

4.2.2 Luminescence with interband transition

There are numerous types of semiconductor light emission. A typical example is light emission due to the recombination (pair annihilation) of electron-hole pairs. Minority carriers excited by various methods, including the above light absorption, emit their energy as photons by **radiative recombination** with the majority carriers. When the electron-hole pair does not emit a photon and the energy is dissipated to other freedoms, the process is called **non-radiative recombination**. Such emission of photons by radiative recombination is called **luminescence**. Among them the ones with comparatively short lifetime are called **fluorescence** while those with very long lifetime is called **phosphorescence**. Luminescence is also classified with the origin of the electron-hole pair creation. The photon-absorption originated emission is called **photoluminescence**, the electrically stimulated emission (electric field activation of recombination center, injection of minority carriers, etc.) is called **electroluminescence**. By some reason minority carriers are trapped in impurities and some heat pulses cause release of them and lead to luminescence, which phenomenon is called **thermoluminescence**^{*1}.

As we saw in the previous section, there are two kinds of photon-emission, **stimulated emission** and **spontaneous emission**. In the former the emission probability is proportional to the photon density in the surrounding space while in the latter the probability is independent of that. If we include the zero-point fluctuation into the photon density, there is no difference in these two. In practice, however because the former is significant under limited conditions, causing peculiar phenomena like laser light emission etc., we usually discuss these separately. As this indicates, the density of photons is a very important factor in the treatment of light emission.

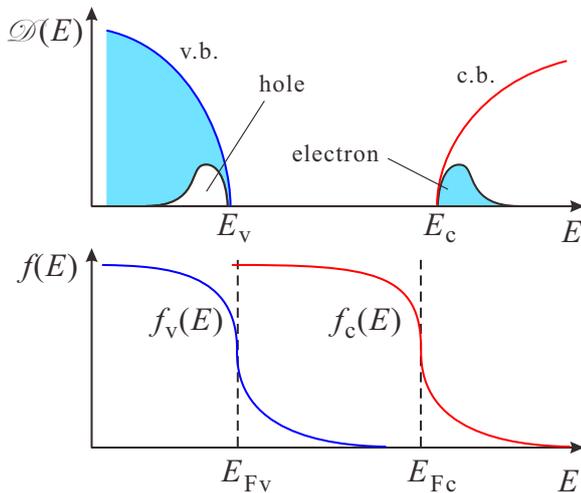


Fig. 4.3 Illustration of the concept of pseudo-Fermi levels.

When minority carriers are generated by photoexcitation under light irradiation, the carrier distribution deviates from the thermal equilibrium, which is described by single chemical potential and temperature. Even in such a case, if the system is steady in balance, we consider the energy distribution function f_c of electrons in the conduction band, that of electrons in the valence band f_v . Because in most cases, relaxation of distribution by carrier-to-carrier interaction and relaxation by intra-band carrier-lattice interaction are much faster processes than the inter-band carrier recombination, we adopt the approximation described in the following. In a semiconductor under steady light irradiation, the electrons in the conduction band and those in the valence band are in quasi-thermal equilibrium state described by the Fermi distribution functions with the same temperature but with the

The Planck's law of radiation gives the density of photons with energy E in a material with refractive index \bar{n} (we assume a real number ignoring the absorption) as

$$P(E) = \frac{8\pi\bar{n}^3 E^3}{h^3 c^3} \frac{1}{\exp(E/k_B T) - 1}. \quad (4.70)$$

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^{*1} There are many other excitation factors around us, such as electron beams, sound, friction, and chemical reactions, etc.

different chemical potentials called **quasi-Fermi levels**. The difference is caused by the excitation by the light and the slow inter-band transition. Then we write

$$f_c(E) = \left[\exp\left(\frac{E - E_{Fc}}{k_B T}\right) + 1 \right]^{-1}, \quad f_v(E) = \left[\exp\left(\frac{E - E_{Fv}}{k_B T}\right) + 1 \right]^{-1}. \quad (4.71)$$

Let us consider the process of the photon absorption (energy $\hbar\omega$) and the excitation of an electron from the valence band (energy E_1) to the conduction band (energy E_2). The frequency of such transition is written as

$$R(1 \rightarrow 2) = B_{12} f_v(1 - f_c) P(\hbar\omega), \quad (4.72)$$

where B_{12} is the transition probability of $1 \rightarrow 2$. Conversely, the frequency of spontaneous emission with the electron relaxation from E_2 to E_1 is

$$R(sp, 2 \rightarrow 1) = A_{21} f_c(E_2)(1 - f_v(E_1)), \quad (4.73)$$

independently of the photon density. The frequency of the stimulated emission is proportional to the photon density as

$$R(st, 2 \rightarrow 1) = B_{21} f_c(E_2)(1 - f_v(E_1)) P(\hbar\omega). \quad (4.74)$$

They should fulfill the balance equation

$$R(1 \rightarrow 2) = R(sp, 2 \rightarrow 1) + R(st, 2 \rightarrow 1). \quad (4.75)$$

Substituting equations (4.70)–(4.74) to the above and the comparison of LHS and RHS gives the following **Einstein relations**.

$$\begin{cases} A_{21} = \frac{8\pi\bar{n}^3 E_{21}^3}{h^3 c^3} B_{21}, & (4.76a) \\ B_{12} = B_{21}. & (4.76b) \end{cases}$$

These are identical with eq.(4A.9). Equation (4A.9) is for the angular frequency spectrum and there is the difference in the conversion factor \hbar .

4.3 Phenomenological treatment of electromagnetic field in materials

In the above we have considered the optical response caused by the photon absorption by interband transition of electrons based on the knowledge of two-level systems. This is very important of course, but there are many other optical processes in real crystals. It is also important to look at the optical phenomena from macroscopic perspectives. For example, the refractive index can be viewed as a parameter that modifies the speed of light. We have a brief look at such a classical macroscopic approach.

Let us begin with the Maxwell equations:

$$\operatorname{div} \mathbf{D} = \rho, \quad \operatorname{div} \mathbf{B} = 0, \quad (4.77a)$$

$$\operatorname{rot} \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \quad \operatorname{rot} \mathbf{H} = \mathbf{j} + \frac{\partial \mathbf{D}}{\partial t}, \quad (4.77b)$$

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}, \quad \mathbf{B} = \mu_0 \mathbf{H} + \mathbf{M}. \quad (4.77c)$$

Here we assume a non-magnetic insulating material and drop the magnetization $\mathbf{M} = \vec{0}$, and the current $|\mathbf{j}| \ll |\partial \mathbf{D} / \partial t|$ ^{*2}. These simplifications lead to the following wave equation.

$$\Delta \mathbf{E} - \epsilon_0 \mu_0 \frac{\partial^2 \mathbf{E}}{\partial t^2} = \mu_0 \frac{\partial^2 \mathbf{P}}{\partial t^2}, \quad (4.78)$$

^{*2} When these are finite, various interesting phenomena are expected even in this macroscopic level. On the microscopic level, we can find numerous subjects. These are called **magneto-optical effects**. They are the targets of researches as well as the sources of many useful experimental techniques. [2, 3] are recommended for advanced study.

which is the same as that for the vacuum when $\mathbf{P} = \vec{0}$. This means that the polarization \mathbf{P} represents the effect of dielectric material in this macroscopic model. In the linear response approximation, \mathbf{P} is written with the electric susceptibility tensor χ as

$$\mathbf{P} = \epsilon_0 \chi \mathbf{E}. \quad (4.79)$$

Equation (4.77c) leads to $\mathbf{D} = \epsilon_0(1 + \chi_r)\mathbf{E}$ and **relative dielectric function** or relative permittivity is defined as follows^{*3}.

$$\mathbf{D} = \epsilon_0 \epsilon_r \mathbf{E}, \quad \epsilon_r = 1 + \chi. \quad (4.80)$$

Below for simplicity, we consider isotropic materials and the tensor ϵ_r can be treated as a scalar ϵ_r . From eq.(4.79) and (4.80), eq.(4.78) becomes

$$\Delta \mathbf{E} - \epsilon_0 \mu_0 \frac{\partial^2 \mathbf{E}}{\partial t^2} = \epsilon_0 \mu_0 (\epsilon_r - 1) \frac{\partial^2 \mathbf{E}}{\partial t^2}.$$

Then we obtain

$$\Delta \mathbf{E} - \frac{\epsilon_r}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0. \quad (4.81)$$

In the above simplest approximation, the effect of polarization in the material can be taken into account with changing the light speed c with $c' = c/\sqrt{\epsilon_r}$. Hence the dispersion relation in the vacuum $\omega = ck$ is modified as

$$c^2 \mathbf{k}^2 = \omega^2 \epsilon_r(\omega, \mathbf{k}). \quad (4.82)$$

Here ϵ_r depends on ω_r, \mathbf{k} , reflecting the properties of materials.

As above, the association of the polarization with the electromagnetic wave inside materials can be taken into account phenomenologically by considering the relative dielectric function $\epsilon_r(\omega, \mathbf{k})$ or the refractive index $\tilde{n} = \sqrt{\epsilon_r}$. Above that, the absorption we saw in Sec.4.2.1 can be phenomenologically taken into account with adding the imaginary part to the refractive index. Then the **complex refractive index** is defined as

$$\tilde{n}(\omega, \mathbf{k}) = n(\omega, \mathbf{k}) + i\kappa(\omega, \mathbf{k}). \quad (4.83)$$

Then from eq.(4.59), or from the definition $I(z) = I_0 \exp(-\alpha z)$, the absorption coefficient α is expressed as

$$\alpha = \frac{2\omega}{c} \kappa(\omega, \mathbf{k}). \quad (4.84)$$

Let us go into a bit “model” of materials. In the Lorentz model, the electromagnetic field in the materials is a set of harmonic oscillators. In the model the mass, the charge, and the spring constant is common as (m, e, ξ) and the electromagnetic wave interacts with the oscillators through the Coulomb interaction with the charges. The frequency of the electromagnetic wave is ω and the wavelength is much longer than the distance between the oscillators and the electromagnetic wave can be approximated by uniform time-dependent electric field, which is written as $eE_0 e^{-i\omega t}$. The equation of motion for each oscillator is written as

$$m \frac{d^2 x}{dt^2} + \Gamma m \frac{dx}{dt} + \xi x = eE_0 \exp(-i\omega t), \quad (4.85)$$

where Γm is the coefficient representing the energy dissipation (friction in a classical model).

The eigenfrequency of each oscillator is $\omega_h = \sqrt{\xi/m}$. In order to find the long-term stable solution of (4.85), we substitute $x(t) = x_p \exp(-i\omega t)$. Then

$$x_p(\omega) = \frac{eE_0}{m} \frac{1}{\omega_h^2 - \omega^2 - i\omega\Gamma} \quad (4.86)$$

^{*3} Various expressions are use for the dielectric funtion. Here we put the expression “relative” to clarify the unit is taken as the vacuum dielectric constant ϵ_0 . The units in electromagnetism often cause confusions. Textbooks [5, 6, 7] are recommended for those who are intrested in the problem.

is obtained. Let N be the spatial density of the oscillators and we get

$$P = N(\epsilon x_p(\omega)) = \frac{Ne^2}{m} \frac{1}{\omega_h^2 - \omega^2 - i\omega\Gamma} E_0. \quad (4.87)$$

The coefficient of E_0 in r.h.s. corresponds to χ in (4.79). Then the definition in (4.80) leads to the relative dielectric function

$$\epsilon_r(\omega) = 1 + \frac{Ne^2}{\epsilon_0 m} \frac{1}{\omega_h^2 - \omega^2 - i\omega\Gamma}. \quad (4.88)$$

In the above we consider the case of single mode oscillator. If the oscillator has multiple mode and we write f_j as the portion of the mode indicated by index j , (4.88) is

$$\epsilon_r(\omega) = 1 + \frac{Ne^2}{\epsilon_0 m} \sum_j \frac{f_j}{\omega_h^2 - \omega^2 - i\omega\Gamma_j}. \quad (4.89)$$

This f_j is the oscillator strength we've already seen, but with this treatment we understand the wording of "oscillator strength."

4.4 Optical response of excitons

The excitons introduced at the end of the last chapter have discrete energy levels below the band gap. In many cases they appear as prominent peak structures in the absorption/emission spectrum. In bulk semiconductors, they appear mostly at low temperatures but the situation changes in quantum structures discussed later in this lecture. We do not have time to go into but the Frenkel-type excitons are now the main origin of the electroluminescence in organic semiconductors. Let us begin with the excitons in bulk semiconductors.

4.4.1 Absorption/emission by excitons

As we saw in Sec.3.3.2, the kinetic freedoms in excitons can be specified by the electron-hole relative spatial coordinate \mathbf{r} and coordinate of the parallel motion \mathbf{R} . Then the wavefunction can be written in the effective mass approximation as

$$\Phi_{n\mathbf{K}}(\mathbf{r}, \mathbf{R}) = \frac{1}{\sqrt{V}} \exp(i\mathbf{K} \cdot \mathbf{R}) \phi_n(\mathbf{r}). \quad (4.90)$$

The Fourier transform of the above is

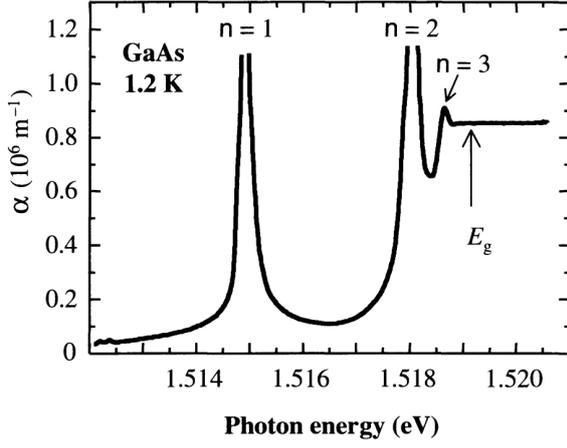
$$\begin{aligned} F_{n\mathbf{K}}(\mathbf{k}_e, \mathbf{k}_h) &= \frac{1}{V} \int d^3\mathbf{r}_e d^3\mathbf{r}_h e^{-i\mathbf{k}_e \cdot \mathbf{r}_e} e^{-i\mathbf{k}_h \cdot \mathbf{r}_h} \Phi_{n\mathbf{K}}(\mathbf{r}, \mathbf{R}) \\ &= \frac{1}{\sqrt{V}} \int d^3\mathbf{r} d^3\mathbf{R} e^{-i\mathbf{R} \cdot (\mathbf{k}_e + \mathbf{k}_h - \mathbf{K})} \phi_n(\mathbf{r}) e^{-i\mathbf{k}^* \cdot \mathbf{r}} \\ &= \frac{1}{\sqrt{V}} \int d^3\mathbf{r} e^{-i\mathbf{k}^* \cdot \mathbf{r}} \phi_n(\mathbf{r}) \delta_{\mathbf{K}, \mathbf{k}_e + \mathbf{k}_h}, \quad \mathbf{k}^* \equiv \frac{m_h \mathbf{k}_e - m_e \mathbf{k}_h}{m_e + m_h}. \end{aligned} \quad (4.91)$$

The total wavenumber of the excitation \mathbf{K} is thus turned out to be

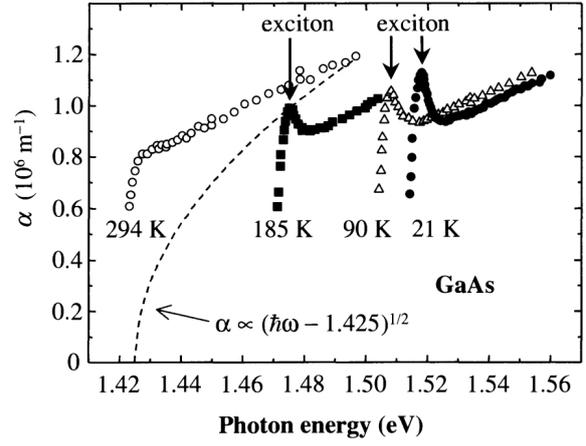
$$\mathbf{K} = \mathbf{k}_e + \mathbf{k}_h. \quad (4.92)$$

For the treatment of optical absorption, we take the initial state before the electron-hole excitation as the ground state $\Phi_0 = \phi_{c\mathbf{k}_e} \phi_{v\mathbf{k}_e}$ and calculate the transition probability w_{if} to the state represented as eq.(4.90) with taking $\mathbf{k}_p = \vec{0}$, $\mathbf{k}_e = -\mathbf{k}_h$ and along with the line shown for the case of two-level systems.

$$\begin{aligned} w_{if} &= \frac{2\pi}{\hbar} \frac{e^2}{m^2} |A_0|^2 \frac{1}{V} \sum_{\lambda} |\langle \Phi_{\lambda\mathbf{K}} | \exp(i\mathbf{k}_p \cdot \mathbf{r}) \mathbf{e} \cdot \mathbf{p} | \Phi_0 \rangle|^2 \delta(E_g + E_{\lambda} - \hbar\omega) \\ &= \frac{2\pi}{\hbar} \frac{e^2}{m^2} |A_0|^2 \frac{1}{V} \sum_{\mathbf{k}_e \lambda} |F_{\lambda\mathbf{K}}(\mathbf{k}_e, -\mathbf{k}_e) \langle \phi_{c\mathbf{k}_e} | \mathbf{e} \cdot \mathbf{p} | \phi_{v\mathbf{k}_e} \rangle|^2 \delta(E_g + E_{\lambda} - \hbar\omega). \end{aligned} \quad (4.93)$$



(a)



(b)

Fig. 4.4 (a) Optical absorption peaks by excitons at lower side in the energy than the fundamental absorption edge in GaAs[9]. (b) Absorption anomaly by excitons around the fundamental edge in GaAs[10].

From $\mathbf{k}_e = -\mathbf{k}_h$,

$$F_{n\mathbf{K}}(\mathbf{k}_e, -\mathbf{k}_h) = \frac{1}{V} \int d^3\mathbf{r}_e d^3\mathbf{r}_h \exp[-i\mathbf{k}_e \cdot (\mathbf{r}_e - \mathbf{r}_h)] \Phi_{\lambda\mathbf{K}}(\mathbf{r}_e, \mathbf{r}_h). \quad (4.94)$$

In (4.93), the summation over \mathbf{k}_e results in $\mathbf{r}_e = \mathbf{r}_h$. $F_{n\mathbf{K}}$ takes large values only in a narrow region of \mathbf{k}_e around $\mathbf{k}_e \approx \vec{0}$. In that region, $\langle \phi_{c\mathbf{k}_e} | e \cdot \mathbf{p} | \phi_{v\mathbf{k}_e} \rangle$ is almost constant and is M in (4.62). We then obtain

$$\omega_{if} = \frac{2\pi}{\hbar} \frac{e^2}{m^2} |A_0|^2 \sum_{\lambda} |M|^2 |\phi_{\lambda}(0)|^2 \delta(E_g + E_{\lambda} - \hbar\omega). \quad (4.95)$$

Again for simplicity we consider an isotropic system. Because $\phi_{\lambda}(0)$ is not zero only for s -state,

$$|\phi_n(0)|^2 = \frac{1}{\pi a_{ex}^3 n^3}, \quad E_n = -\frac{E_{ex}}{n^2}. \quad (4.96)$$

The imaginary part of the relative dielectric function $\epsilon_{r2}(\omega) = 2in(\omega)\kappa(\omega)$ is

$$\epsilon_{r2}(\omega) = \frac{\pi e^2}{\epsilon_0 m^2 \omega^2} |M|^2 \frac{1}{\pi a_{ex}^3} \sum_n \frac{1}{n^3} \delta\left(E_g - \frac{E_{ex}}{n^2} - \hbar\omega\right). \quad (4.97)$$

In the above the spin degree of freedom 2 is not considered and the result should be multiplied by two.

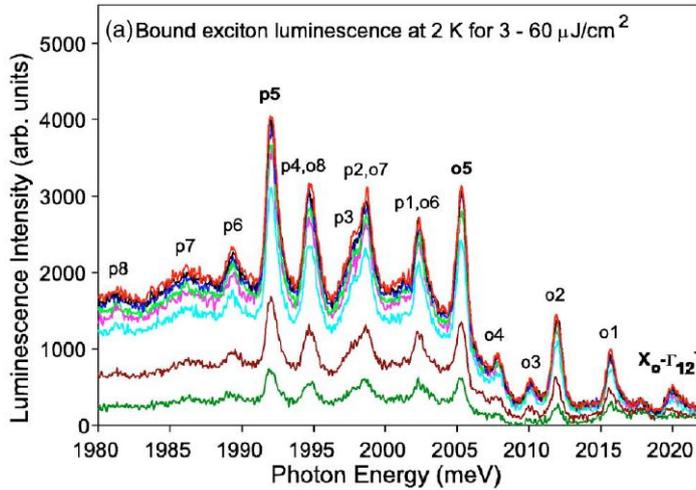


Fig. 4.5 Emission spectra of bound excitons in Cu_2O [11].

We do not go into calculation details (see *e.g.* [8]), but the twice of (4.97) agrees with (4.68) at the boundary $\hbar\omega = E_g$ between discrete states and continuum. Hence we can confirm how good is the approximation by the comparison of the spectra in experiments.

In eq.(4.97), the part other than δ -functions is common and we write it as the constant C .

$$\epsilon_{r2} = C \delta\left(E_g - \frac{E_{ex}}{n^2} - \hbar\omega\right). \quad (4.98)$$

Mathematical identity

$$\lim_{\Gamma \rightarrow +0} \frac{1}{x_0 - x - i\Gamma} = \mathcal{P} \frac{1}{x_0 - x} + i\pi\delta(x_0 - x) \quad (4.99)$$

tells

$$\epsilon_{r2} = \text{Im} \left\{ \frac{C/\pi}{E_g - \frac{E_{\text{ex}}}{n^2} - (\hbar\omega + i\delta)} \right\}. \quad (4.100)$$

Here we write $\Gamma \rightarrow +0$ as δ . And the Kramers-Kronig relation (4B.2) leads to

$$\epsilon_r = \frac{C/\pi}{E_g - \frac{E_{\text{ex}}}{n^2} - (\hbar\omega + i\Gamma)}, \quad (4.101)$$

with which we can try fitting the data in, *e.g.* Fig. 4.4(b).

The emission is the reversal process of the absorption and just as the absorption, discrete emission peaks appear at lower energies than the fundamental emission edge. Figure 4.5 shows an example of photoluminescence spectra of Cu_2O .

4.4.2 Exciton-polariton

Well known as “polaritons” are the quasiparticle created by the combination of optical phonons and photons. Here we consider, however the combination of photons and excitons. The concept of **exciton-polariton** is illustrated in Fig. 4.6. As mentioned in the previous section, an absorption and an emission of photon with an exciton are reversal process to each other. In an exciton-polariton these processes form a continuous chain. The cycle period of the processes is as short as a few fs and both the exciton and the photon keep their quantum coherence and the resultant quasiparticle propagates inside the crystal as a coherent state.

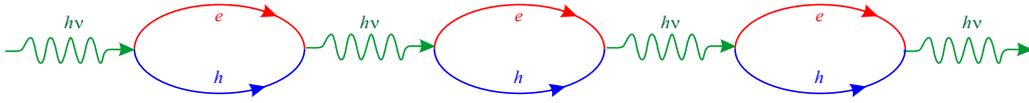


Fig. 4.6 Illustration of the concept of exciton-polariton. A photon creates an exciton and the recombination of the electron-hole pair recreates a photon. These processes occur in series.

We consider the ground state of $n = 1$ in eq.(4.101), define ω_0 as $E_g - E_{\text{ex}} \equiv \hbar\omega_0$, and the contribution to the dielectric function other than the excitons as ϵ_s . Then with $\gamma = \Gamma/\hbar$, the relative dielectric function is written as

$$\epsilon_r(\omega) = \epsilon_s \left(1 + \frac{\Delta_{\text{ex}}}{\omega_0 - \omega - i\gamma} \right). \quad (4.102)$$

For the transverse wave with $\mathbf{k} \cdot \mathbf{E} = 0$, the angular frequency $\omega_t = \omega_0$, the polariton equation (4.82) holds. On the other hand, for the longitudinal wave $\epsilon_r(\omega) = 0$, the angular frequency ω_l is given as

$$\omega_l = \omega_0 + \Delta_{\text{ex}} = \omega_t + \Delta_{\text{ex}}. \quad (4.103)$$

Δ_{ex} is called longitudinal-transverse splitting.

Now we consider the wavenumber $k = k_1 + ik_2$, then from (4.82), (4.102) we get

$$\begin{cases} \frac{\omega^2 \epsilon_s}{c^2} \left(1 + \frac{\Delta_{\text{ex}}}{\omega_0 - \omega} \right) = k_1^2 - k_2^2, & (4.104a) \\ \pi \delta(\omega - \omega_0) \frac{\omega_0^2 \epsilon_s}{c^2} = 2k_1 k_2. & (4.104b) \end{cases}$$

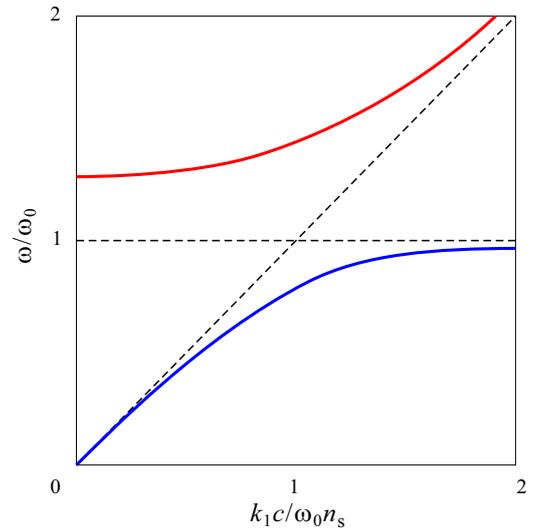


Fig. 4.7 Schematic drawing of the dispersion relation of exciton-polariton.

Equation (4.104b) represents the resonance at $\omega = \omega_0$, then we ignore k_2 in (4.104a) to get

$$\omega \sqrt{\frac{\omega - \omega - \Delta_{\text{ex}}}{\omega - \omega_0}} = \frac{ek_1}{\sqrt{\epsilon_s}}, \quad (4.105)$$

which gives the dispersion relation of exciton-polariton.

Appendix 4B: Kramers-Kronig relation

Here we just show well-known Kramers-Kronig relation. Let us consider a complex function with a complex argument ω as

$$\chi(\omega) = \chi_1(\omega) + i\chi_2(\omega), \quad \chi_1, \chi_2 \in \mathbb{R}. \quad (4B.1)$$

$\chi(\omega)$ is analytic in the upper half of ω -plane and diminish faster than $1/|\omega|$ for large $|\omega|$. Then there hold relations between χ_1 and χ_2 as

$$\chi_1(\omega) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\chi_2(\omega')}{\omega' - \omega} d\omega', \quad \chi_2(\omega) = -\frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\chi_1(\omega')}{\omega' - \omega} d\omega'. \quad (4B.2)$$

Here \mathcal{P} represents the Cauchy's principal value. The above are the Kramers-Kronig relation.

Appendix 4C: Lattice vibration in semiconductors

Lattice vibration is a phenomenon in which an atom vibrates around it with kinetic energy while being localized at an equilibrium position as a time average position. This is an important subject in semiconductor physics, should be discussed using at least one whole chapter, but that is impossible due to the lecture time. Here we take a minimum look at very basics.

4C.1 Lattice vibration in one-dimensional system

Just as in the electron system, we introduce basic concepts in one-dimensional systems.

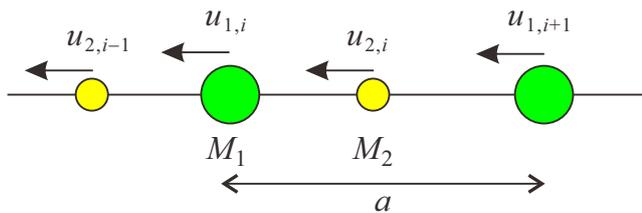


Fig. 4C.1 Schematic diagram of one-dimensional lattice vibration.

We consider a one-dimensional lattice with the unit cell of length a , which has two atoms with masses M_1 and M_2 . The shifts of the atoms from the equilibrium positions are written as u_{1j}, u_{2j} (j : integer). The force working on the atoms is assumed to be harmonic oscillator-like, that is, the force proportional to the shift of the distance between neighboring atoms from the equilibrium value $a/2$. Let α be the coefficient for the force then we get the equation of motion as

$$M_1 \frac{d^2 u_{1,j}}{dt^2} = -\alpha(u_{1,j} - u_{2,j-1}) + \alpha(u_{2,j} + u_{2,j-1}) = \alpha[-2u_{1,j} + (u_{2,j} - u_{2,j-1})], \quad (4C.1a)$$

$$M_2 \frac{d^2 u_{2,j}}{dt^2} = \alpha[-2u_{2,j} + (u_{1,j} - u_{1,j-1})]. \quad (4C.1b)$$

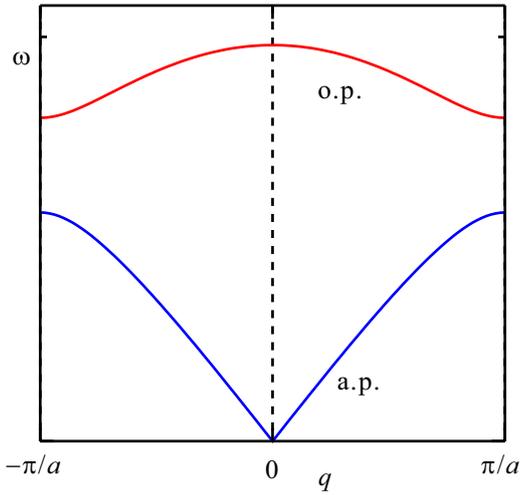


Fig. 4C.2 Dispersion relation of one dimensional lattice vibration $\omega(q)$ obtained from eq.(4C.5) is plotted for the case $M_1 = 2M_2$.

The equation (4C.1) remains unchanged with the parallel shift operation $j \rightarrow j + n$ (n is an integer) and the solution can be written in the form of Bloch function. Let us take x coordinate along the lattice direction and the equations for the wavenumber q are

$$\begin{cases} u_{1,j}(x_j) = e^{iqx_j} u_{1,q}, \\ u_{2,j}(x_j + a/2) = e^{iq(x_j + a/2)} u_{2,q}. \end{cases} \quad (4C.2)$$

Substituting the above into (4C.1) we obtain

$$\begin{cases} M_1 \frac{d^2 u_{1,q}}{dt^2} = 2\alpha(-u_{1,q} + \cos \frac{ja}{2} u_{2,q}), \\ M_2 \frac{d^2 u_{2,q}}{dt^2} = 2\alpha(-u_{2,q} + \cos \frac{ja}{2} u_{1,q}). \end{cases} \quad (4C.3)$$

In order to find the solution we assume $u_{(1,2),q} \propto \exp(i\omega t)$ to write down

$$\begin{pmatrix} 2\alpha - M_1\omega^2 & -2\alpha \cos \frac{qa}{2} \\ -2\alpha \cos \frac{qa}{2} & 2\alpha - M_2\omega^2 \end{pmatrix} \begin{pmatrix} u_{1,q} \\ u_{2,q} \end{pmatrix} \equiv \mathbf{A} \begin{pmatrix} u_{1,q} \\ u_{2,q} \end{pmatrix} = \vec{0}. \quad (4C.4)$$

For the equations to have non-trivial solution $\{u_{i,q}\}$ other than $\vec{0}$, $|\mathbf{A}| = 0$ leads to

$$\frac{\omega_{\pm}^2}{\alpha} = \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \pm \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2} \right)^2 - 4 \frac{\sin^2(qa/2)}{M_1 M_2}}. \quad (4C.5)$$

We consider non-negative ω , and eq.(4C.5) has two modes, the dispersion relations of which are shown in Fig. 4C.2.

The following description of wording does not depend on the dimension.

The modes with linear dispersion around $q \approx 0$ are called **acoustic modes**, those with finite ω and $d\omega/dq = 0$ for $q = 0$ are called **optical modes**. The naming acoustic mode comes from the property that the group velocity does not depend on the frequency just like sound in the air or electromagnetic wave in the vacuum. The naming optical mode comes from the interaction with photons as the small wavenumber and the large energy. The quantized particles of them are called **acoustic phonon** and **optical phonon** respectively.

4C.2 Lattice vibration in zinc-blende crystals

We consider zinc-blende (ZB) crystals as an example of three-dimensional crystal which has two species of atoms in the unit cell. The Bravais lattice is fcc but the ZB crystalline structure can be considered as an overlapp of two ‘‘fcc crystals’’, in which one atom is placed at the lattice point of fcc lattice.

(to be continued in the next lecture note.)

References

- [1] 櫛田孝司「光物性物理学」(朝倉書店, 2009).
- [2] 佐藤勝昭「光と磁気」(朝倉書店, 1988).
- [3] S. Sugano ed., “Magneto-optics” (Springer, 1999).
- [4] A. K. Zvezdin and V. A. Kotov, “Modern Magneto-optics and Magneto-optical Materials” (IOPP, 1997).
- [5] 青野 修「電磁気学の単位系」(丸善, 1990).
- [6] 高梨弘毅「磁気工学入門」(共立出版, 2008)
- [7] 2018 年の SI 単位改定については, 沢山解説が出ているが, 改定自身というより単位系全般の話を非常に易しく解説したものとして, 和田純夫, 大上雅史, 根本和昭「単位がわかると物理がわかる」(ベレ出版, 2002).
- [8] 浜口智尋「半導体物理」(朝倉書店, 2001). 英語版は C. Hamaguchi, “Basic Semiconductor Physics” (Springer, 2017).
- [9] G.W. Fehrenbach, W. Schafer, and R. G. Ulbrich, *J. Luminescence*, **30**, 154 (1985).
- [10] M. D. Sturge, *Phys. Rev.* **127**, 768 (1962).
- [11] J. I. Jang, Y. Sun, B. Watkins, and J. B. Ketterson, *Phys. Rev. B* **74**, 235204 (2006).