# 能带理论(下)

## (I) 晶格电子的平均速度

① 布洛赫波 $\psi_{nk}$，计算平均速度

$$\begin{cases} \vec{v}_n(\vec{k}) = \dfrac{1}{m}\int \psi_{nk}^{*}\,\hat{p}\,\psi_{nk}\,d\vec{r} \\ \hat{p} = -i\hbar\vec{\nabla} \end{cases}$$

代入布洛赫波形式 $\psi_{nk} = e^{i\vec{k}\cdot\vec{r}}\,u_{nk}(\vec{r})$

$$\Rightarrow \vec{v}_n(k) = \frac{1}{m}\int e^{-i\vec{k}\cdot\vec{r}}u_{nk}^{*}(\vec{r})\,(-i\hbar\vec{\nabla})\left[e^{ikr}u_{nk}(\vec{r})\right]d\vec{r}$$

$$= \frac{1}{m}\int \cancel{e^{-i\vec{k}\cdot\vec{r}}}\,u_{nk}^{*}(\vec{r})\left[\hbar\vec{k}\,\cancel{e^{i\vec{k}\cdot\vec{r}}}\,u_{nk} + \cancel{e^{i\vec{k}\cdot\vec{r}}}\,(-i\hbar\nabla u_{nk})\right]$$

$$= \frac{1}{m}\int u_{nk}^{*}(r)\,(\hbar\vec{k} - i\hbar\vec{\nabla})\,u_{nk}(r)\,d\vec{r}$$

$$= \frac{1}{m}\int u_{nk}^{*}(r)\,(\hbar\vec{k} + \hat{p})\,u_{nk}(\vec{r})\,d\vec{r}$$

$$\vec{v}_n(k) = \frac{1}{m}\langle u_{nk}|\,\hbar\vec{k} + \hat{p}\,|u_{nk}\rangle$$

周期部分

② $u_{nk}(r)$ 的 Schrödinger Equation

$$\left[\frac{(\vec{p}+\hbar\vec{k})^2}{2m} + V(r)\right]u_{nk}(\vec{r}) = \varepsilon_n(k)\,u_{nk}(\vec{r})$$

$$H_k = \frac{(\vec{p}+\hbar\vec{k})^2}{2m} + V(r),$$

$$H_k\cdot u_{nk}(\vec{r}) = \varepsilon_n(k)\,u_{nk}(r)$$

两边 $\nabla_k$： 左边 $= (\nabla_k H_k)\,u_{nk}(r) + H_k\,\nabla_k u_{nk}(r)$

$$\hbar\cdot\frac{(\hbar\vec{k}+\vec{p})}{m}u_{nk}(\vec{r})+H_k\vec{\nabla}_k u_{nk}(\vec{r})$$

右边 $=\nabla_k[\varepsilon_n(k)u_{nk}(r)]$

$$=\vec{\nabla}_k\varepsilon_n(k)\,u_{nk}(r)+\varepsilon_n(k)\nabla_k u_{nk}(r)$$

$$\frac{\hbar}{m}(\hbar\vec{k}+\vec{p})u_{nk}(\vec{r})+H_k\vec{\nabla}_k u_{nk}(\vec{r})=\vec{\nabla}_k\varepsilon_n(k)u_{nk}+\varepsilon_n(k)\nabla_k u_{nk}$$

左乘 $u^*_{nk}(r)$，并积分 (Dirac notation)

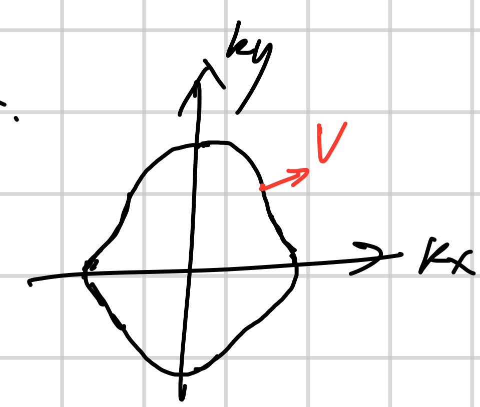
$$\frac{\hbar}{m}\cdot\langle u_{nk}|\hbar\vec{k}+\vec{p}|u_{nk}\rangle+\langle u_{nk}|H_k|\cancel{\vec{\nabla}_k}u_{nk}\rangle$$

$$=\langle u_{nk}\cancel{|u_{nk}\rangle}\cdot\vec{\nabla}_k\cdot\varepsilon_n(k)+\varepsilon_n(k)\cancel{\langle u_{nk}|}\vec{\nabla}_k u_{nk}\rangle$$

$$\Rightarrow\quad\frac{1}{m}\langle\hbar\vec{k}+\vec{p}\rangle=\frac{1}{\hbar}\vec{\nabla}_k\varepsilon_n(k)$$

得到 $\quad\vec{V}_n(k)=\frac{1}{\hbar}\vec{\nabla}_k\varepsilon_n(k)$ 晶格电子平均速度.

③ 讨论 • $\varepsilon\sim\hbar\omega$，$v_n\sim\nabla_k\omega$ 波包群速度.




• 沿等能面梯度方向

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

$$V(k)=\frac{1}{\hbar}\nabla_k\left(\frac{\hbar^2k^2}{2m}\right)=\hbar\vec{k}/m$$

II. 电子运动的半经典模型/运动方程.

• 晶格电子对外场的响应 $(\vec{E},\vec{B})\Rightarrow$ 经典处理

• 晶格电子的运动状态 $\Rightarrow$ 量子力学（能带理论）

(1) $\vec{F}$ 外力作用下，布洛赫电子运动方程.

电子能量的改变 = 外力做功

$\Delta\mathcal{E}(k) = \vec{f}\cdot\Delta\vec{s}$ $\qquad \frac{d\mathcal{E}(k)}{dt} = \vec{f}\cdot\vec{v}$

左边: $\frac{d\mathcal{E}(k)}{dt} = \nabla_k \mathcal{E}(k)\cdot\frac{d\vec{k}}{dt} = \hbar\vec{v}\cdot\frac{d\vec{k}}{dt} = \frac{d(\hbar\vec{k})}{dt}\cdot\vec{v}$

右边: $\vec{f}\cdot\vec{v}$

$\Rightarrow \quad \frac{d(\hbar\vec{k})}{dt} = \vec{f}$ 运动方程.

讨论: ① $\vec{f}$ 仅包含外力 (不包含晶格势场)

电磁场中: $\frac{d(\hbar\vec{k})}{dt} = -e\underbrace{[\vec{E}(\vec{r},t) + \vec{v}_n(\vec{k})\times\vec{B}(\vec{r},t)]}_{\equiv f}$

② 牛顿运动方程 (经典)

$\hbar\vec{k}$ 描述电子状态 (量子)

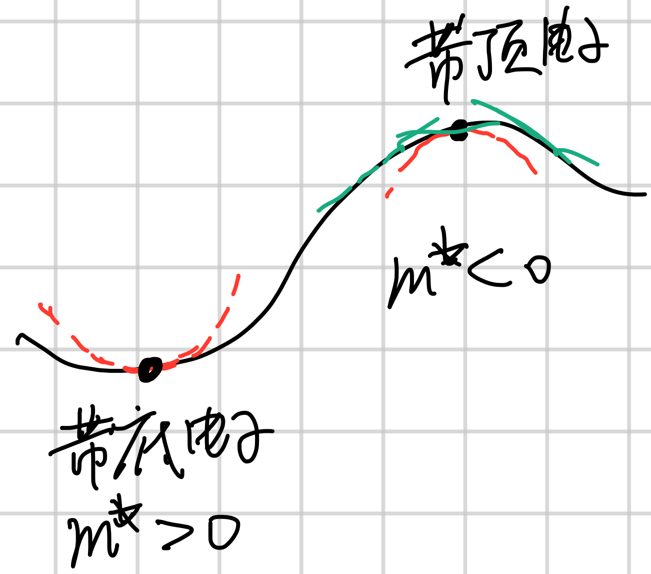
(2) 加速度与有效质量

$\vec{a} = \frac{d\vec{v}}{dt} = \frac{d}{dt}\left[\frac{1}{\hbar}\nabla_k\mathcal{E}_n(k)\right]$

$= \frac{1}{\hbar}\nabla_k\left[\nabla_k\mathcal{E}_n(k)\right]\cdot\frac{d\vec{k}}{dt}$

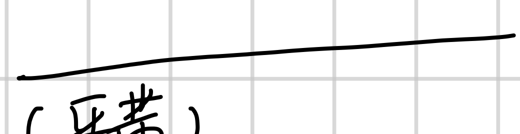
$\boxed{(f = m^* a)}$ $\quad = \frac{1}{\hbar^2}\left[\nabla_k^2\mathcal{E}_n(k)\right]\cdot\vec{f}$

$\Rightarrow$ 有效质量 $m^* = \hbar^2/\nabla_k^2\mathcal{E}_n(k)$




讨论: ① 1D, $m^* = \hbar^2\cdot\frac{1}{d^2\mathcal{E}_n(k)/dk^2}$

平坦能带 $m^* = \hbar^2\cdot\frac{1}{d^2/dk^2\to 0}\to\infty$




$\Rightarrow$ 局域 (实空间)

③ 3D 情况

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

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

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）

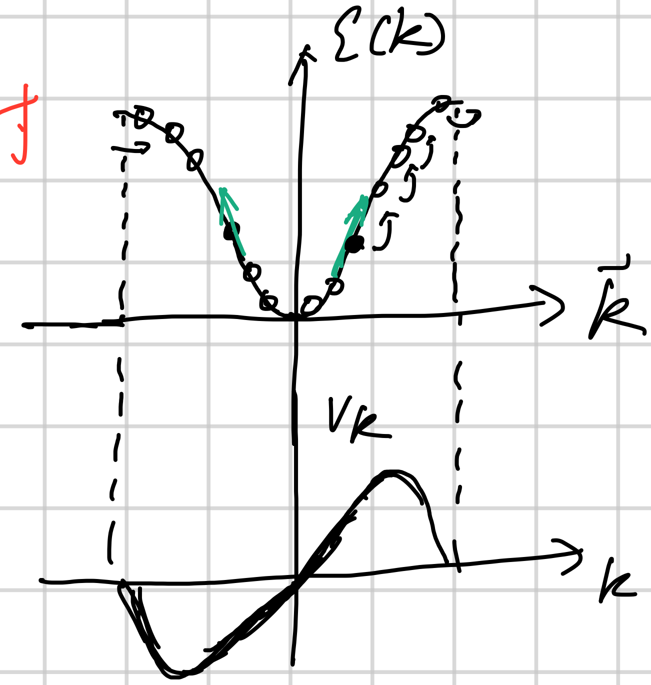
## Ⅲ. 稳恒电场中的电子运动

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

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

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

稳恒电场下，电子波矢匀速移动




② 运动速度分析（半正，半负）

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

（$k$ 和 $-k$ 处运动速度相反）

✓ 无外场，对称填充 ⇒ 无电流（满或不满）