Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.4.28 Lecture 04

10:25 – 11:55

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Review of lecture in the last week

Envelope function (effective mass approximation)

Chapter 3 Carrier statistics and chemical doping

Density of states

Definition and properties of valence band hole states

Carrier distribution in intrinsic semiconductors

Shallow hydrogen-like impurity states

Shallow impurity states in Si

Contents today

Doping and carrier distribution

Temperature dependence of carrier concentration

Exciton

Chapter 4 Optical properties (bulk)

Quantization of electromagnetic field

Number state, coherent state

Optical response of two-level system

Optical absorption with inter-band transition

Doping and carrier distribution

Uniform donor concentration N_D

n: excited electrons,
n_D: captured electrons

$$n + n_D = N_D$$

Entropy $S = k_B \ln W$

Helmholtz free energy

$$F = U - TS = E_D n_D - k_B T \ln \left[2^{n_D} \frac{N_D!}{n_D!(N_D - n_D)!} \right]$$

Starling approximation

$\ln N! \sim N \ln N - N$

$$\mu = E_F = \frac{\partial F}{\partial n_D} = E_D - k_B T \ln \left[\frac{2(N_D - n_D)}{n_D} \right]$$

Donor level

$$n_D = N_D \left[1 + \frac{1}{2} \exp\left(\frac{E_D - E_F}{k_B T} \right) \right]^{-1}$$

For acceptors

$$n_A = N_A \left[1 + 2 \exp\left(\frac{E_A - E_F}{k_B T} \right) \right]^{-1}$$

note: the formula is symmetric if we introduce captured hole concentration $p_A = N_A - n_A$

Doping and carrier distribution

E_F is given from n or p as
$$\begin{cases} E_\mathrm{F} \approx E_C + k_\mathrm{B}T\left[\ln\left(\frac{n}{N_C}\right) + 2^{-3/2}\left(\frac{n}{N_C}\right)\right], \\ E_\mathrm{F} \approx E_V - k_\mathrm{B}T\left[\ln\left(\frac{p}{N_V}\right) + 2^{-3/2}\left(\frac{p}{N_V}\right)\right] \end{cases}$$

In the case of n-type semiconductor with compensation $n + N_A = N_\mathrm{D} - n_\mathrm{D}$

$$\frac{n + N_\mathrm{A}}{N_\mathrm{D} - N_\mathrm{A} - n} = \frac{1}{2}\exp\left(\frac{E_\mathrm{D} - E_\mathrm{F}}{k_\mathrm{F}T}\right)$$

$$\frac{n(n + N_\mathrm{A})}{N_\mathrm{D} - N_\mathrm{A} - n} = \frac{1}{2}N_c\exp\left(-\frac{\Delta E_\mathrm{D}}{k_\mathrm{B}T}\right), \quad \Delta E_\mathrm{D} \equiv E_c - E_\mathrm{D}$$

Temperature dependence of carrier concentration

(I) Impurity regime I: Temperature is very low.

$$n \ll N_\mathrm{A} \ll N_\mathrm{D}$$

$$n \approx \frac{N_\mathrm{D} N_c}{2N_\mathrm{A}} \exp\left(-\frac{\Delta E_\mathrm{D}}{k_\mathrm{B} T}\right)$$

(II) Impurity regime II:

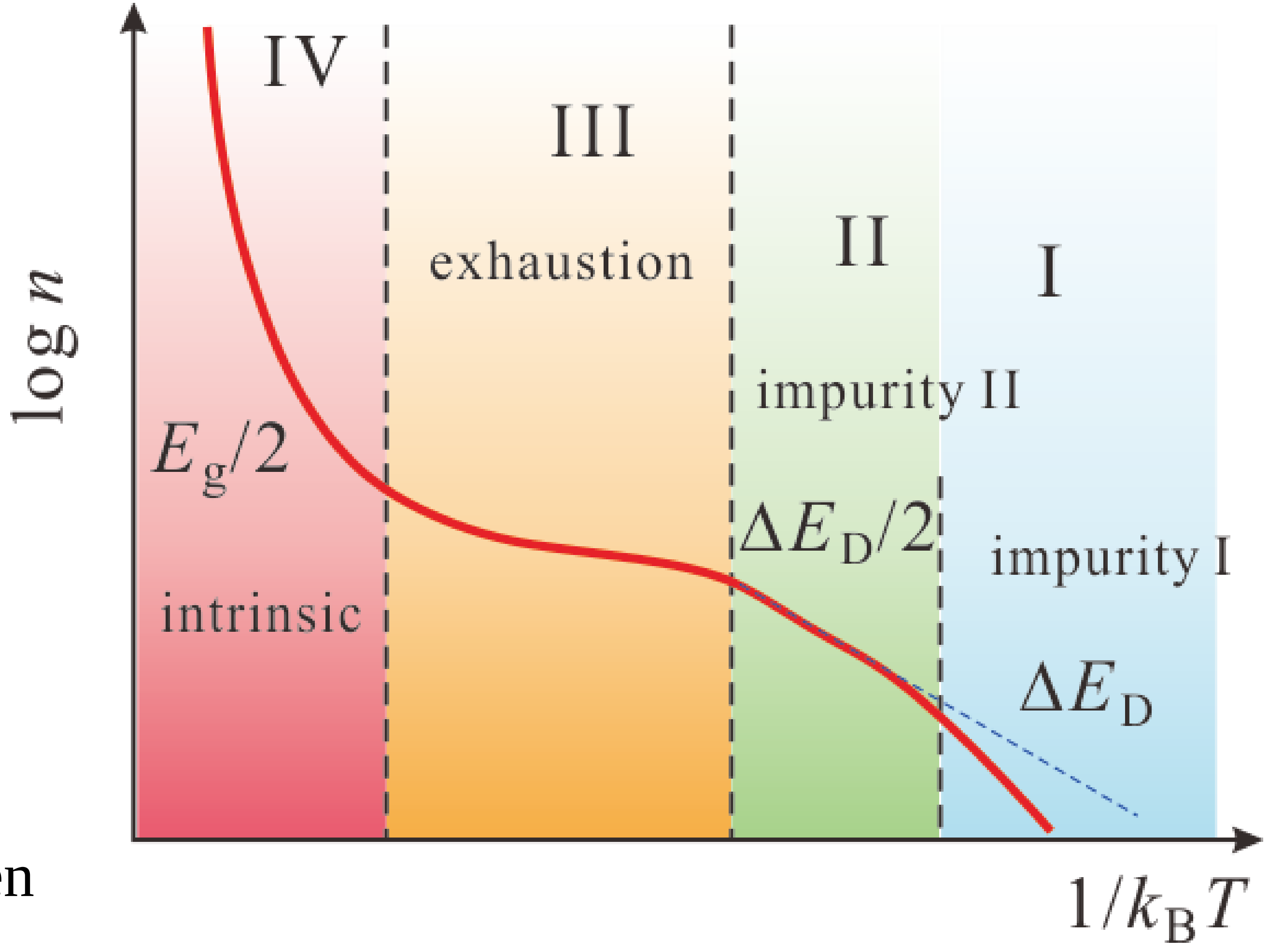
T is a bit higher. $N_\mathrm{A} \ll n \ll N_\mathrm{D}$

$$n \approx \left(\frac{N_c N_\mathrm{D}}{2}\right)^{1/2} \exp\left(-\frac{\Delta E_\mathrm{D}}{2k_\mathrm{B} T}\right)$$

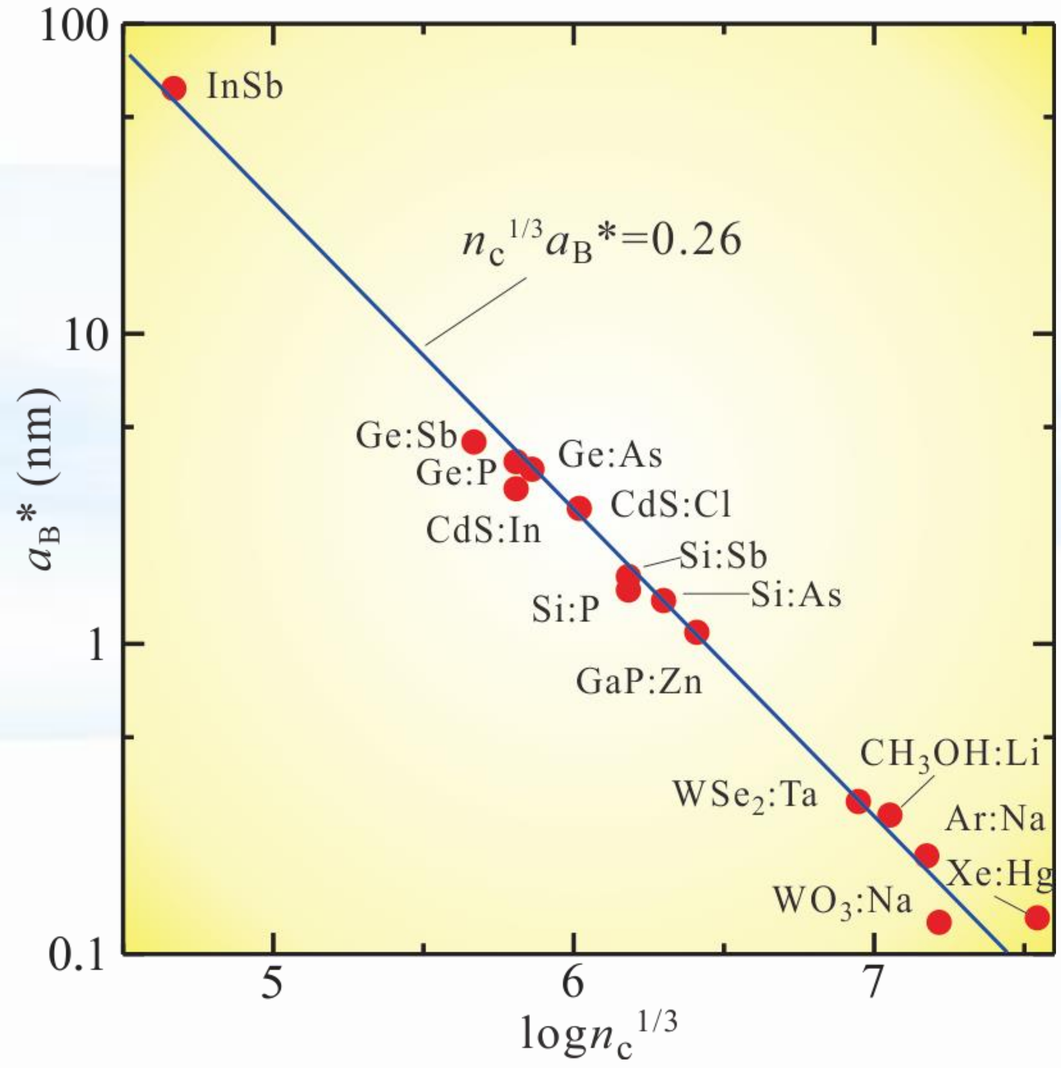
(III) Exhaustion regime:

$k_\mathrm{B} T > \Delta E_\mathrm{D}$ $\quad n \approx N_\mathrm{D} - N_\mathrm{A}$

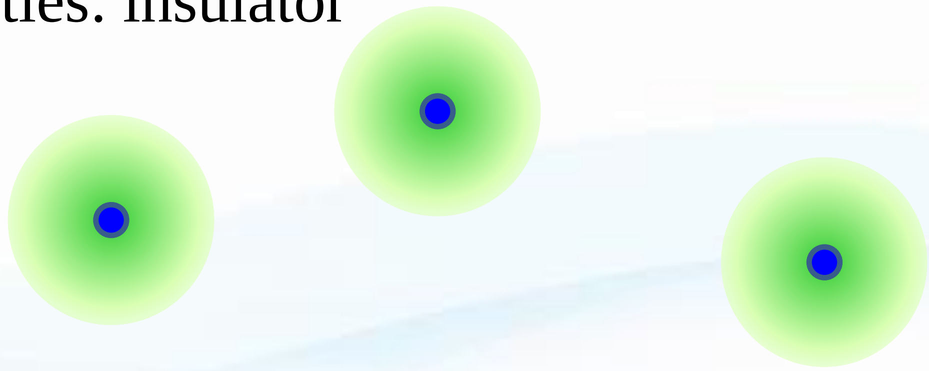
(IV) Intrinsic regime: direct excitation between the v.b. and the c.b. is not negligible.



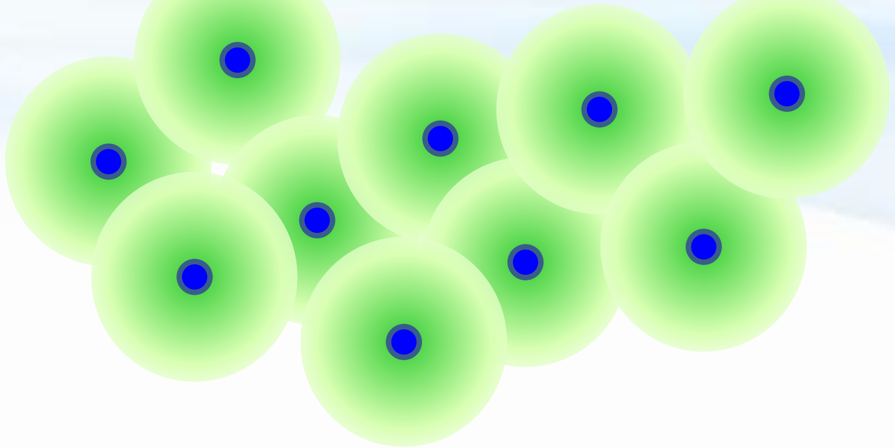
Degenerate semiconductors



sparse impurities: insulator



dense impurities: metal

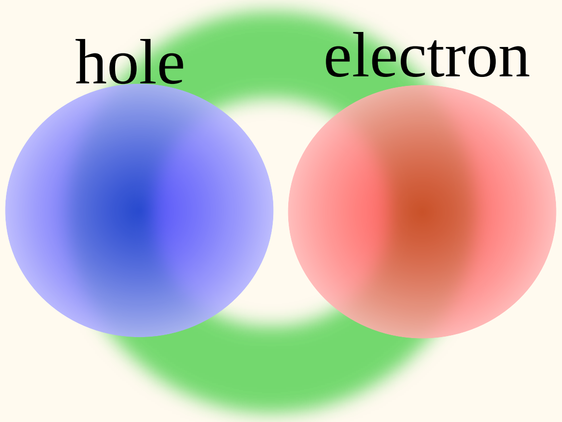


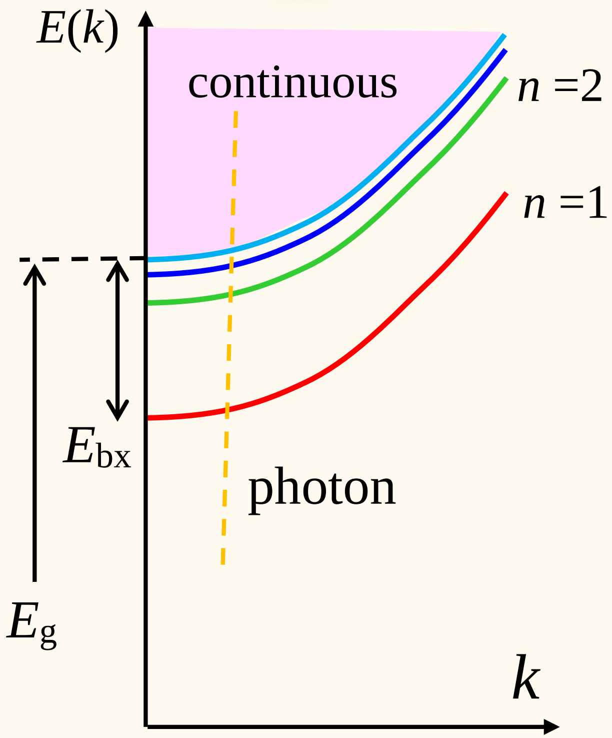
Empirical metal-insulator criterion

$$n_c^{1/3} a_{\mathrm{B}}^* = 0.26$$

Excitons (Wannier type)

Free excitons





Binding energy $$E_{bx} = -\frac{m_r^* e^4}{8h^2(\epsilon_0\epsilon)^2}\frac{1}{n^2}$$

Reduced mass $$\frac{1}{m_r^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

Exciton kinetic energy $$E_{kx} = \frac{\hbar^2 k^2}{2(m_e + m_h)}$$

Energy for exciton creation $$E_{ex} = E_g + \frac{\hbar^2 k^2}{2(m_e + m_h)} - \frac{m_r^* e^4}{8h^2(\epsilon_0\epsilon)^2}\frac{1}{n^2}$$

Excitonic complexes

(+) : donor + : hole – : electron

(+)	+	–		H_2^+	Excitonic ions
(+)	–	–		H^-	
+	+	–		H_2^+	
+	+	–	–	H_2	Excitonic molecule (bi-exciton, trion)
(+)	+	–	–	H_2	

Chapter 4 Optical properties (bulk)

Luminescence from CdTe quantum dots (Sigma-Aldrich)

Quantization of electromagnetic field

1-d harmonic oscillator $\frac{\hbar\omega}{2}\left(-\frac{d^2}{dq^2}+q^2\right)\phi = E\phi \rightarrow \hbar\omega\left(a^\dagger a+\frac{1}{2}\right)\phi = E\phi$

up/down operators $a = \frac{1}{\sqrt{2}}\left(\frac{d}{dq}+q\right), \quad a^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{d}{dq}+q\right), \quad [a, a^\dagger] = 1$

Eigenenergy $E_n = \hbar\omega\left(n+\frac{1}{2}\right) \; (n = 0, 1, 2, \cdots)$ $\frac{\hbar\omega}{2}$: Zero-point energy

Starting point: Electro-magnetic field is a set of harmonic oscillators (Jeans theorem)

$$E = \int\left(\epsilon_0 \boldsymbol{E}^2 + \frac{\boldsymbol{H}^2}{\mu_0}\right)\frac{d\boldsymbol{r}}{4} \rightarrow \boldsymbol{A}_{\boldsymbol{k}\lambda} = \frac{\boldsymbol{e}_{\boldsymbol{k}\lambda}}{\sqrt{4\epsilon_0 V\omega_{\boldsymbol{k}}^2}}(iP_{\boldsymbol{k}\lambda}+\omega_{\boldsymbol{k}}Q_{\boldsymbol{k}\lambda}), \quad E = \frac{1}{2}\sum_{\boldsymbol{k}\lambda}(P_{\boldsymbol{k}\lambda}^2+\omega_{\boldsymbol{k}}^2 Q_{\boldsymbol{k}\lambda}^2)$$

Quantization: $\rightarrow \hat{H} = \frac{1}{2}\sum_{\boldsymbol{k}\lambda}(\hat{P}_{\boldsymbol{k}\lambda}^2+\omega_{\boldsymbol{k}}^2\hat{Q}_{\boldsymbol{k}\lambda}^2), \quad [\hat{Q}_{\boldsymbol{k}'\lambda'}, \hat{P}_{\boldsymbol{k}\lambda}] = i\hbar\delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\delta\delta'}$

Creation/annihilation operators

$$a_{\boldsymbol{k}\lambda}^\dagger = \frac{1}{\sqrt{2\hbar\omega_{\boldsymbol{k}}}}(\omega_{\boldsymbol{k}}\hat{Q}_{\boldsymbol{k}\lambda}-i\hat{P}_{\boldsymbol{k}\lambda}), \quad a_{\boldsymbol{k}\lambda} = \frac{1}{\sqrt{2\hbar\omega_{\boldsymbol{k}}}}(\omega_{\boldsymbol{k}}\hat{Q}_{\boldsymbol{k}\lambda}+i\hat{P}_{\boldsymbol{k}\lambda})$$

$$[a_{\boldsymbol{k}\lambda}, a_{\boldsymbol{k}'\lambda'}^\dagger] = \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\lambda\lambda'}, \quad (\text{others}) = 0$$

Quantization of electromagnetic field (2)

$$\hat{H} = \sum_{\boldsymbol{k}\lambda} \hbar\omega_{\boldsymbol{k}} \left(a^\dagger_{\boldsymbol{k}\lambda} a_{\boldsymbol{k}\lambda} + \frac{1}{2} \right)$$

$$\hat{\boldsymbol{A}}(\boldsymbol{r}, t) = \sum_{\boldsymbol{k}\lambda} \sqrt{\frac{\hbar}{2\epsilon_0 \omega_{\boldsymbol{k}} V}} \boldsymbol{e}_{\boldsymbol{k}\lambda} \left[a_{\boldsymbol{k}\lambda} e^{i(\boldsymbol{k}\boldsymbol{r} - \omega_{\boldsymbol{k}} t)} + a^\dagger_{\boldsymbol{k}\lambda} e^{-i(\boldsymbol{k}\boldsymbol{r} - \omega_{\boldsymbol{k}} t)} \right]$$

$$|\{n_{\boldsymbol{k}\lambda}\}\rangle = \left[\prod_{\boldsymbol{k}\lambda} \frac{(a^\dagger_{\boldsymbol{k}\lambda})^{n_{\boldsymbol{k}\lambda}}}{\sqrt{n_{\boldsymbol{k}\lambda}!}} \right] |0\rangle$$

$$\langle \{n_{\boldsymbol{k}\lambda}\} | \hat{H} | \{n_{\boldsymbol{k}\lambda}\} \rangle = \sum_{\boldsymbol{k}\lambda} \hbar\omega_{\boldsymbol{k}} \left(n_{\boldsymbol{k}\lambda} + \frac{1}{2} \right)$$

$$|v\rangle = \exp(-|v|^2/2) \exp(v a^\dagger) |0\rangle = \exp(-|v|^2/2) \sum_{n=0}^{\infty} \frac{v^n}{\sqrt{n!}} |n\rangle$$

Properties of number state, coherent state

Number state

Expectation value of electromagnetic field is zero

$$\langle\{n_{\boldsymbol{k}\lambda}\}|\hat{\boldsymbol{E}}|\{n_{\boldsymbol{k}\lambda}\}\rangle = -\langle\{n_{\boldsymbol{k}\lambda}\}|(\partial\hat{\mathbf{A}}/\partial t)|\{n_{\boldsymbol{k}\lambda}\}\rangle = 0$$

Quantum fluctuation is non-zero even for |0⟩

$$\langle\{n_{\boldsymbol{k}\lambda}\}|\hat{\boldsymbol{E}}^2|\{n_{\boldsymbol{k}\lambda}\}\rangle = \sum_{\boldsymbol{k}\lambda}\frac{\hbar\omega_{\boldsymbol{k}}}{\epsilon_0 V}\left(n_{\boldsymbol{k}\lambda}+\frac{1}{2}\right) = \frac{1}{\epsilon_0 V}\langle\{n_{\boldsymbol{k}\lambda}\}|H|\{n_{\boldsymbol{k}\lambda}\}\rangle$$

Coherent state

$$|\alpha\rangle = \exp\left(-\frac{|\alpha|^2}{2}\right)\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

Probability of *n*-photons $P(n) = \dfrac{e^{-|\alpha|^2}|\alpha|^{2n}}{n!}$ Poisson distribution

If we write $\alpha = |\alpha|e^{i\phi}$

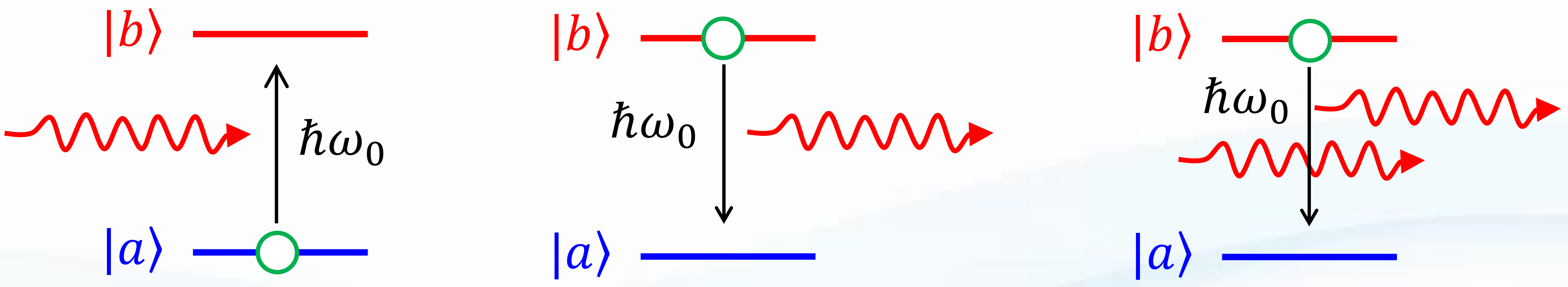
$$\langle\alpha|\hat{\boldsymbol{E}}(\boldsymbol{r},t)|\alpha\rangle = -\sqrt{\frac{2\hbar\omega_{\boldsymbol{k}}}{\epsilon_0 V}}|\alpha|\boldsymbol{e}_{\boldsymbol{k}\lambda}\sin(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t+\phi)$$

$$\langle\alpha|\hat{\boldsymbol{B}}(\boldsymbol{r},t)|\alpha\rangle = -\sqrt{\frac{2\hbar}{\epsilon_0\omega_{\boldsymbol{k}}V}}|\alpha|\boldsymbol{k}\times\boldsymbol{e}_{\boldsymbol{k}\lambda}\sin(\boldsymbol{k}\cdot\boldsymbol{r}-\omega_{\boldsymbol{k}}t+\phi)$$

Expectation value: classical electromagnetic field

Optical response of two-level system

Three fundamental processes



(a) absorption (b) spontaneous emission (c) stimulated emission

$$\mathscr{H}_0|a\rangle = E_a|a\rangle, \quad \mathscr{H}_0|b\rangle = E_b|b\rangle$$

$$\psi(t) = c_a(t)e^{-E_a t/\hbar}|a\rangle + c_b(t)e^{-E_b t/\hbar}|b\rangle$$

Hamiltonian with electromagnetic field $\mathscr{H}_{\text{op}} = \dfrac{(\boldsymbol{p}+e\boldsymbol{A})^2}{2m} + V(\boldsymbol{r}) \approx \mathscr{H}_0 + \dfrac{e}{m}\boldsymbol{A}\cdot\boldsymbol{p}$

Light absorption process $\boldsymbol{A} = A_0\vec{e}\cos(\boldsymbol{k}_{\text{p}}\cdot\boldsymbol{r} - \omega t)$

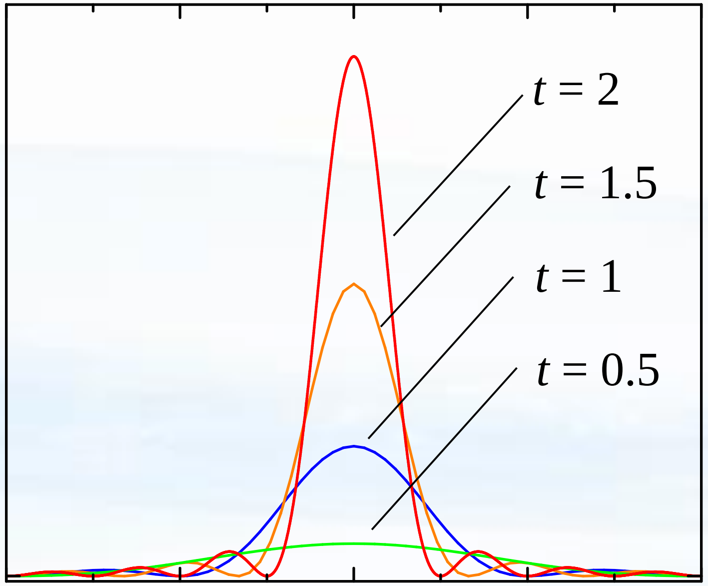
Perturbation part in $\mathscr{H}_{\text{op}}$ $\mathscr{H}' = \dfrac{eA_0}{m}\vec{e}\cdot\hat{\boldsymbol{p}}\cos(\boldsymbol{k}_{\text{p}}\cdot\boldsymbol{r} - \omega t)$

assumption

$$\langle a|\mathscr{H}'|a\rangle = \langle b|\mathscr{H}'|b\rangle = 0$$

Optical response of two-level system (2)

Schrödinger equation: $$i\hbar\left[\frac{dc_a}{dt}|a\rangle e^{-iE_at/\hbar}+\frac{dc_b}{dt}|b\rangle e^{-iE_bt/\hbar}\right]=c_a\mathscr{H}'|a\rangle e^{-iE_at/\hbar}+c_b\mathscr{H}'|b\rangle e^{-iE_bt/\hbar}$$



$$\begin{cases}\dfrac{dc_a}{dt}=-\dfrac{i}{\hbar}c_b\langle a|\mathscr{H}'|b\rangle e^{-i\omega_0t},\\ \dfrac{dc_b}{dt}=-\dfrac{i}{\hbar}c_a\langle b|\mathscr{H}'|a\rangle e^{i\omega_0t}.\end{cases}\qquad \omega_0\equiv\frac{E_b-E_a}{\hbar}$$

$$c_a^{(1)}(t)=1,\quad c_b^{(1)}(t)=-\frac{i}{\hbar}\int_0^t\langle b|\mathscr{H}'|a\rangle(t')e^{i\omega_0t'}dt'(=c_b^{(2)}(t))$$

$$c_a^{(2)}(t)=1-\frac{1}{\hbar^2}\int_0^t dt'\langle a|\mathscr{H}'|b\rangle(t')e^{-i\omega_0t'}\left[\int_0^{t'}dt''\langle b|\mathscr{H}'|a\rangle(t'')e^{i\omega_0t''}\right]$$

$$\mathscr{H}'=\frac{eA_0}{m}\vec{e}\cdot\hat{\boldsymbol{p}}\cos(\boldsymbol{k}_{\rm p}\cdot\boldsymbol{r}-\omega t)$$

Ignore $\boldsymbol{k}_{\rm p}$

$$V_{ba}\equiv\langle b|\frac{eA_0}{m}\vec{e}\cdot\hat{\boldsymbol{p}}|a\rangle$$

$$c_b(t)\simeq-\frac{i}{\hbar}V_{ba}\int_0^t dt'\cos\omega t'e^{i\omega_0t'}=-\frac{V_{ba}}{2\hbar}\left[\frac{e^{i(\omega_0+\omega)t}-1}{\omega_0+\omega}+\frac{e^{i(\omega_0-\omega)t}-1}{\omega_0-\omega}\right]$$

$$\simeq-i\frac{V_{ba}}{\hbar}\frac{\sin[(\omega_0-\omega)t/2]}{\omega_0-\omega}e^{i(\omega_0-\omega)t/2}$$

$$P_b(t)=|c_b(t)|^2\simeq\frac{|V_{ba}|^2}{\hbar^2}\frac{\sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2}$$

Energy conservation

Rabi oscillation

Rotating wave approximation (drop $e^{-i\omega t}$)

$$\langle a|\mathscr{H}'|b\rangle = \frac{V_{ab}}{2} e^{i\omega t}$$

$$\begin{cases} \dfrac{dc_a}{dt} = -\dfrac{i}{2\hbar} c_b V_{ab} e^{-i(\omega_0 - \omega)t}, \\ \dfrac{dc_b}{dt} = -\dfrac{i}{2\hbar} c_a V_{ba} e^{i(\omega_0 - \omega)t}. \end{cases}$$

$$\frac{d^2 c_b}{dt^2} + i(\omega - \omega_0)\frac{dc_a}{dt} + \frac{|V_{ab}|^2}{(2\hbar)^2} = 0$$

solution $c_b(t) = c_+ e^{i\lambda_+ t} + c_- e^{\lambda_- t}$ $\quad \lambda_\pm \equiv \frac{1}{2}(\delta \pm \sqrt{\delta^2 + |V_{ab}|^2/\hbar^2}), \quad \delta \equiv \omega_0 - \omega$

initial condition $|c_a(0)| = 1,\ c_b(0) = 0$

Rabi oscillation

$$\begin{cases} c_b(t) = \dfrac{i|V_{ab}|}{\omega_R \hbar} e^{i\delta t/2} \sin(\omega_R t/2), \\ c_a(t) = e^{i\delta t/2}\left[\cos\left(\dfrac{\omega_R t}{2}\right) - i\dfrac{\delta}{\omega_R}\sin\left(\dfrac{\omega_R t}{2}\right)\right] \end{cases}$$

Rabi frequency $\omega_R \equiv \sqrt{\delta^2 + |V_{ab}|^2/\hbar^2}$

Oscillator strength and selection rule

Oscillation strength for $|0\rangle \to |\Phi_{\rm ex}\rangle$

$$\frac{|V_{ba}|^2}{\hbar^2} = \left(\frac{eA_0}{m\hbar}\right)^2 |\langle \Phi_{\rm ex}|\vec{e}\cdot\hat{p}\,|0\rangle|^2 \equiv \left(\frac{eA_0}{m\hbar}\right)^2 P_{\rm p}$$

Application to an electron-hole localized system (with main, angular momentum quantum number)

(wavefunction)=(lattice periodic)×(envelope) $\Phi_{\rm e}(\boldsymbol{r}_{\rm e}) = u_{\rm c} f_{\rm e}(\boldsymbol{r}_{\rm e}), \quad \Phi_{\rm h}(\boldsymbol{r}_{\rm h}) = u_{\rm v} f_{\rm h}(\boldsymbol{r}_{\rm h})$

Envelope functions varies slowly
→ the momentum can be ignored

$$P_{\rm p} = |\langle \Phi_{\rm e}|\vec{e}\cdot\hat{p}\,|\Phi_{\rm h}\rangle|^2 = |\langle u_{\rm c}|\vec{e}\cdot\hat{p}\,|u_{\rm v}\rangle|^2 |\langle f_{\rm e}|f_{\rm h}\rangle|^2$$
$$= |\langle u_{\rm c}|\vec{e}\cdot\hat{p}\,|u_{\rm v}\rangle|^2 \underline{\delta_{n_{\rm e},n_{\rm h}}\delta_{L_{\rm e},L_{\rm h}}}$$

Selection rule

$n_{\rm e} = n_{\rm h},\ L_{\rm e} = L_{\rm h}$

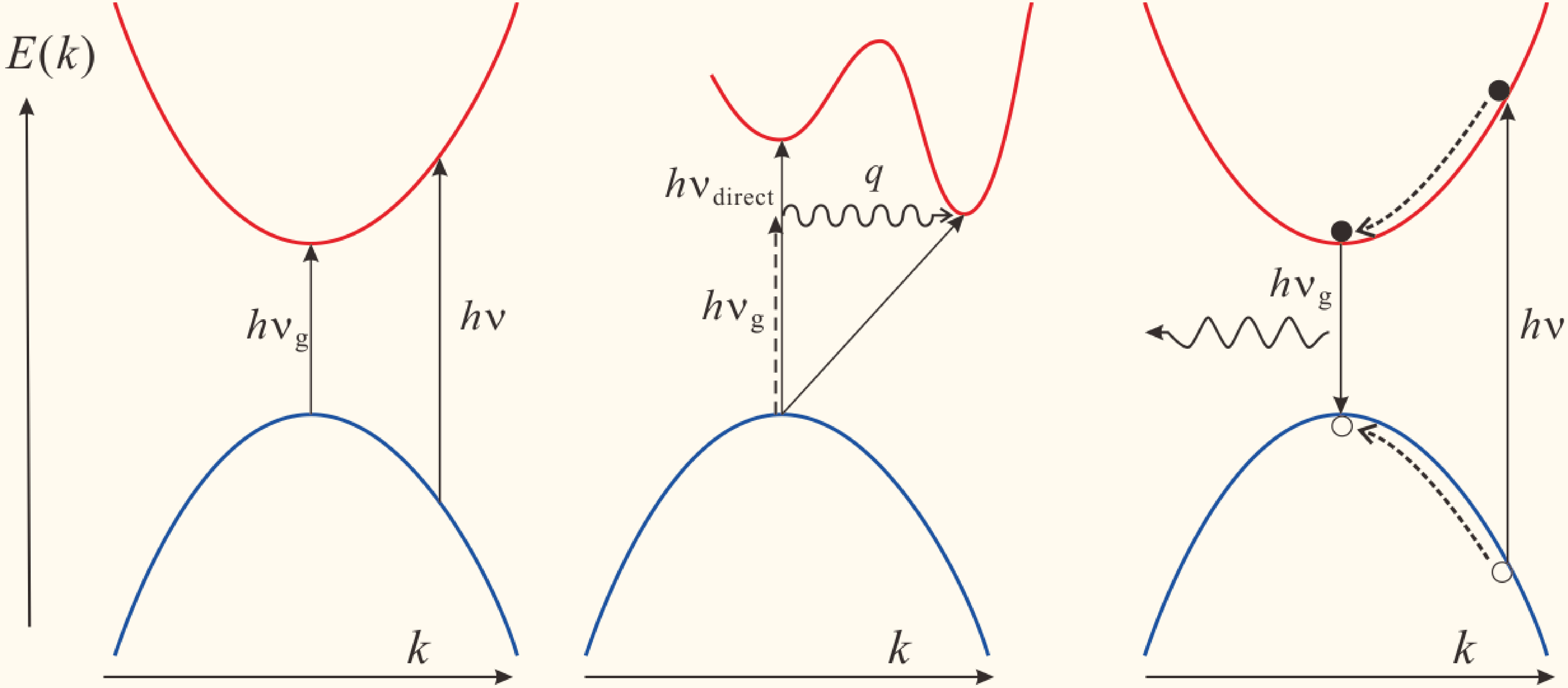
Oscillation strength
(absorption, stimulated emission)

$$\left(\frac{eA_0}{m\hbar}\right)^2 |\langle u_{\rm c}|\vec{e}\cdot\hat{p}\,|u_{\rm v}\rangle|^2 \delta_{n_{\rm e},n_{\rm h}}\delta_{L_{\rm e},L_{\rm h}} \frac{\sin^2[(\omega_{\rm g}-\omega)t/2]}{(\omega_{\rm g}-\omega)^2}$$

For spontaneous emission
(photon number part → 1/2)

$$\frac{e^2}{2m^2\epsilon_0\hbar\omega} |\langle u_{\rm c}|\vec{e}\cdot\hat{p}\,|u_{\rm v}\rangle|^2 \delta_{n_{\rm e},n_{\rm h}}\delta_{L_{\rm e},L_{\rm h}} \frac{\sin^2[(\omega_{\rm g}-\omega)t/2]}{(\omega_{\rm g}-\omega)^2}$$

Application to extended states



(a) direct absorption (b) indirect absorption (c) photoluminescence

Optical absorption with transition from valence to conduction

Plane wave vector potential $\boldsymbol{A} = A_0 \boldsymbol{e} \cos(\boldsymbol{k}_p \cdot \boldsymbol{r} - \omega t)$ $\quad \boldsymbol{k}_{\rm p} = (0, 0, k_{\rm p}),\ \boldsymbol{e} = (1, 0, 0)$

$$\boldsymbol{E} = -\frac{\partial \boldsymbol{A}}{\partial t}, \quad \boldsymbol{H} = \frac{\mathrm{rot}\,\boldsymbol{A}}{\mu}$$

Poyinting vector $\boldsymbol{I} = \langle \boldsymbol{E} \times \boldsymbol{H} \rangle = \dfrac{\epsilon_0 c \bar{n} \omega^2 A_0^2}{2} \boldsymbol{e}_z$ $\quad \bar{n} = c/c' = \sqrt{\epsilon_1 \mu_1}$

$I(z) = I_0 \exp(-\alpha z)$ Definition of absorption coefficient α

W: number of photons absorbed per unit time

$$\alpha = \frac{\hbar \omega W}{I} = \frac{2\hbar\omega W}{\epsilon_0 c \bar{n} \omega^2 A_0^2}$$

perturbation

$$\mathscr{H}' = \frac{e A_0}{m_0} \boldsymbol{e} \cdot \boldsymbol{p}$$

Conduction electron $|c\boldsymbol{k}\rangle$, valence hole $|v\boldsymbol{k}'\rangle$
Transition probability is

$$W_{\rm vc} = \frac{2\pi e A_0^2}{\hbar m_0} |\langle c\boldsymbol{k}|\boldsymbol{e} \cdot \boldsymbol{p}|v\boldsymbol{k}'\rangle|^2 \delta(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}') - \hbar\omega)$$
$$= \frac{\pi e^2 A_0^2}{2\hbar m_0^2} |M|^2 \delta(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}') - \hbar\omega)$$

Optical absorption with transition from valence to conduction (2)

Bloch electrons

$$|c\boldsymbol{k}\rangle = u_{c\boldsymbol{k}} e^{i\boldsymbol{kr}}, \quad |v\boldsymbol{k}\rangle = u_{v\boldsymbol{k}} e^{i\boldsymbol{kr}}$$

$$M = \int_V \frac{d^3r}{V} e^{i(\boldsymbol{k}_p+\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} u^*_{c\boldsymbol{k}}(\boldsymbol{r})\boldsymbol{e}\cdot(\boldsymbol{p}+\hbar\boldsymbol{k}')u_{v\boldsymbol{k}'}(\boldsymbol{r})$$

$$= \frac{\sum_l e^{i(\boldsymbol{k}_p+\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{R}_l}}{V} \int_\Omega d^3r u^*_{c\boldsymbol{k}}(\boldsymbol{r})\boldsymbol{e}\cdot(\boldsymbol{p}+\hbar\boldsymbol{k}')u_{v\boldsymbol{k}'}(\boldsymbol{r})$$

$$= \frac{N}{V}\delta_{\boldsymbol{k}_p+\boldsymbol{k}'-\boldsymbol{k},\boldsymbol{K}} \int_\Omega d^3r u^*_{c\boldsymbol{k}}(\boldsymbol{r})\boldsymbol{e}\cdot(\boldsymbol{p}+\hbar\boldsymbol{k}')u_{v\boldsymbol{k}'}(\boldsymbol{r})$$

$$M = \int_\Omega \frac{d^3r}{\Omega} u^*_{c\boldsymbol{k}}(\boldsymbol{r})\boldsymbol{e}\cdot\boldsymbol{p}u_{v\boldsymbol{k}}(\boldsymbol{r})$$

Absorption coefficient
for direct absorption

$$\alpha_{\mathrm{da}} = \frac{\pi e^2}{\bar{n}\epsilon_0\omega c m_0^2}|M|^2 \underline{\sum_{\boldsymbol{k}} \delta(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}) - \hbar\omega)}$$

joint density of states $\equiv J_{cv}(\hbar\omega)$

$$E_{cv}(\boldsymbol{k}) \equiv E_c(\boldsymbol{k}) - E_v(\boldsymbol{k})$$

Γ point $\quad E_{cv}(\vec{0}) = E_{\mathrm{g}}(\Gamma)$

$$J_{cv}(\hbar\omega) = \sum_{\boldsymbol{k}} \delta(E_{cv}(\boldsymbol{k}) - \hbar\omega) = 2\int \frac{d^3k}{(2\pi)^3}\delta(E_{cv}(\boldsymbol{k}) - \hbar\omega)$$

Optical absorption with transition from valence to conduction (3)

$$d^3k = dS dk_\perp = dS \frac{dk_\perp}{dE_{cv}} dE_{cv} = dS |\boldsymbol{\nabla}_{\boldsymbol{k}} E_{cv}|^{-1} dE_{cv}$$

$$\therefore\ J_{cv}(\hbar\omega) = \frac{2}{(2\pi)^3} \int \frac{dS}{|\boldsymbol{\nabla}_{\boldsymbol{k}} E_{cv}(\boldsymbol{k})|_{E_{cv}=\hbar\omega}}$$

Minimum at $\boldsymbol{k}_0$

$$E_{cv}(\boldsymbol{k}_0) = E_{\mathrm{g}}, \quad \boldsymbol{\nabla}_{\boldsymbol{k}} E_{cv} = \boldsymbol{0}$$

$$E_{cv}(\boldsymbol{k}) = E_{\mathrm{g}} + \sum_i \frac{\hbar^2}{2\xi_i}(k_i - k_{i0})^2, \quad \xi_i > 0 (i = 1, 2, 3) \text{ for simplicity.}$$

Change of variables

$$(\hbar/(2\xi_i)^{1/2})(k_i - k_{i0}) = s_i$$

$$E_{cv} = E_{\mathrm{g}} + \sum_i s_i^2 \equiv E_{\mathrm{g}} + s^2, \quad d^3k = \frac{\sqrt{8\xi_1\xi_2\xi_3}}{\hbar^3} ds_1 ds_2 ds_3$$

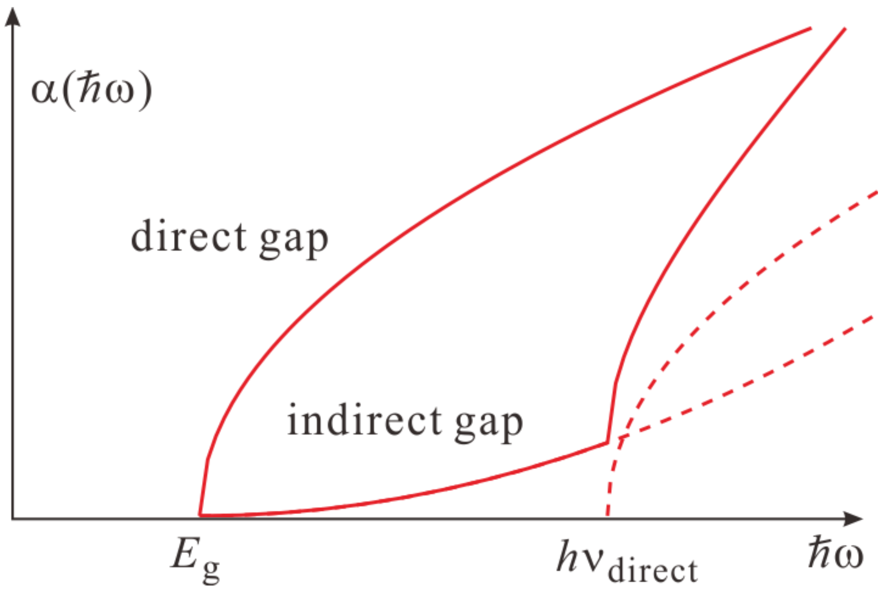
$$|\boldsymbol{\nabla}_{\boldsymbol{s}} E_{cv}| = 2s$$

$$J_{cv} = \frac{2}{(2\pi)^3} \frac{\sqrt{8\xi_1\xi_2\xi_3}}{\hbar^3} \int \frac{dS}{2s} = \frac{1}{2\pi^2} \frac{\sqrt{8\xi_1\xi_2\xi_3}}{\hbar^3} \sqrt{\hbar\omega - E_{\mathrm{g}}}$$

$$\frac{1}{m_r} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

$$= \frac{\sqrt{2}}{\pi^2} \frac{m_r^{3/2}}{\hbar^3} \sqrt{\hbar\omega - E_{\mathrm{g}}}$$

Optical absorption with transition from valence to conduction (4)



Absorption coefficient $\alpha(\hbar\omega) = \frac{e^2(2m_r)^{3/2}|M|^2}{2\pi\epsilon_0 m_0^2 \bar{n}\omega c\hbar^3}\sqrt{\hbar\omega - E_g}$

Oscillator strength $f_{vc} = \frac{2|M|^2}{m_0\hbar\omega}$

Indirect gap semiconductors $\alpha_{id}(\hbar\omega) \propto (\hbar\omega - E_g)^2$

Example GaAs