$

$\Rightarrow \quad \sigma = \frac{ne^2\tau}{m}$.

✓ 能带电子. $m \to m^*$, $\sigma = ne^2\tau/m^*$.

② 近满带填充与空穴 (nearly full band and hole)

(i) 整条能带中除k点外均填充电子—近满带.

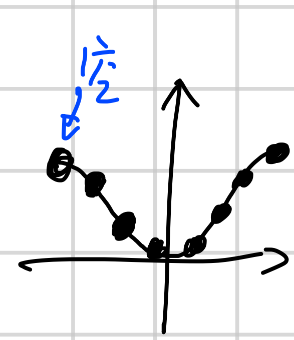
(ii) 施加电场$\vec{E}$ → 趋动电流 $I_k$

⇒ 假设k点放电子 → 补充成满带. ($I = I_k + \tilde{I}_k = 0$)

$\tilde{I}_k = -e\cdot\vec{v}_k \Rightarrow I_k = -\tilde{I}_k = e\vec{v}_k$

空穴带有正电荷"e".

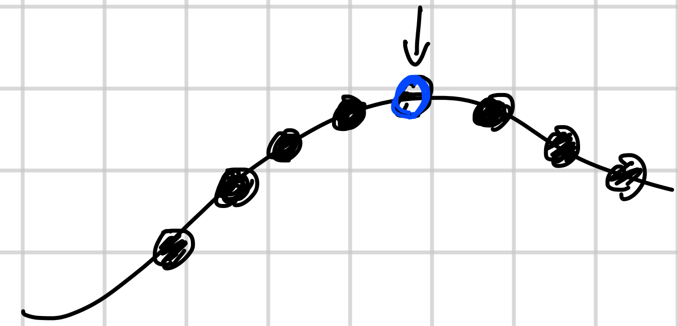
⇒ 电子集体运动用空穴代表.



(iii) 空穴有效质量 (运动方程)

$$\frac{dv_k}{dt} = \frac{1}{m_e^*}(-e\vec{E}) \quad \text{(填至顶处时)}$$

$$\Rightarrow \frac{dv_k}{dt} = \frac{e\vec{E}}{(-m_e^*)} = \frac{e\vec{E}}{m_h^*}.$$



$m_e^* < 0$

$m_h^* = -m_e^* > 0$

定义 $m_h^* = -m_e^*$ ← 电子有效质量.

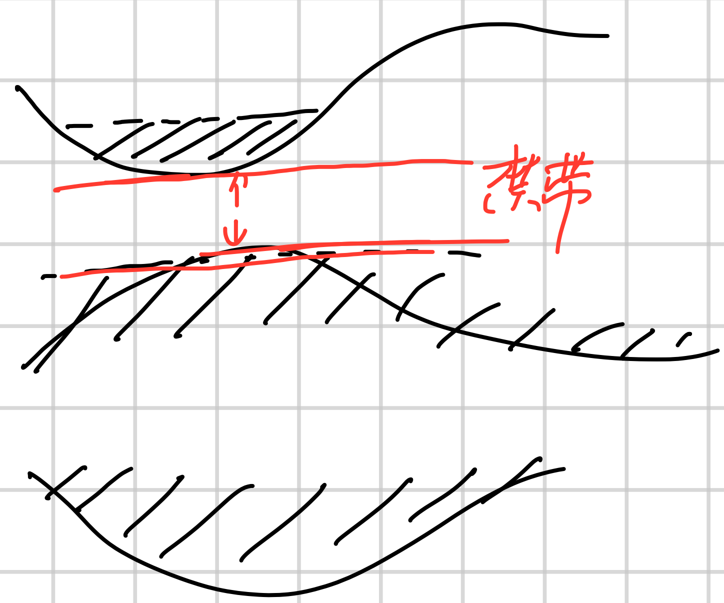
↑ 空穴有效质量.

空穴携带正电荷(往往也是)正质量.

⇒ "演生准粒子" Emergent Quasi-Particle

金属 半导体与绝缘体

✓ 能带填充从低往高，最高能带存在部分填充 ⇒ 导带



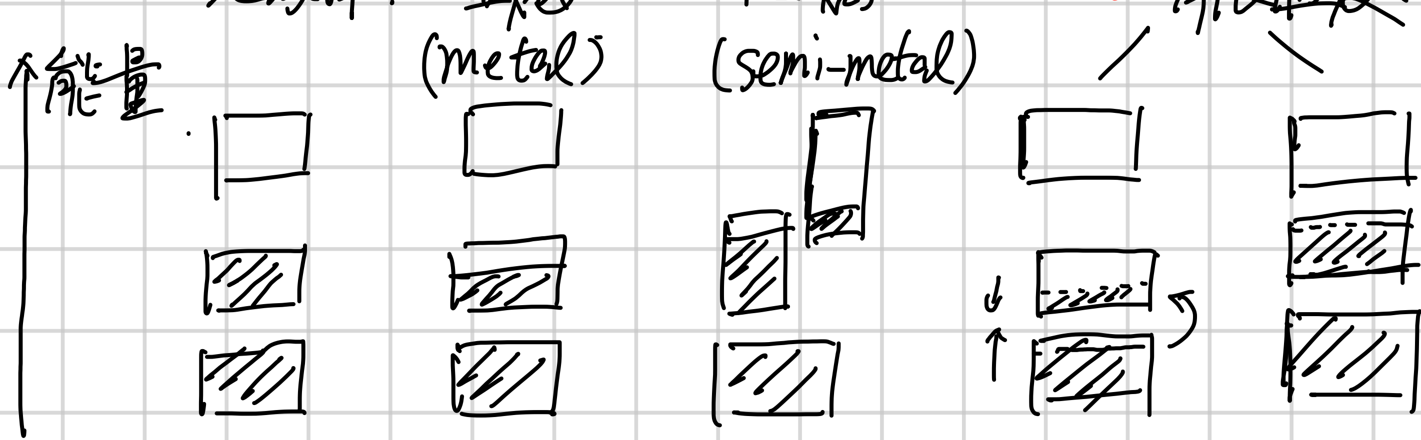

✓ 若为空带，则存在一禁带 (forbidden band)

✓ 金属：导带部分填充. (金属：存在费米面)

(正方)　(六角)

绝缘体.　金属 (metal)　半金属 (semi-metal)　半导体 (semi-conductor)

✓有限温度(掺杂)



# IV. 稳恒磁场中的能带电子.

提纲：① 一般介绍. ② 自由电子磁场中运动. ③ 布洛赫电子在磁场中的运动
(费米面及其测量, dHvA效应)

(1) 磁场中的半经典运动

$$\hbar \frac{d\vec{k}}{dt} = -\frac{e}{c}\vec{v}_k \times \vec{B}$$

← 洛仑兹力 (经典)

布洛赫波矢

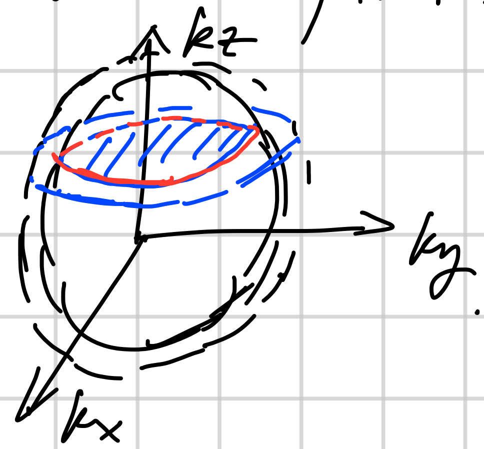
其中 $\vec{v}_k = \frac{1}{\hbar}\nabla_k \varepsilon(k)$ 群速度.

假设磁场沿 z 方向. $\hat{B} = B_z \hat{z}$

① $\frac{d\vec{k}}{dt} \perp \hat{z}$ , $\frac{dk_z}{dt} = 0$ (电子的运动局限在 $k_x$-$k_y$ 平面内)

② $\frac{d\vec{k}}{dt} \perp \vec{v}_k$ , 运动处于等能面.

$$\frac{d\vec{k}}{dt} \cdot \vec{v}_k = \cancel{\frac{dk}{dt}} \cdot \frac{d\varepsilon}{\cancel{dk}} \cdot \frac{1}{\hbar} = \frac{d\varepsilon}{dt} \cdot \frac{1}{\hbar} = 0$$




✓ 综上, 电子在k空间的轨道为等能面与 $k_x$-$k_y$ 平面的交线.

(2) 自由电子 $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$

代入运动方程. $\left(\vec{v}_k = \frac{1}{\hbar}\nabla_k \varepsilon(k) = \frac{\hbar \vec{k}}{m}\right)$

$$\hookrightarrow \hbar \frac{d\vec{k}}{dt} = -e\frac{\hbar \vec{k}}{mc} \times \vec{B} . \quad (\vec{B} = B \cdot \hat{z})$$

① 分量:

$$\begin{cases} \cancel{\hbar}\frac{dk_x}{dt} = -\frac{e\cancel{\hbar}}{mc} \cdot k_y \cdot B_z \\ \cancel{\hbar} \cdot \frac{dk_y}{dt} = \frac{e\cancel{\hbar}}{mc} k_x \cdot B_z \end{cases} \Rightarrow \begin{array}{l} \frac{dk_x}{dt} = -\frac{e}{mc} B \cdot k_y \\ \frac{dk_y}{dt} = \frac{e}{mc} \cdot B \cdot k_x . \end{array}$$

$$\Rightarrow \begin{cases} k_x = A\cdot\cos(\omega t) \\ k_y = A\cdot\sin(\omega t) \end{cases} \quad \left( \omega_c = \frac{eB}{mc} \ , \ T = \frac{2\pi}{\omega} = \frac{2\pi mc}{eB} \right).$$

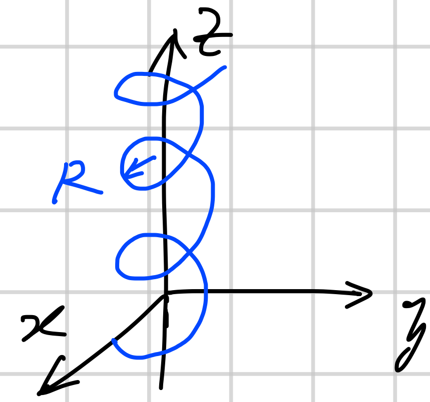
② $$\begin{cases} V_x = X\cos(\omega t) \\ V_y = X\sin(\omega t) \end{cases} \Rightarrow \begin{cases} x = x_0 + \frac{X}{\omega}\sin(\omega t) \\ y = y_0 - \frac{X}{\omega}\cos(\omega t) \\ z = z_0 - C_0 t . \end{cases}$$

$, V_z = C_0 \sim$ 常数.

③ 实空间：以 $(x_0, y_0)$ 为中心圆周运动. 同时沿 $z$ 方向匀速运动.

螺旋线. $\frac{1}{2}m(V_x^2+V_y^2) = \frac{1}{2}m\cdot X^2$ 常数 $= \frac{1}{2}m|V|^2$

$$|V| = \frac{2\pi R}{T} = \frac{eB}{mc}\cdot R.$$




(3) 布洛赫电子.

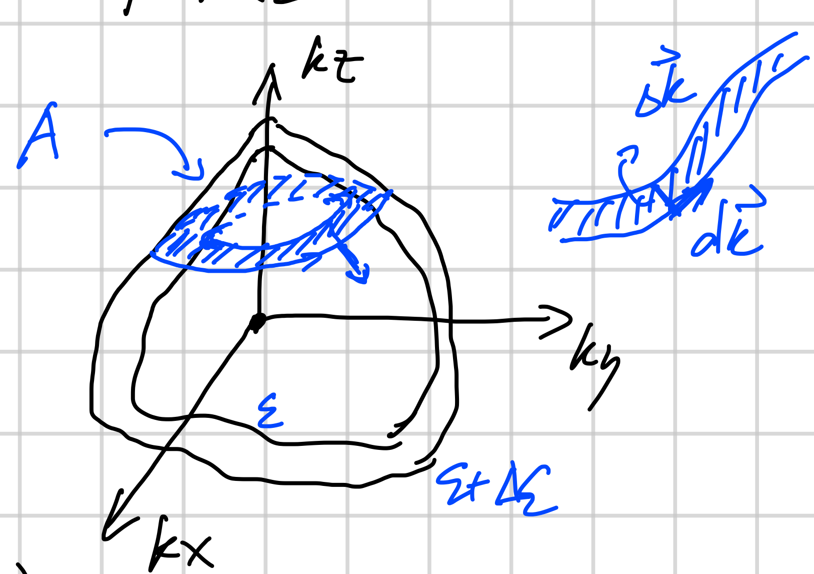
等能面一般地非球面, $m \to m^*$ (有效质量)

回旋频率 $\omega_c = \frac{eB}{m^* c}$.

回旋周期

$$T = \frac{2\pi}{\omega_c} = \oint dt = \oint d\vec{k}\Big/\left(\frac{d\vec{k}}{dt}\right)$$

$$= \oint \frac{d\vec{k}}{|V_\perp|}\frac{\hbar c}{eB} \quad \text{(半经典运动方程)}$$




两等能面能量差: $\Delta\varepsilon = \hbar|V_\perp|\cdot\Delta k$ ($\Delta k$ 等能面的梯度方向)

$$T = \oint d\vec{k}\cdot\frac{1}{\Delta\varepsilon}(\hbar\cdot\Delta k)\cdot\frac{\hbar c}{eB} = \oint\frac{d\vec{k}}{\Delta\varepsilon}\cdot\frac{\hbar^2 c}{eB}\Delta k.$$

$$= \left[\oint d\vec{k}\cdot\Delta k\Big/\Delta\varepsilon\right]\cdot\frac{\hbar^2 c}{eB} = \frac{\partial A(\varepsilon,k_z)}{\partial\varepsilon}\cdot\frac{\hbar^2 c}{eB}$$

$$\omega_c = \frac{2\pi}{T} = \frac{2\pi}{\hbar^2 c} \cdot \frac{eB}{\partial_\varepsilon A(\varepsilon, k_z)} \left[ = \frac{eB}{m^* c} \right]$$

$$\Rightarrow m^* = \partial_\varepsilon A(\varepsilon, k_z) \cdot \frac{\hbar^2}{2\pi}.$$

② 实空间轨道.

$$\vec{B} \times \hbar \frac{d\vec{k}}{dt} = \vec{B} \times \left(-\frac{e}{c} \vec{v} \times \vec{B}\right)$$

$$= B\hat{z} \times \left(-\frac{e}{c} \cdot B\right)\left(-v_x \cdot \hat{y} + v_y \hat{x}\right)$$

$$= B^2 \left(\frac{-e}{c} v_x \hat{x} - \frac{e}{c} \cdot v_y \hat{y}\right)$$

$$= B^2 \cdot \frac{-e}{c} \left(v_x \cdot \hat{x} + v_y \cdot \hat{y}\right) = B^2 \cdot \left(\frac{-e}{c}\right) \cdot \vec{v} = B^2 \left(-\frac{e}{c}\right) \frac{d\vec{r}_\perp}{dt}.$$

$\left(\vec{v} = \frac{d\vec{r}_\perp}{dt}\right)$ $\vec{r}_\perp$ 表示 xy 面的位置矢量.

$$\left[\vec{r}_\perp(t) - \vec{r}_\perp(0)\right] = \left(-\frac{c}{e}\right) \frac{1}{B^2} \cdot \vec{B} \times \left[\vec{k}(t) - \vec{k}(0)\right]$$

$$\Rightarrow \underbrace{\left[\vec{r}_\perp(t) - \vec{r}_\perp(0)\right]}_{\text{实空间轨道 (xy平面)}} = -\frac{\hat{B} \cdot c}{eB} \times \underbrace{\left[\vec{k}(t) - \vec{k}(0)\right]}_{k\text{-空间轨道 (xy平面)}}$$

✓ 实空间轨道是 k-空间轨道以 z 为轴转动 90° 并做缩放 $\left(\frac{c}{eB}\right)$

✓ z 方向运动

$$z(t) = z(0) + \int_0^t \underbrace{v_z(t)}_{\to \text{不一定匀速}} dt$$

$$\left(v_z = \frac{1}{\hbar} \cdot \frac{\partial \varepsilon}{\partial k_z}.\right)$$

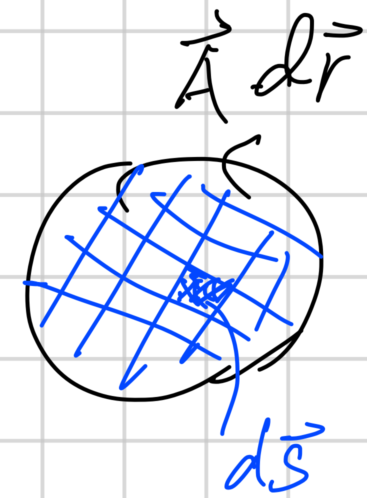
(4) 磁场中电子运动的量子理论.

② 无磁场时: $\hat{H} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$.

加磁场后: $\hat{H} = \frac{1}{2m}(\underbrace{\hat{p}}_{\text{机械动量}} + \underbrace{\tfrac{e}{c}\vec{A}}_{\text{正则动量}})^2$

机械动量.

粒子速度: $\begin{cases} \vec{v} = \frac{1}{m}(\vec{p} + \frac{e}{c}\vec{A}) \\ \vec{p} = m\vec{v} - \frac{e}{c}\vec{A} \end{cases}$




引入 Bohr-Sommerfeld 轨道量子化.

$\Rightarrow \oint \vec{p}\cdot d\vec{r} = (j+\frac{1}{2})h. \quad j = 0, 1, 2, \cdots$

$\oint (m\vec{v} - \frac{e}{c}\vec{A})\, d\vec{r} = (j+\frac{1}{2})h.$

✓ $|v| = \frac{eB}{mc}\cdot R \Rightarrow \cancel{m}\cdot\frac{eB}{\cancel{m}c}\cdot 2\pi\cdot R^2 = \frac{2e}{c}B\pi\cdot R^2$

✓ $\oint(-\frac{e}{c})\cdot\vec{A}\, d\vec{r} = (-\frac{e}{c})\oint \vec{A}\, d\vec{r} = -\frac{e}{c}\iint_S (\nabla\times\vec{A})\cdot d\vec{S}$

$= (-\frac{e}{c})\cdot\iint_S \vec{B}\cdot d\vec{S}$

$= (-\frac{e}{c})\cdot B\cdot\pi\cdot R^2$

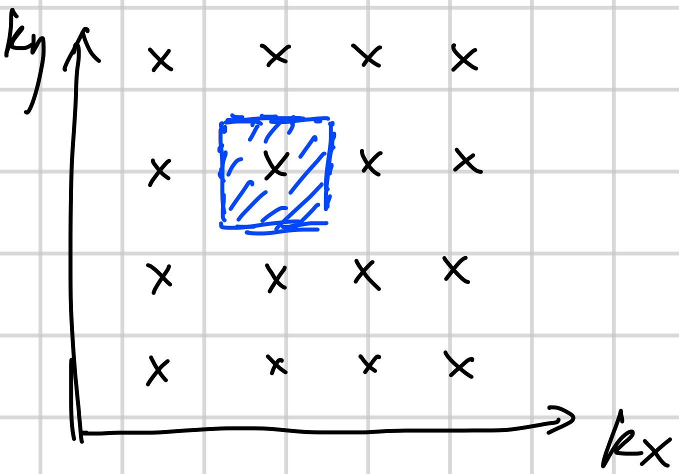
$\frac{2e}{c}\cdot B\cdot\pi R^2 - \frac{e}{c}B\cdot\pi R^2 = (j+\frac{1}{2})h$

$\Rightarrow \frac{e}{c}B\cdot\pi R^2 = (j+\frac{1}{2})h.$

$\Rightarrow R^2 = \frac{2c}{eB}(j+\frac{1}{2})\hbar.$ (轨道量子化)

能量 $\varepsilon = \frac{1}{2}m\cdot\frac{e^2B^2}{m^2c^2}R^2 = \frac{eB}{mc}(j+\frac{1}{2})\hbar = (j+\frac{1}{2})\hbar\omega_c.$

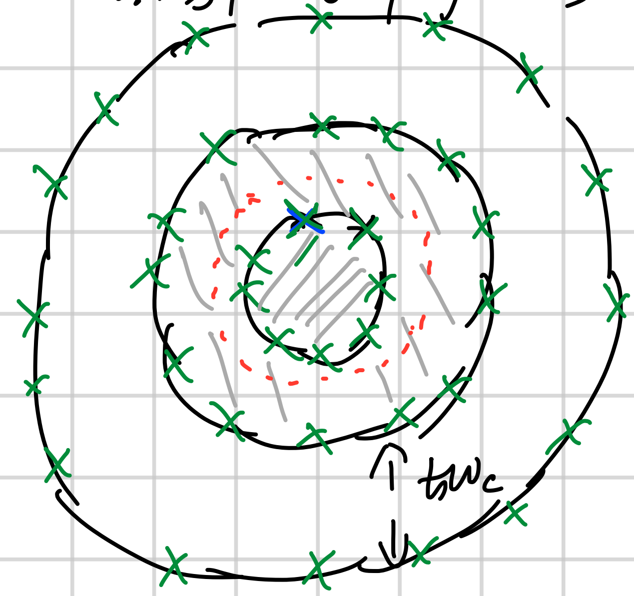
## 自由电子k空间



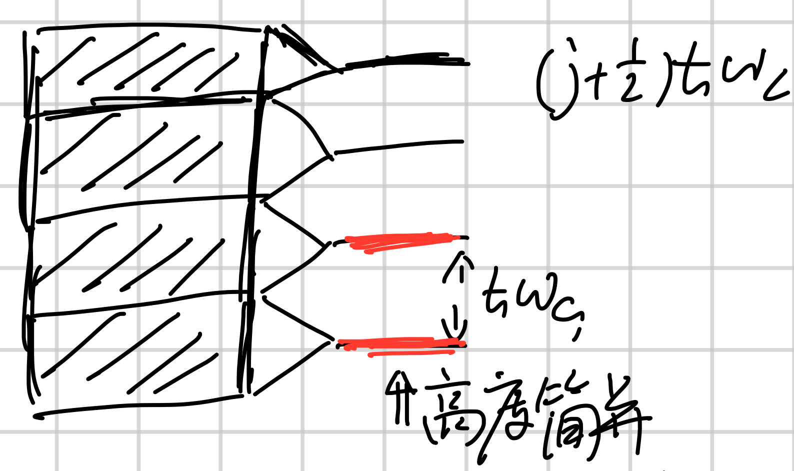

$\left(\frac{2\pi}{L}\right)^2\cdot\frac{1}{2}$

$\Rightarrow (k_x^2+k_y^2)/2m$

$\Rightarrow$ 磁场中电子许可态




(准)连续 $\rightarrow$ 分立




## 朗道能级简并度 $g$

$$g=\frac{\text{轨道间}k\text{空间面积}}{\text{单位面积}}$$

$$g=\frac{\pi\,\Delta(k^2)}{\left(\frac{2\pi}{L}\right)^2\cdot\frac{1}{2}}$$

$$\left(\frac{\hbar^2\Delta k^2}{2m}=\hbar\omega_c\right)$$

$$g=\frac{\pi\cdot 2m\cdot\hbar\omega_c\cdot\frac{1}{\hbar^2}}{2\pi^2/L^2}=\frac{L^2}{2\pi^2}\cdot\frac{2m\omega_c}{\hbar}\cdot\cancel{\pi}$$

$$\boxed{g=\frac{L^2}{h}\cdot 2\cancel{m}\cdot\frac{eB}{\cancel{m}c}=\frac{2e}{hc}\cdot B\cdot L^2}$$

朗道能级简并度 $\propto B$，$\propto L^2$ 宏观简并度.

讨论：$B$极大，$g$极大 $> N$. 所有电子填充第一朗道能级.
(LLL)