Notes of 141A
Solid State Physics

hebrewsnabla

2018年11月28日

目录

7 Energy Bands

7.1 Nearly Free Elec Model

$$\begin{aligned} U(x) &= U_0\left[\cos^4\frac{\pi x}{a} - \frac{3}{8}\right] \\ &= \ldots \\ &= U_0\left(\frac{1}{2}\cos\frac{2\pi x}{a} + \frac{1}{8}\cos\frac{4\pi x}{a}\right) \end{aligned} \tag{7.1}$$

$$(\lambda_k - \epsilon)C_k + \sum_G U_G C_{k-G} = 0 \tag{7.2}$$

solve reduced problem near degenerate points

$$\begin{pmatrix} \lambda_k - \epsilon & U_g \\ U_g^* & \lambda_{k-g} - \epsilon \end{pmatrix}\begin{pmatrix} C_k \\ C_{k-g} \end{pmatrix} = 0 \quad (g = \frac{2\pi}{a}) \tag{7.3}$$

$$(\lambda_k - \epsilon)^2 - |U_g|^2 = 0 \tag{7.4}$$

$$\epsilon = \frac{\hbar^2 k^2}{2m} \pm \frac{U_0}{4} \tag{7.5}$$

or

$$\epsilon = \frac{\hbar^2 (k + G_1)^2}{2m} \pm \frac{U_0}{16} \tag{7.6}$$

7.2 Bloch Oscillators

Semi-classical eq. of motion

$$\hbar\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t} = \mathbf{F} = -e\mathbf{E} \tag{7.7}$$

$$v_{grp} = \frac{1}{\hbar}\frac{\mathrm{d}\varepsilon}{\mathrm{d}k} \tag{7.8}$$

consider

$$\varepsilon(k) = \varepsilon_0(1 - \cos ka) \tag{7.9}$$

$$v = \frac{a\varepsilon_0}{\hbar}\sin ka \tag{7.10}$$

$$\begin{aligned} x &= \int \frac{a\varepsilon_0}{\hbar}\sin ka \mathrm{d}t \\ &= \frac{a\varepsilon_0}{\hbar}\int \sin ka \mathrm{d}k\frac{\mathrm{d}t}{\mathrm{d}k} \\ &= \ldots \\ &= -\frac{\varepsilon_0}{eE}\left(\cos\frac{-eEa}{\hbar} - 1\right) \end{aligned} \tag{7.11}$$

$$T = \frac{\Delta k}{\mathrm{d}k/\mathrm{d}t} = \frac{2\pi/a}{eE/\hbar} = ... \tag{7.12}$$

scattering time $\tau >> T$.

suppose $\mathbf{F} = m^* \mathbf{a}$

$$m^* = \hbar \frac{\mathrm{d}k/\mathrm{d}t}{\mathrm{d}v_g/\mathrm{d}t} = \hbar \left(\frac{\mathrm{d}v_g}{\mathrm{d}k} \right)^{-1} = \hbar^2 \left(\frac{\partial^2 \varepsilon}{\partial k^2} \right)^{-1} \tag{7.13}$$

7.3 Consequence of Band Structure

even # of elec's per unit cell – insulator – $\mathrm{C}, \mathrm{Si}, \mathrm{Ge}$
odd # of elec's per unit cell – metal – $\mathrm{Cu}, \mathrm{Ag}, \mathrm{Au}$
Ins – $E_g > 2\ eV$
Semiconductor – $E_g < 2; eV$

7.3.1 Density of States

Van Hove Singularities of DoS

8 Semiconductors

8.1 Photoconductivity

$$\mathbf{J}_n = \frac{1}{V} \int_{unocc} eD(\mathbf{k}_e) \mathbf{v}_e(\mathbf{k}_e) \mathrm{d}^3 \mathbf{k}_e \tag{8.1}$$

$$\frac{\mathrm{d}\mathbf{k}_e}{\mathrm{d}t} = \frac{-e}{\hbar} (\mathbf{E} + \frac{1}{c} \mathbf{v}_e \times \mathbf{B}) \tag{8.2}$$

$$\mathbf{v}_e(\mathbf{k}_e) = \frac{1}{\hbar} \frac{\partial E_v(\mathbf{k}_e)}{\partial \mathbf{k}_e} \tag{8.3}$$

Holes: Def

$$\mathbf{k}_n = -\mathbf{k}_e \quad E_n = -E_v \tag{8.4}$$

$$\mathbf{v}_n(\mathbf{k}_n) = \frac{1}{\hbar} \frac{\partial E_n(\mathbf{k}_n)}{\partial \mathbf{k}_n} = \frac{1}{\hbar} \frac{\partial(-E_v(-\mathbf{k}_e))}{\partial(-\mathbf{k}_e)} = \mathbf{v}_e(\mathbf{k}_e) \tag{8.5}$$

Holes: + charge, evolves like particle, $m^* > 0$

8.2 Intrinsic Mobility

$$\mathbf{J}_{tot} = \mathbf{J}_e + \mathbf{J}_h \tag{8.6}$$

$$\sigma_{tot} = \sigma_e + \sigma_h \tag{8.7}$$

$$\sigma_e = \frac{n_e e^2 \tau_e}{|m_e^*|} \tag{8.8}$$

$$\sigma_h = \frac{n_h e^2 \tau_h}{|m_h^*|} \tag{8.9}$$

def: mobility

$$\mu = \frac{e\tau}{m^*} \tag{8.10}$$

$$\sigma_{tot} = n_e e \mu_e + n_h e \mu_h \tag{8.11}$$

8.3 Impurity Conductivity / Doping

$$n_e(T) \neq n_h(T) \quad \Rightarrow \quad \text{doping} \tag{8.12}$$

Impurity atoms that can give up an electron are called donors.

8.3.1 Donor States

the donated elec moves in the coulomb potential $-e/\epsilon r$

$$N_d = \frac{\#donors}{Vol.} \quad N_a = \frac{\#acceptors}{Vol.} \tag{8.13}$$

$$n_e(T) = 2\left(\frac{m_e k_B T}{2\pi\hbar^2}\right)^{3/2} \mathrm{e}^{-(E_c-\mu)/k_B T} \tag{8.14}$$

$$n_p(T) = 2\left(\frac{m_h k_B T}{2\pi\hbar^2}\right)^{3/2} \mathrm{e}^{-(\mu-E_v)/k_B T} \tag{8.15}$$

Intrinsic:

$$n_i(T) = \sqrt{n_e(T) n_p(T)} \tag{8.16}$$

$$\mu_i(T) = E_v + \frac{1}{2}E_g + \frac{3}{4}k_B T \ln\frac{m_h}{m_e} \tag{8.17}$$

$$\frac{N_d - N_a}{n_i(T)} = 2\sinh\frac{\mu - \mu_i}{k_B T} \tag{8.18}$$

8.4 Hall Effect w/ 2 Carrier Types

Kittel 8.3
mobilities:

$$\mu_e = \frac{e\tau_e}{m_e} \quad \mu_h = \frac{e\tau_h}{m_h} \tag{8.19}$$

(m_e is eff mass)
Recall conductivity tensor w/ B-field

$$\sigma = \frac{\sigma_0}{(1+\omega_c^2\tau^2)^2}\begin{pmatrix} 1 & -\omega_c\tau \\ -\omega_c\tau & 1 \end{pmatrix} \tag{8.20}$$

where $\sigma_0 = \dfrac{ne^2\tau_e}{m_e}$, $\omega_c = \dfrac{eB}{m_e c}$.
transverse current ($\omega_c\tau << 1$)

$$j_y(e) = \sigma_0(\omega_c\tau E_x + E_y) = ne\mu_e(\frac{\mu_e B}{c}E_x + E_y) \tag{8.21}$$

$$j_y(h) = pe\mu_h(\frac{-\mu_h B}{c}E_x + E_y) \tag{8.22}$$

longitudinal curr

$$j_x = j_x(e) + j_x(h) = (ne\mu_e + pe\mu_h)E_x \tag{8.23}$$

tot transverse curr = 0, thus

$$(n\mu_e^2 - p\mu_h^2)\frac{eB}{c}E_x + (n\mu_e + p\mu_h)eE_y = 0 \tag{8.24}$$

$$E_y = -E_x\frac{B}{c}\frac{n\mu_e^2 - p\mu_h^2}{n\mu_e + p\mu_h} \tag{8.25}$$

$$R_H = \frac{E_y}{j_x B} = -\frac{1}{ec}\frac{n\mu_e^2 - p\mu_h^2}{(n\mu_e + p\mu_h)^2} \tag{8.26}$$

8.5 Tight-binding

start w/ AOs (1-D)

$$\psi_k(r) = \sum_j c_j\phi(r - r_j) \tag{8.27}$$

(ϕ is s orb)
Bloch Th.

$$\psi_k(r) = \mathrm{e}^{\mathrm{i}kr}\,u(r) \tag{8.28}$$

if $c_j = \dfrac{1}{\sqrt{N}}\,\mathrm{e}^{\mathrm{i}kr}$

$$\left\langle \psi_k \middle| \hat{\mathbf{H}} \middle| \psi_k \right\rangle = \frac{1}{N}\sum_j\sum_m \mathrm{e}^{\mathrm{i}k(r_j - r_m)}\left\langle \phi_m \middle| \hat{\mathbf{H}} \middle| \phi_j \right\rangle \tag{8.29}$$

let $\rho_m = r_m - r_j$, suppose only nearest neighbor interacts

$$\left\langle \psi_k \middle| \hat{\mathbf{H}} \middle| \psi_k \right\rangle = \frac{1}{N} \sum_m \mathrm{e}^{\mathrm{i}k\rho_m} \int \mathrm{d}V \, \phi^*(r - \rho_m) \, \hat{\mathbf{H}} \, \phi(r) \tag{8.30}$$

$(r - r_j \to r)$

Let

$$-\varepsilon_0 = \int \mathrm{d}V \, \phi^*(r) \, \hat{\mathbf{H}} \, \phi(r) \qquad - t = \int \mathrm{d}V \, \phi^*(r - \rho) \, \hat{\mathbf{H}} \, \phi(r) \tag{8.31}$$

$$E = -\varepsilon_0 - t \sum_{n.n.} \mathrm{e}^{-\mathrm{i}k\rho_{n.n.}} \tag{8.32}$$

for cubic lattice (1-D)

$$E = -\varepsilon_0 - t(1 + 2\cos ka) \tag{8.33}$$

consider a lattice w/ 2-atom basis

$$\psi_k(r) = \alpha_k \psi_k^A(r) + \beta_k \psi_k^B(r) \tag{8.34}$$

$$H_{AB} = \left\langle \psi_k^A \middle| \hat{\mathbf{H}} \middle| \psi_k^B \right\rangle = \begin{pmatrix} AHA & AHB \\ BHA & BHB \end{pmatrix} = \begin{pmatrix} -\varepsilon_1 & \sum_{n.n.} \mathrm{e}^{-\mathrm{i}k\rho_{n.n.}} \\ \sum_{n.n.} \mathrm{e}^{\mathrm{i}k\rho_{n.n.}} & -\varepsilon_2 \end{pmatrix} \tag{8.35}$$

$$H_{AB} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E_k \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{8.36}$$

$$H = \begin{pmatrix} -\varepsilon_1 & t(1 + \mathrm{e}^{-\mathrm{i}ka}) \\ t(1 + \mathrm{e}^{\mathrm{i}ka}) & -\varepsilon_2 \end{pmatrix} \tag{8.37}$$

$$\det(H - E_k I) = 0 \tag{8.38}$$

$$E_k = \frac{1}{2}(\varepsilon_1 + \varepsilon_2) \pm \sqrt{\dots} \tag{8.39}$$

8.6 p-n Junctions

p-n jcn

– diode

– half-transistor

– solar cell

– LED

– laser

$$I = I_{CB} + I_{VB} \tag{8.40}$$

conduction band, valence band

$$I_{CB} = I_{nr} - I_{ng} \tag{8.41}$$

recomb, generation

$$I_{nr} \sim \mathrm{e}^{-e(\Delta\phi - V)\beta} \tag{8.42}$$

$$I_{ng} \sim \mathrm{e}^{-e\Delta\phi\beta} \tag{8.43}$$

$$ICB = Ing(\mathrm{e}^{eV\beta} - 1) \tag{8.44}$$

$$IVB = Ihr - Ihg \tag{8.45}$$

$$IVB = Ihg(\mathrm{e}^{eV\beta} - 1) \tag{8.46}$$

$$I = (Ing + Ihg)(\mathrm{e}^{eV\beta} - 1) \tag{8.47}$$

LED

Solar cell

Schottkey barrier

p-n-p jcn

9 Tight Binding

Start: Localized picture

$$\begin{aligned} \Psi_{\mathbf{k}} &= \frac{1}{\sqrt{N}} \sum_{j=1}^{N} C_{\mathbf{k},j} \phi(\mathbf{r} - \mathbf{r}_j) \\ &= \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_j}\, \phi(\mathbf{r} - \mathbf{r}_j) \quad \text{(Bloch Th.)} \end{aligned} \tag{9.1}$$

$$\begin{aligned} \varepsilon(\mathbf{k}) = \left\langle \Psi_{\mathbf{k}} \middle| \hat{\mathbf{H}} \middle| \Psi_{\mathbf{k}} \right\rangle &= \frac{1}{N} \left\langle \sum_{j=1}^{N} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_j}\, \phi(\mathbf{r} - \mathbf{r}_j) \middle| \hat{\mathbf{H}} \middle| \sum_{j=1}^{N} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_j}\, \phi(\mathbf{r} - \mathbf{r}_j) \right\rangle \\ &= \frac{1}{N} \sum_{j} \sum_{n} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_n)} \left\langle \phi(\mathbf{r} - \mathbf{r}_n) \middle| \hat{\mathbf{H}} \middle| \phi(\mathbf{r} - \mathbf{r}_j) \right\rangle \end{aligned} \tag{9.2}$$

Let

$$\boldsymbol{\rho}_m = \mathbf{r}_j - \mathbf{r}_n \quad \boldsymbol{\xi}_n = \mathbf{r} - \mathbf{r}_n \tag{9.3}$$

$$\begin{aligned} \varepsilon(\mathbf{k}) &= \frac{1}{N} \sum_{m} \sum_{n} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\rho}_m} \left\langle \phi(\boldsymbol{\xi}_n) \middle| \hat{\mathbf{H}} \middle| \phi(\boldsymbol{\xi}_n - \boldsymbol{\rho}_m) \right\rangle \\ &= \sum_{m} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\rho}_m} \left\langle \phi(\boldsymbol{\xi}) \middle| \hat{\mathbf{H}} \middle| \phi(\boldsymbol{\xi} - \boldsymbol{\rho}_m) \right\rangle \\ &\equiv \sum_{m} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\rho}_m}\, I(\rho_m) \end{aligned} \tag{9.4}$$

Overlap integral

$$I(\rho_m) = \left\langle \phi(\mathbf{r}) \,\middle|\, \hat{\mathbf{H}} \,\middle|\, \phi(\mathbf{r} - \boldsymbol{\rho}_m) \right\rangle \tag{9.5}$$

Now neglect all non-neighbor interaction.
when $\rho_m = \rho$(t: hopping amplitude.)

$$-t = I(\rho) = \left\langle \phi(\mathbf{r}) \,\middle|\, \hat{\mathbf{H}} \,\middle|\, \phi(\mathbf{r} - \boldsymbol{\rho}) \right\rangle \tag{9.6}$$

when $\rho_m = 0$

$$-\alpha = \left\langle \phi(\mathbf{r}) \,\middle|\, \hat{\mathbf{H}} \,\middle|\, \phi(\mathbf{r}) \right\rangle \tag{9.7}$$

thus

$$\varepsilon(\mathbf{k}) = -\alpha - t \sum_m \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\rho}_m} \tag{9.8}$$

9.0.1 1-D Crystal

$$\begin{aligned} \varepsilon(k) &= ... = -\alpha - 2t\cos ka \\ &= -\alpha - 2t\left(1 - \frac{k^2a^2}{2}\right) \\ &= -\alpha - 2t + tk^2a^2 \end{aligned} \tag{9.9}$$

let

$$m^* = \frac{\hbar^2}{2ta^2} \tag{9.10}$$

$$\varepsilon(k) = -\alpha - 2t + \frac{\hbar^2k^2}{2m^*} \tag{9.11}$$

10 Screening

$$D(k,\omega) = \varepsilon(k,\omega)E(k,\omega) \tag{10.1}$$

10.0.1 Static Screening

$\omega = 0$

$$E(r) = \sum_k \mathrm{e}^{\mathrm{i}k\cdot r}\, E(k) \tag{10.2}$$

$$\rho(r) = \sum_k \mathrm{e}^{\mathrm{i}k\cdot r}\, \rho(k) \tag{10.3}$$

$$D(r) = \sum_k \mathrm{e}^{\mathrm{i}k\cdot r}\, D(k) \tag{10.4}$$

$$\boldsymbol{\nabla}\cdot E = \boldsymbol{\nabla}\cdot\left(\sum_k \mathrm{e}^{\mathrm{i}k\cdot r}\, E(k)\right) = 4\pi \sum_k \mathrm{e}^{\mathrm{i}k\cdot r}\, \rho(k) \tag{10.5}$$

$$\nabla \cdot D = \nabla \cdot \left(\sum_k \mathrm{e}^{\mathrm{i}k \cdot r} \, \varepsilon(k) E(k) \right) = 4\pi \sum_k \mathrm{e}^{\mathrm{i}k \cdot r} \, \rho_{ext}(k) \tag{10.6}$$

$\therefore$

$$\varepsilon(k) = \frac{\rho_{ext}(k)}{\rho(k)} = 1 - \frac{\rho_{ind}(k)}{\rho(k)} \tag{10.7}$$

In terms of potential, ...

10.0.2 Calculating ρ_{ind} Using Thomas-Fermi Theory of Screening

$$-\frac{\hbar^2}{2\mathrm{m}} \frac{\mathrm{d}^2}{\mathrm{dx}^2} \, \psi_i(r) = E_i \psi_i(r) \tag{10.8}$$

$$V = -e\phi(r) \tag{10.9}$$

$\phi(r)$ varies slowly enough that

$$E_i = \frac{\hbar^2 k^2}{2m} - e\phi(r) \tag{10.10}$$

10.1 Graphene Tight-binding

General tight-binding for 2 atom-basis

$$\psi_k = a_k \psi_k^{(A)}(r) + b_k \psi_k^{(B)}(r) \tag{10.11}$$

$$\psi_k^{(B)}(r) = \sum_j c_j \phi^{(B)}(r - r_j) \tag{10.12}$$