

3.3.1 Degenerate semiconductors

So far we treat the impurity states in semiconductors as isolated. In such cases, as shown in Fig.3.2, charge carriers disappear at low temperatures, the conductivity is lost, and the system is insulating. Now we consider doping to higher impurity densities, where the average distance between the dopants is similar to or less than the spatial size of the wavefunctions. Then the overlapping of wavefunctions enables tunneling between the impurity sites. Such tunnelings may form a kind of conducting network in the crystal and with further increasing the impurity concentration finally spreads the network over the whole crystal, which now has a finite conductance at the lowest temperature, thus is a metal.

This problem – **metal-insulator transitions, MIT** – has been one of the most important problems in condensed matter physics, and huge amount of efforts have been devoted for years. The field of MIT extends over various phenomena in condensed matter physics, far beyond the doped semiconductors. We have not reached the final answer through great amount of knowledges have been accumulated. There are so many textbooks, very few of which are listed in references ([1]~[5]).

In the above we have defined the MIT as the spatial size of the wavefunctions at the Fermi level. The phenomenon is observed in the energy space as follows. With overlapping of neighboring wavefunctions, as we have seen in the tight binding model (regular, coherent case), the energy levels broadened and a band is formed, which we call an **impurity band**. Even under the formation of impurity band, in which the density of states is continuous, the wavefunction at the Fermi level is not necessarily spread over the entire crystal. It was first pointed out by Anderson that the electrons in a potential with a certain degree of disorder are spatially localized. This is called **Anderson localization**. Hence, some lower part of the impurity band is usually localized and the boundary is called a mobility edge.

It is well known that as shown in Fig. 3.6, in many matrix crystals and species of dopants, an empirical relation,

$$n_c^{1/3} a_B^* = 0.26 \quad (3.32)$$

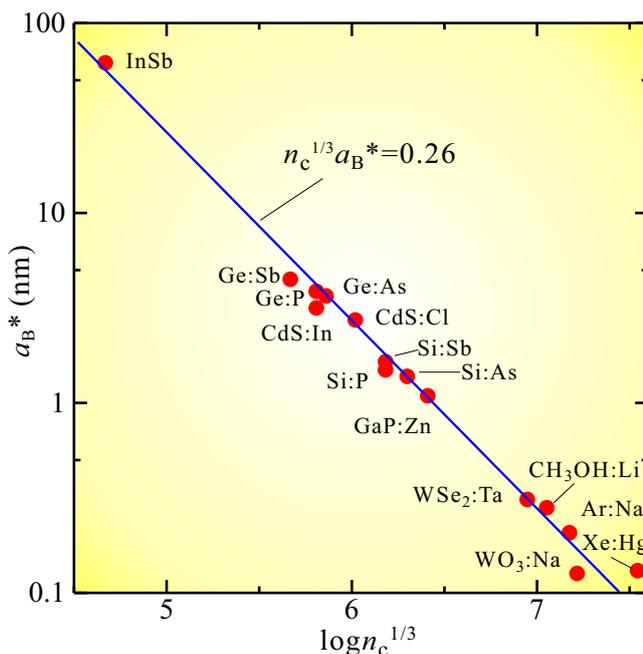


Fig. 3.6 Experimental values for the critical concentrations of the MIT and the effective Bohr radiuses for various matrix semiconductors and dopants (the element symbols put after the colons). The data are plotted in log scale. The unit for n_c is cm^{-3} . The line indicates the empirical relation in eq.(3.32). The data are taken from P. Edwards and M. Sienko, Phys. Rev. B 17, 2575 (1978).

holds between the critical impurity concentration n_c for the MIT and the effective Bohr radius a_B^* . This criterion is natural from the view of impurity band formation and there are many trials to derive it from more rigorous theoretical background.

The largest difficulty in solving this problem lies in the treatment of disorder, which makes it impossible to utilize the coherence of the scattering from the crystal lattice. In the band theory, the coherence brings about great simplicity. In the case of MIT in disordered systems, one should directly treat the disorder itself.

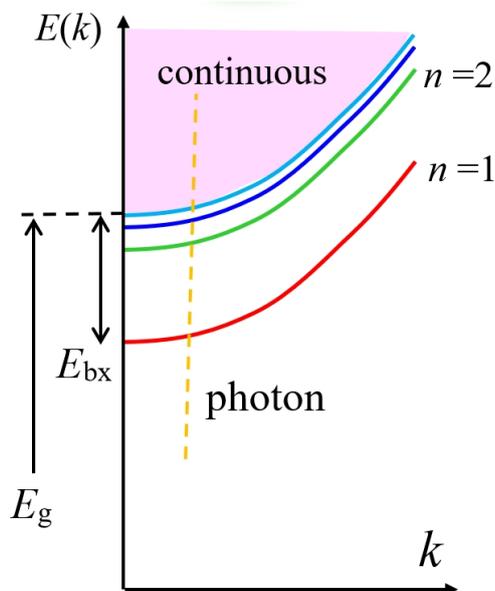
Though the final answer has not been found, or it is not even known whether there is such one or not, many new physical idea have been developed, which have greatly expanded our knowledges on random systems. The concepts have been applied various fields such as organic semiconductors. We do not go into this problem further due to the space-time limitations.

The MIT in ordered systems is also an important and difficult problem, particularly in so called strongly correlated systems. Here I just list a review paper[6], which was published a quarter century ago. I will not go into this problem in this lecture.

There are a number of devices which utilize such degenerate semiconductors. A representative is the Esaki diode (tunnel diode), which first attracted attentions as a device for fast switching and actually was used in counter circuits in the experiments of high energy physics. Recently, the Esaki diode is also used in the interfacial connection of multiple junction solar cells. In many of ordinary solar cells, highly-doped degenerate semiconductors are used as the upper layers of the junctions. The high level doping is also used in the IMPATT diodes for high-frequency use, and $p-i-n$ type photo-diode, etc.

3.3.2 Excitons

Here we introduce the concept of exciton, which is a bit tail subject as “carrier statistics” but we can view it as an application of the effective mass approximation. Exciton has long been the central theme of optical properties[7], but even more extensive research is still underway, such as the BEC of exciton polaritons. In solids, the bound states formed by Coulomb force between quasiparticles of positive and negative charges are called **exciton**.



When the quasiparticles are spread over several lattice constants, the exciton is called “Wannier type.” When the charge polarization occurs within a molecule or over very few lattice points, it is called “Frenkel type.” The latter often found in organic semiconductors, in which the molecules at the lattice points are comparatively well separated. Here we concentrate ourselves on the Wannier type.

Let us consider an exciton state with an electron excited to the conduction band, and a hole excited to the valence band. These spread over several lattice points or more, and effective mass approximation can be applied. Based on the free state of both electrons and holes, even if they create a bound state, the degree of freedom of the movement of the center of mass remains, and the “wave number” and kinetic energy due to this remain. This wavenumber should be derived from the overall wavenumber conservation since the concept of holes is also introduced by considering the conservation of the total wavenumber. The “mass” of the exciton also would be introduced simply by taking the sum of effective masses of electrons

and holes, as $m_e + m_h$. I have used the expression “would” because the Coulomb force, which is most natural candidate

for the force in the equation of motion for electrons and holes, works in the opposite directions, the accelerations for two kinds of particles with different effective masses is a bit complicated for the treatment. Anyway we assume that the effective mass approximation holds. Then the creation energy of an exciton from the state without the electron and the hole, hence including the electron-hole pair creation energy, is written as

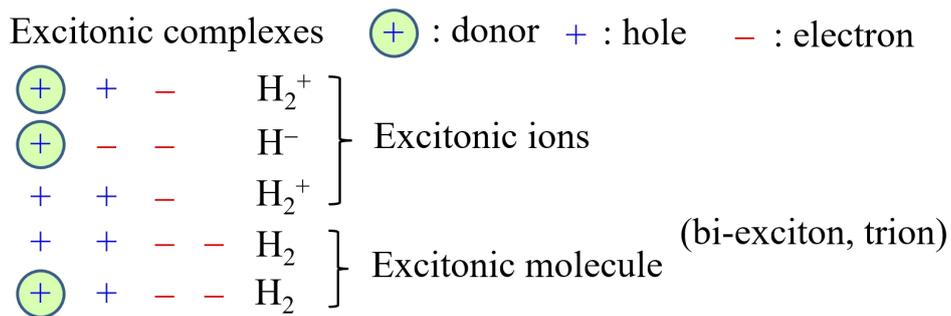
$$E_{\text{ex}}^{(n)}(k) = E_g + \frac{\hbar^2 k^2}{2(m_e + m_h)} - \frac{e^4 m_r^*}{2\hbar^2} \frac{1}{n^2}, \quad n = 1, 2, \dots, \quad (3.33)$$

where the third term is the binding energy of the electron and the hole. We assume the system is isotropic and the exciton is hydrogen-like. m_r is the reduced mass defined as

$$\frac{1}{m_r^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*}. \quad (3.34)$$

The second term in (3.33) is the kinetic energy of the parallel motion. The dispersion described in eq.(3.33) is illustrated in the figure in the previous page. The existence of such bound states can be confirmed by checking, *e.g.* the optical absorption spectra, which we will see in the next chapter.

However, for example in optical absorption experiments, there often appear many absorption peak spectra which cannot be interpreted simply with eq.(3.33). The candidates for the interpretation of those observations are, the excitons trapped by impurity potentials (bound excitons), the exciton molecules made of more than two excitons, or such complicated excited states.



In the above illustration, the cases for the number of charged excitation including zero or single donor is from three to four (corresponding to hydrogen molecule or its charged state) are listed. Such excited states are called **excitonic complexes**.

In this chapter, we introduced electrons excited in the conduction band, holes excited in the valence band, and excitons, which are bound states of these excitations.

All of them are many-body states of electrons, but they can be treated as if “particles” are freely moving in the space of a crystal, which is different from the vacuum. Such free particle-like pictures, in which many-body effects are renormalized are called **quasi-particle**.



Chapter 4 Optical response of bulk semiconductors

Many of the substances called “semiconductors” have bandgaps around the energy region of electromagnetic wave called “light”, and have characteristic optical responses. The optical response is one of the most important subject as well as the carrier transport. In the optical devices such as detectors or emitters, semiconductors are mostly used as active materials. In this chapter, as the first look, we see basic optical properties of semiconductor bulk materials.

4.1 Optical response of two-level systems

In order to consider the optical response of semiconductor bulk, we should investigate the relationship between light and the transition between the extended electronic states of the valence band and conduction band that we have seen so far. But here, we begin with the optical response of a much simpler “two-level system.” The reason why we devote our pages to such basic matters here is that we want to confirm the zero-point oscillation of the electromagnetic field and the state of photons in particular. The following two sections are for the lecture to be just self-contained. For more complete description, see the textbooks listed in [8]. If the reader already has such knowledge, the skip to Sec.4.1.3 is recommended. In addition, if he/she is already used to the two-level systems, a further skip to Sec.4.2 is also OK.

4.1.1 Quantization of electromagnetic field

We have a very short look at the quantization of electromagnetic field to consider the states of photons[8]. As the basics we start with the one-dimensional harmonic oscillator, which subject appears in the beginning part of elementary quantum mechanics. The problem is described as the Schrödinger equation;

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega_h^2 x^2}{2} \right] \phi = E\phi. \quad (4.1)$$

The second term in the parenthesis in the left hand side represents the potential characteristic for the harmonic oscillator. We define a dimensionless variable q with

$$x = \sqrt{\frac{\hbar}{\omega_h m}} q, \quad (4.2)$$

and rewrite (4.1) as

$$\frac{\hbar\omega_h}{2} \left(-\frac{d^2}{dq^2} + q^2 \right) \phi = E\phi. \quad (4.3)$$

We introduce down and up operators

$$a = \frac{1}{\sqrt{2}} \left(\frac{d}{dq} + q \right), \quad a^\dagger = \frac{1}{\sqrt{2}} \left(-\frac{d}{dq} + q \right), \quad [a, a^\dagger] = 1, \quad (\text{others}) = 0, \quad (4.4)$$

where the commutation relation is readily derived from the definition. Then eq.(4.3) is further rewritten as

$$\hbar\omega_h \left(a^\dagger a + \frac{1}{2} \right) \phi \equiv \hat{H}\phi = E\phi. \quad (4.5)$$

If we define the **number operator** as

$$\hat{n} \equiv a^\dagger a. \quad (4.6)$$

Because \hat{n} and \hat{H} commute with each other ($[\hat{n}, \hat{H}] = [\hat{H}, \hat{n}] = 0$), they have common eigenfunctions. Here we assume $|w\rangle$ is a eigen function common for \hat{H} and \hat{n} with eigen[values ϵ, γ respectively. From the commutation relation eq.(4.4), we see

$$\hat{H}(a^\dagger|w\rangle) = (\gamma + \hbar\omega_h)(a^\dagger|w\rangle), \quad \hat{H}(a|w\rangle) = (\gamma - \hbar\omega_h)(a|w\rangle), \quad (4.7)$$

that is, $a^\dagger|w\rangle, a|w\rangle$ are also such simultaneous eigenfunctions with the energy eigenvalues of up and down shifts by $\hbar\omega_h$ respectively. Let $|0\rangle$ be the simultaneous eigenstate with the lowest energy eigenstate ϵ_0 . Since there is no eigenstate with energy eigenvalue of $\epsilon_0 - \hbar\omega_h$, the above equation leads to $a|0\rangle = 0$. Furthermore, $\epsilon_0 = \hbar\omega_h/2$ is concluded.

On the other hand, the eigenstates with higher energy eigenvalues than ϵ_0 can be obtained by sequential application of a^\dagger to $|0\rangle$. The eigenvalues are

$$E_n = \hbar\omega_h \left(n + \frac{1}{2} \right) \quad (n = 0, 1, 2, \dots). \quad (4.8)$$

And the commutation relation tells that the operator $a^n (a^\dagger)^n$ works as multiplication of $n!$. Then the normalized eigenfunction for the eigenvalue E_n can be obtained from the normalized $|0\rangle$ is written as

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle. \quad (4.9)$$

Also from $a|0\rangle = 0$, a solution of $|0\rangle = \varphi_0(q)$ is straightforwardly obtained as

$$\frac{d\varphi_0}{dq} + q^2\varphi_0 = 0 \quad \therefore \varphi_0 = \frac{1}{\pi^{1/4}} \exp\left(-\frac{q^2}{2}\right). \quad (4.10)$$

Based on the above knowledge, we go to the electromagnetic field. Our starting point here is the fact that the electromagnetic field is mathematically equivalent to a set of harmonic oscillators^{*1}. We take Coulomb gage ($\text{div}\mathbf{A} = \vec{0}$), and expand the vector potential \mathbf{A} with the plane waves as follows.

$$\begin{aligned} \mathbf{A}(\mathbf{r}, t) &= \sum_{\mathbf{k}, \lambda} (\mathbf{A}_{\mathbf{k}\lambda} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}\lambda}t)} + \mathbf{A}_{\mathbf{k}\lambda}^* e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}\lambda}t)}), \\ (\omega_{\mathbf{k}} &= c|\mathbf{k}|, \quad \mathbf{A}_{\mathbf{k}\lambda}^* = \mathbf{A}_{-\mathbf{k}\lambda}). \end{aligned} \quad (4.11)$$

Here λ represents the freedom of polarization. From the selection of Coulomb gauge, the electromagnetic wave should be transverse and λ represents two-dimensional freedom. From the Maxwell equaiton $\mathbf{E} = \partial\mathbf{A}/\partial t$, $\mathbf{B} = \text{rot}\mathbf{A}$, the energy of electromagnetic field \mathcal{E} in volume V is written as

$$\mathcal{E} = \int_V [\epsilon_0 \mathbf{E}^2(\mathbf{r}, t) + \mu_0^{-1} \mathbf{B}^2(\mathbf{r}, t)] \frac{d^3\mathbf{r}}{2} = 2\epsilon_0 V \sum_{\mathbf{k}, \lambda} \omega_{\mathbf{k}\lambda} (\mathbf{A}_{\mathbf{k}\lambda} \cdot \mathbf{A}_{\mathbf{k}\lambda}^*), \quad (4.12)$$

because the terms with $\exp(\pm 2i\mathbf{k} \cdot \mathbf{r})$ vanish with spatial integration.

Then we introduce variables(vectors) $\mathbf{Q}_{\mathbf{k}\lambda}, \mathbf{P}_{\mathbf{k}\lambda}$ as

$$\mathbf{Q}_{\mathbf{k}\lambda} = \sqrt{\epsilon_0 V} (\mathbf{A}_{\mathbf{k}\lambda} e^{-i\omega_{\mathbf{k}\lambda}t} + \mathbf{A}_{\mathbf{k}\lambda}^* e^{i\omega_{\mathbf{k}\lambda}t}), \quad \mathbf{P}_{\mathbf{k}\lambda} = d\mathbf{Q}_{\mathbf{k}\lambda}/dt = i\omega_{\mathbf{k}\lambda} \sqrt{\epsilon_0 V} (-\mathbf{A}_{\mathbf{k}\lambda} e^{-i\omega_{\mathbf{k}\lambda}t} + \mathbf{A}_{\mathbf{k}\lambda}^* e^{i\omega_{\mathbf{k}\lambda}t}). \quad (4.13)$$

\mathcal{E} is expressed as

$$\mathcal{E} = \frac{1}{2} \sum_{\mathbf{k}\lambda} (\mathbf{P}_{\mathbf{k}\lambda}^2 + \omega_{\mathbf{k}\lambda}^2 \mathbf{Q}_{\mathbf{k}\lambda}^2), \quad (4.14)$$

which tells the electromagnetic field is described as a set of harmonic oscillators in \mathbf{Q} space. Then the field can be quantized with changing \mathbf{P}, \mathbf{Q} to operators and require the following commutation relations.

$$[\hat{Q}_{\mathbf{k}'\lambda'}, \hat{P}_{\mathbf{k}\lambda}] = i\hbar\delta_{\mathbf{k}\mathbf{k}'}\delta_{\lambda\lambda'}, \quad (\text{others}) = 0. \quad (4.15)$$

^{*1} According to the literature[10], this is called "Jeans theorem." Actually, in ref.[9], that "theorem" is proven. The discussion then leads to the Rayleigh-Jeans law. However, there is more famous "Jeans theorem", which is on the distribution of particles with gravitational interactions[9, 10]

The Hamiltonian is in the same form with (4.3).

$$\hat{H} = \frac{1}{2} \sum_{\mathbf{k}\lambda} (\hat{P}_{\mathbf{k}\lambda}^2 + \omega_{\mathbf{k}}^2 \hat{Q}_{\mathbf{k}\lambda}^2). \quad (4.16)$$

creation/annihilation operators, which corresponds to up/down operators, are

$$a_{\mathbf{k}\lambda}^\dagger = \frac{1}{\sqrt{2\hbar\omega_{\mathbf{k}}}} (\omega_{\mathbf{k}} \hat{Q}_{\mathbf{k}\lambda} - i\hat{P}_{\mathbf{k}\lambda}), \quad a_{\mathbf{k}\lambda} = \frac{1}{\sqrt{2\hbar\omega_{\mathbf{k}}}} (\omega_{\mathbf{k}} \hat{Q}_{\mathbf{k}\lambda} + i\hat{P}_{\mathbf{k}\lambda}). \quad (4.17)$$

From (4.15), the commutation relations

$$[a_{\mathbf{k}\lambda}, a_{\mathbf{k}'\lambda'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'}, \quad (\text{others}) = 0 \quad (4.18)$$

are derived. Finally (4.16) can be quantized in the Hamiltonian form as

$$\hat{H} = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}} \left(a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda} + \frac{1}{2} \right). \quad (4.19)$$

The vector potential, for example, can also be written in the form of operator as

$$\hat{\mathbf{A}}(\mathbf{r}, t) = \sum_{\mathbf{k}\lambda} \sqrt{\frac{\hbar}{2\epsilon_0\omega_{\mathbf{k}}V}} e_{\mathbf{k}\lambda} \left[a_{\mathbf{k}\lambda} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} + a_{\mathbf{k}\lambda}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} \right]. \quad (4.20)$$

4.1.2 States of photons

Corresponding to eq.(4.6), the operator

$$\hat{n}_{\mathbf{k}\lambda} \equiv a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda} \quad (4.21)$$

represents the level of excitation in the mode (\mathbf{k}, λ) from the ground state $|0\rangle_{\mathbf{k}\lambda}$. Single step of the excitation corresponds to the energy of $\hbar\omega_{\mathbf{k}}$, which is also the energy of single photon in the Einstein relation of photon quantum. Hence $\hat{n}_{\mathbf{k}\lambda}$ in (4.21) can be interpreted as **photon number operator** in mode (\mathbf{k}, λ) . As in (4.9), there are eigenfunctions of (4.19) in which the number of photons in mode (\mathbf{k}, λ) is $n_{\mathbf{k}\lambda}$. We use the expression that the symbol $\{\cdot\cdot\cdot\}_\alpha$ represents the set of elements with α as the index. Then the state is represented as $|\{n_{\mathbf{k}\lambda}\}\rangle$.

From (4.9), we call the state described in the form

Number state

$$|\{n_{\mathbf{k}\lambda}\}\rangle = \left[\prod_{\mathbf{k}\lambda} \frac{(a_{\mathbf{k}\lambda}^\dagger)^{n_{\mathbf{k}\lambda}}}{\sqrt{n_{\mathbf{k}\lambda}!}} \right] |0\rangle \quad (4.22)$$

as **number state**.

The expectation value of the energy of the number state is

$$\langle \{n_{\mathbf{k}\lambda}\} | \hat{H} | \{n_{\mathbf{k}\lambda}\} \rangle = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}} \left(n_{\mathbf{k}\lambda} + \frac{1}{2} \right). \quad (4.23)$$

A state with multiple mode is a superposition of eigenstates with different eigenvalues and is not an eigenstate of the total Hamiltonian. On the other hand, the expectation value of the electric field is from (4.20),

$$\langle \{n_{\mathbf{k}\lambda}\} | \hat{\mathbf{E}} | \{n_{\mathbf{k}\lambda}\} \rangle = -\langle \{n_{\mathbf{k}\lambda}\} | (\partial\hat{\mathbf{A}}/\partial t) | \{n_{\mathbf{k}\lambda}\} \rangle = 0. \quad (4.24)$$

That is the expectation value of the electric field is zero. This does not mean the time-average makes it zero. Even for the measurements in very short time, the average over many measurements is zero. Just the same for the magnetic field. On the other hand the quantum fluctuation in the electric field is

$$\langle \{n_{\mathbf{k}\lambda}\} | \hat{\mathbf{E}}^2 | \{n_{\mathbf{k}\lambda}\} \rangle = \sum_{\mathbf{k}\lambda} \frac{\hbar\omega_{\mathbf{k}}}{\epsilon_0 V} \left(n_{\mathbf{k}\lambda} + \frac{1}{2} \right) = \frac{1}{\epsilon_0 V} \langle \{n_{\mathbf{k}\lambda}\} | H | \{n_{\mathbf{k}\lambda}\} \rangle, \quad (4.25)$$

which is non-zero. Furthermore, even for the photon number zero state, each mode has the fluctuation of $\hbar\omega_{\mathbf{k}}/(2\epsilon_0V)$, which is called **zero-point motion** of electromagnetic field. The zero-point fluctuation corresponds to 1/2 in the energy expression of (4.23). This is very important property for the spontaneous emission of photon. The reason of using space for free electromagnetic field is to describe this clearly.

The properties of number state described above indicate that it is difficult to coherently superimpose the oscillating electromagnetic field of multiple photons to obtain the oscillating electromagnetic field as in the classical picture in the energy eigenstate where the number of photons is fixed. On the other hand, by superimposing several states, it is possible to create a state with a finite expected value of the electromagnetic field. For example, the number states for a single mode (hence for a while we omit writing the mode index as $|n\rangle$) can be summed up with Gaussian weight to get

Coherent state

$$|\alpha\rangle = \exp\left(-\frac{|\alpha|^2}{2}\right) \exp(\alpha a^\dagger)|0\rangle = \exp\left(-\frac{|\alpha|^2}{2}\right) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle, \quad (4.26)$$

where α is a complex parameter. The state expressed as (4.26) is called **coherent state**. When the annihilation operator is applied, from $a|n\rangle = \sqrt{n}|n-1\rangle$,

$$a|\alpha\rangle = \alpha|\alpha\rangle, \quad (4.27)$$

that is the coherent state is the eigenstate of the annihilation operator with the eigenvalue of α . This means that the coherent state is a superposition of an infinite number of states, and even if quantum mechanical "measurement" is performed on the single photon in it, the whole state remains unchanged. If we measure the photon number in this state, the probability of detecting n -photons is

$$P(n) = \langle n|\alpha\rangle = \frac{e^{-|\alpha|^2} |\alpha|^{2n}}{n!}, \quad (4.28)$$

which is a Poissonian distribution. We write the complex parameter α in the amplitude and the phase as $\alpha = |\alpha|e^{i\phi}$. Then the expectation values of the electric field and the magnetic field are

$$\langle\alpha|\hat{\mathbf{E}}(\mathbf{r}, t)|\alpha\rangle = -\sqrt{\frac{2\hbar\omega_{\mathbf{k}}}{\epsilon_0V}} |\alpha| e_{\mathbf{k}\lambda} \sin(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}}t + \phi), \quad (4.29a)$$

$$\langle\alpha|\hat{\mathbf{B}}(\mathbf{r}, t)|\alpha\rangle = -\sqrt{\frac{2\hbar}{\epsilon_0\omega_{\mathbf{k}}V}} |\alpha| \mathbf{k} \times e_{\mathbf{k}\lambda} \sin(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}}t + \phi). \quad (4.29b)$$

This means classical electromagnetic wave is reproduced in the coherent state.

4.1.3 Basic optical processes in two-level systems

The **two-level system** composed of two quantum states is also called qubit in the field of quantum information and is the most basic quantum system. As in Fig. 4.1, we consider a two-level electronics system of ($|a\rangle, |b\rangle$) with the energy eigenvalues (E_a, E_b). We take these

$$\mathcal{H}_0|a\rangle = E_a|a\rangle, \quad \mathcal{H}_0|b\rangle = E_b|b\rangle \quad (4.30)$$

as the basis and the general state can be written as

$$\psi(t) = c_a(t)e^{-E_a t/\hbar}|a\rangle + c_b(t)e^{-E_b t/\hbar}|b\rangle. \quad (4.31)$$

In Fig. 4.1, three basic optical processes in the two-level system are illustrated. (a) is the **optical absorption**, in which the electron absorbs the photon energy and makes transition of $|a\rangle \rightarrow |b\rangle$. (b) is the **spontaneous emission** of photon associated with the transition $|b\rangle \rightarrow |a\rangle$ of the electron initially excited to $|b\rangle$. (c) is the **stimulated emission**, in which the first photon comes to the excited state $|b\rangle$ to stimulate the emission of the second photon coherent to the first one.

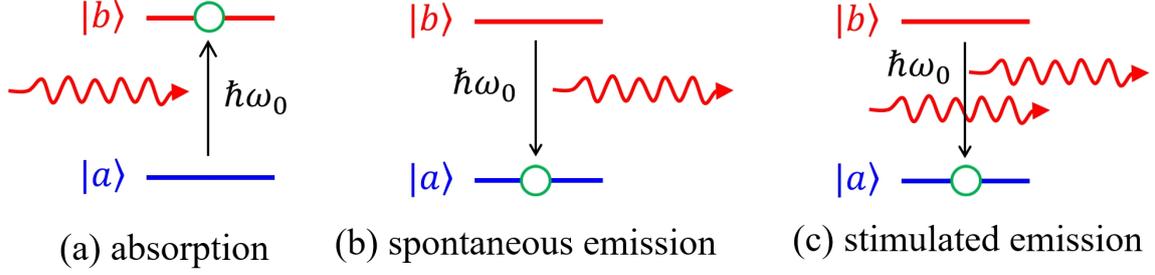


Fig. 4.1 Three basic optical processes in two-level systems (a) optical absorption, (b) spontaneous emission of a photon, (c) stimulated emission of a photon

We write the Hamiltonian of the system with electromagnetic field in non-relativistic approximation as

$$\mathcal{H}_{\text{op}} = \frac{(\mathbf{p} + e\mathbf{A})^2}{2m} + V(\mathbf{r}), \quad (4.32)$$

where \mathbf{A} is the vector potential and we treat it as perturbation. We then drop the term of \mathbf{A}^2 and the perturbation Hamiltonian \mathcal{H}' can be defined as

$$\mathcal{H}_{\text{op}} \approx \mathcal{H}_0 + \frac{e}{m} \mathbf{A} \cdot \mathbf{p} \equiv \mathcal{H}_0 + \mathcal{H}'. \quad (4.33)$$

For simplicity, we assume \mathcal{H}' does not have the diagonal terms.

$$\langle a | \mathcal{H}' | a \rangle = \langle b | \mathcal{H}' | b \rangle = 0. \quad (4.34)$$

We consider the case that a plane electromagnetic wave is applied to the two-level system, which wave is described in Coulomb gauge ($\text{div } \mathbf{A} = 0$) as

$$\mathbf{A} = A_0 \mathbf{e}_p \cos(\mathbf{k}_p \cdot \mathbf{r} - \omega t). \quad (4.35)$$

As we saw in the previous section, this means a coherent state comes to the two-level system. The perturbation Hamiltonian is

$$\mathcal{H}' = \frac{eA_0}{m} \mathbf{e}_p \cdot \hat{\mathbf{p}} \cos(\mathbf{k}_p \cdot \mathbf{r} - \omega t). \quad (4.36)$$

This approximation is called **dipole approximation** from the following reason. The matrix element of \mathcal{H}' for $|a\rangle \rightarrow |b\rangle$ is with writing $A_0 \cos(\mathbf{k}_p \cdot \mathbf{r} - \omega t)$ as A ,

$$\frac{eA}{m} \mathbf{e}_p \cdot \langle b | \hat{\mathbf{p}} | a \rangle = \frac{eA}{m} \langle b | \mathbf{e}_p \cdot \frac{m}{i\hbar} [\hat{\mathbf{r}}, \mathcal{H}_0] | a \rangle = \frac{iA}{\hbar} (E_b - E_a) \mathbf{e}_p \cdot \langle b | (-e) \hat{\mathbf{r}} | a \rangle. \quad (4.37)$$

The last term is the transition element of the electric dipole moment operator and the transition by the Hamiltonian (4.36) is called dipole transition.

Substituting (4.30) to the Schrödinger equation $i\hbar \partial \psi / \partial t = (\mathcal{H}_0 + \mathcal{H}') \psi$, we obtain

$$i\hbar \left[\frac{dc_a}{dt} |a\rangle e^{-iE_a t/\hbar} + \frac{dc_b}{dt} |b\rangle e^{-iE_b t/\hbar} \right] = c_a \mathcal{H}' |a\rangle e^{-iE_a t/\hbar} + c_b \mathcal{H}' |b\rangle e^{-iE_b t/\hbar}. \quad (4.38)$$

Taking inner products with $\langle a |$ and $\langle b |$ leads to the following simultaneous differential equations for (c_a, c_b) .

$$\begin{cases} \frac{dc_a}{dt} = -\frac{i}{\hbar} c_b \langle a | \mathcal{H}' | b \rangle e^{-i\omega_0 t}, \\ \frac{dc_b}{dt} = -\frac{i}{\hbar} c_a \langle b | \mathcal{H}' | a \rangle e^{i\omega_0 t}, \end{cases} \quad \omega_0 \equiv \frac{E_b - E_a}{\hbar}. \quad (4.39)$$

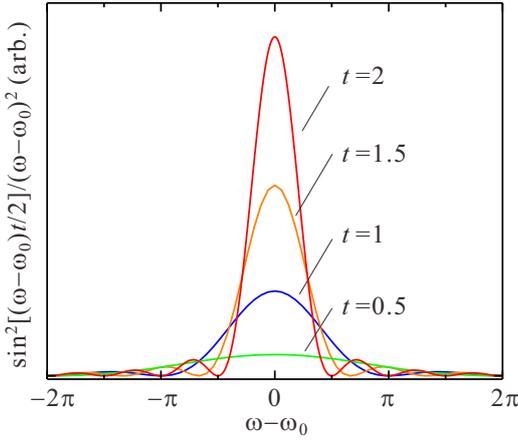
4.1.4 Optical absorption, emission

First we consider the optical absorption in (a). We take $c_a(0) = 1$, $c_b(0) = 0$ as the initial condition and $c_a^{(1)}(t) = 1$ as the starting point of the sequential substitution method to get the approximate solution.

$$\begin{aligned} c_a^{(1)}(t) &= 1, \\ c_b^{(1)}(t) &= -\frac{i}{\hbar} \int_0^t \langle b | \mathcal{H}' | a \rangle(t') e^{i\omega_0 t'} dt', \end{aligned} \quad (4.40a)$$

$$c_a^{(2)}(t) = 1 - \frac{1}{\hbar^2} \int_0^t dt' \langle a | \mathcal{H}' | b \rangle(t') e^{-i\omega_0 t'} \left[\int_0^{t'} dt'' \langle b | \mathcal{H}' | a \rangle(t'') e^{i\omega_0 t''} \right]. \quad (4.40b)$$

The expression $\langle b | \mathcal{H}' | a \rangle(t)$ is to clarify that $\langle b | \mathcal{H}' | a \rangle$ is a function of t .



and from (4.40a),

$$\begin{aligned} c_b(t) &\simeq -\frac{i}{\hbar} V_{ba} \int_0^t dt' \cos \omega t' e^{i\omega_0 t'} = -\frac{V_{ba}}{2\hbar} \left[\frac{e^{i(\omega_0 + \omega)t} - 1}{\omega_0 + \omega} + \frac{e^{i(\omega_0 - \omega)t} - 1}{\omega_0 - \omega} \right] \\ &\simeq -i \frac{V_{ba}}{\hbar} \frac{\sin[(\omega_0 - \omega)t/2]}{\omega_0 - \omega} e^{i(\omega_0 - \omega)t/2}. \end{aligned} \quad (4.42)$$

Then if we apply the oscillating electromagnetic field from $t = 0$, the probability amplitude of $|b\rangle$ at time t is

$$P_b(t) = |c_b(t)|^2 \simeq \frac{|V_{ba}|^2}{\hbar^2} \frac{t \sin^2[(\omega_0 - \omega)t/2]}{2(\omega_0 - \omega)^2(t/2)} \quad (4.43)$$

As is well known the last factor goes to a delta function in the limit of $t \rightarrow \infty$ ($\lim_{t \rightarrow \infty} \sin^2[(\omega_0 - \omega)t/2]/(\omega_0 - \omega)^2(t/2) = \pi\delta(\omega - \omega_0)$). Actually in the plot of $\sin^2[(\omega_0 - \omega)t/2]/(\omega_0 - \omega)^2$, the peak at $\omega - \omega_0 = 0$ grows high and sharp with the increase of t . Hence the factor represents the energy conservation.

When we take the initial condition as $c_b(0) = 1$, $c_a(0) = 0$, that is, the excited state $|b\rangle$ with photon field of ω , the transition $|b\rangle \rightarrow |a\rangle$, which is the reversed process of the optical absorption, occurs with the emission of a photon of ω_0 . This emitted photon is coherent to the existing coherent photon state[11]. This is the stimulated emission in (c).

Then how we treat spontaneous emission in (b) without photon field outside? As we saw in Sec. 4.1.1, even in the vacuum with zero number of photons, the zero-point quantum fluctuation of electromagnetic field exists for each mode. In the spontaneous emission process, the photon emission is “stimulated” by these zero-point fluctuations. Most of the light emission from semiconductor devices (other than lasers) is by this spontaneous emission. In that sense, we are looking at zero-point quantum fluctuation when we are facing electric displays.

4.1.5 Rabi oscillation

In the perturbation term $V_{ba} \cos(\omega t)$, the cosine part can be expressed as $(e^{i\omega t} + e^{-i\omega t})/2$, which means the decomposition into two terms rotation on the complex plane with the angular frequency of $\pm\omega$. Among them, the component important for the transition is with $\omega \sim \omega_0$ and the term of rotation with $-\omega$ has the frequency very far from ω_0 and can be ignored as

$$\langle a | \mathcal{H}' | b \rangle = \frac{V_{ab}}{2} e^{i\omega t}. \quad (4.44)$$

This kind of approximation is called **rotation wave approximation**, in which the simultaneous differential equations are

$$\begin{cases} \frac{dc_a}{dt} = -\frac{i}{2\hbar} c_b V_{ab} e^{-i(\omega_0 - \omega)t}, \\ \frac{dc_b}{dt} = -\frac{i}{2\hbar} c_a V_{ba} e^{i(\omega_0 - \omega)t}. \end{cases} \quad (4.45)$$

This can be written into a differential equation for a single variable as

$$\frac{d^2 c_b}{dt^2} + i(\omega - \omega_0) \frac{dc_a}{dt} + \frac{|V_{ab}|^2}{(2\hbar)^2} = 0. \quad (4.46)$$

The solution is obtained straightforwardly as

$$c_b(t) = c_+ e^{i\lambda_+ t} + c_- e^{i\lambda_- t}, \quad \lambda_{\pm} \equiv \frac{1}{2}(\delta \pm \sqrt{\delta^2 + |V_{ab}|^2/\hbar^2}), \quad \delta \equiv \omega_0 - \omega. \quad (4.47)$$

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

$$\begin{cases} c_b(t) = \frac{i|V_{ab}|}{\omega_R \hbar} e^{i\delta t/2} \sin(\omega_R t/2), \\ c_a(t) = e^{i\delta t/2} \left[\cos\left(\frac{\omega_R t}{2}\right) - i \frac{\delta}{\omega_R} \sin\left(\frac{\omega_R t}{2}\right) \right] \end{cases} \quad (4.48a)$$

$$(4.48b)$$

are obtained where

$$\omega_R \equiv \sqrt{\delta^2 + |V_{ab}|^2/\hbar^2} \quad (4.49)$$

is called **Rabi frequency**.

The oscillation between the two-levels caused by the electromagnetic wave (photon) with energy close to the energy difference between the two levels is called **Rabi oscillation**. When the photon energy is tuned to the energy difference ($\delta = 0$), the Rabi frequency is proportional to the magnitude of the electromagnetic irradiation. The Rabi oscillation is widely used in various resonance phenomena utilized to get information inside materials, or quantum information processing, etc.

4.1.6 Oscillator strength, selection rule

For the one-dimensional harmonic oscillator, which we consider in the beginning of this chapter, from (4.2), (4.4), we can write

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega_h}} (a + a^\dagger), \quad (4.50)$$

which leads to the dipole transition elements of (4.37), corresponding to $|0\rangle \rightarrow |1\rangle$ is

$$\langle 1 | (-e)\hat{x} | 0 \rangle = -e \sqrt{\frac{\hbar}{2m\omega_h}} \equiv \mu_{10}. \quad (4.51)$$

The probability of the dipole transition $|a\rangle \rightarrow |b\rangle$ is indicated by the transition dipole moment;

$$\boldsymbol{\mu}_{ba} \equiv \langle b | (-e)\hat{\mathbf{r}} | a \rangle. \quad (4.52)$$

Then for the “unit” of the strength, we take the transition dipole moment μ_{10} for the one-dimensional harmonic oscillator with the characteristic frequency $\omega_h = (E_b - E_a)/\hbar$. For the probability we need to take the square of the absolute value, we define **oscillator strength** as

$$f_{ba} = \frac{|\mu_{ba}|^2}{|\mu_{10}|^2} = \frac{2m\omega_{ba}}{e^2\hbar} |\mu_{ba}|^2. \quad (4.53)$$

The character f is commonly used and we also call it as “ f -value.”

When there are multiple possible final states $|b\rangle$, we use b as the index of all such states. Then the f -values satisfy the following **sum rule**.

$$\sum_b f_{ba} = 1. \quad (4.54)$$

For the system with N -electrons, the right hand side is N .

When the system has multiple directional oscillators with random directions, the effective transition dipole moment $\langle \mu_{\text{eff}} \rangle$ is given by taking the average as $\mu_{ba}/3$. Then the oscillator strength is expressed as

$$f'_{ba} = \frac{2m\omega_{ba}}{3e^2\hbar} |\mu_{ba}|^2. \quad (4.55)$$

When the system has spatial inversion symmetry, the eigenstates of the Hamiltonian should have the parity for the spatial inversion operation. That is, for an eigenstate $\phi_n(\mathbf{r})$, the following should hold.

$$\phi_n(-\mathbf{r}) = \pm \phi_n(\mathbf{r}). \quad (4.56)$$

$+$, $-$ correspond to even and odd parity respectively. In the expression (4.52), \mathbf{r} has the odd parity then if $|a\rangle$, $|b\rangle$ have the same parity, the integration gives zero for μ_{ba} and the dipole transition is forbidden. As above, the rule that dominates the possibility of a transition along with symmetry, quantum number etc. is called **selection rule**.

4.2 Interband transition and optical response

So far we have seen very basic knowledges on the optical response of two-level systems. We now expand the concepts and the discussions to the electronic states in solids, in which both ground states and excited states are extended over the crystals.

4.2.1 Absorption of light with interband transition

Materials absorb electromagnetic wave in various ways. Free carrier absorption, impurity absorption, absorption by lattice vibration, etc. though the main absorption used in the optical devices is the absorption due to the interband transition of electrons. Thus in this sub-section, we will see the very basics of the interband transition absorption.

For simplicity, we write a plane electromagnetic wave with a linear polarization propagating along z axis with vector potential \mathbf{A} as

$$\mathbf{A} = A_0 \mathbf{e} \exp[i(\mathbf{k}_p \cdot \mathbf{r} - \omega t)]. \quad (4.57)$$

The wavenumber \mathbf{k}_p is $(0, 0, k_p)$, \mathbf{e} is the polarization vector and we put $\mathbf{e}_x = (1, 0, 0)$. The electric field $\mathbf{E} = -\partial\mathbf{A}/\partial t$, the magnetic field $\mathbf{H} = \mu^{-1}\text{rot}\mathbf{A}$ (μ is the permeability of the medium), then the energy flow density (Poynting vector) is

$$\mathbf{I} = \langle \mathbf{E} \times \mathbf{H} \rangle = \frac{\epsilon_0 c \bar{n} \omega^2 A_0^2}{2} \mathbf{e}_z. \quad (4.58)$$

\bar{n} is the refractive index (light speed in the medium is $c' = 1/\sqrt{\epsilon_1\epsilon_0\mu_1\mu_0}$ (ϵ_1, μ_1 are the ratio of dielectric constant and that of magnetic permeability to those of vacuum) $\bar{n} = c/c' = \sqrt{\epsilon_1\mu_1}$), $\mathbf{e}_z = (0, 0, 1)$.

The absorption of light causes the exponential damping of the intensity $|I|$ as $I(z) = I_0 \exp(-\alpha z)$. The damping constant α is the **absorption coefficient**. From this definition $\alpha = -dI/Idz = -dI/Ic'dt$. Thus if we assign the averaged number of photons absorbed in the unit time and the unit volume as W , then the decreasing rate of I is written as $\hbar\omega W$ giving

$$\alpha = \frac{\hbar\omega W}{I} = \frac{2\hbar\omega W}{\epsilon_0 c \bar{n} \omega^2 A_0^2}. \quad (4.59)$$

Among the various absorption mechanisms, that caused by a valence electron absorbing a photon and being excited to the conduction band, is called **fundamental absorption**. The fundamental absorption begins just above the band gap. The absorption just at the band gap is called “band edge absorption”.

We write the Hamiltonian of the system as $\mathcal{H} = (\mathbf{p} + e\mathbf{A})^2/2m_0 + V(\mathbf{r})$ and treat \mathbf{A} as a perturbation. With ignoring \mathbf{A}^2 , $\mathcal{H} = \mathcal{H}_0 + (e/m_0)\mathbf{A} \cdot \mathbf{p}$. Bloch functions in conduction band and valence band are written as $|c\mathbf{k}\rangle = u_{c\mathbf{k}}e^{i\mathbf{k}\mathbf{r}}$, $|v\mathbf{k}\rangle = u_{v\mathbf{k}}e^{i\mathbf{k}\mathbf{r}}$ respectively and the perturbation term causes the transition from the valence band to the conduction band with the probability W_{vc} per unit volume in the Fermi's golden rule approximation as

$$W_{vc} = \frac{2\pi e}{\hbar m_0} |\langle c\mathbf{k} | \mathbf{A} \cdot \mathbf{p} | v\mathbf{k}' \rangle|^2 \delta(E_c(\mathbf{k}) - E_v(\mathbf{k}') - \hbar\omega) = \frac{\pi e^2}{2\hbar m_0^2} A_0^2 |M|^2 \delta(E_c(\mathbf{k}) - E_v(\mathbf{k}') - \hbar\omega), \quad (4.60)$$

$$\begin{aligned} M &= \int_V \frac{d^3r}{V} e^{i(\mathbf{k}_p + \mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}} u_{c\mathbf{k}}^*(\mathbf{r}) \mathbf{e} \cdot (\mathbf{p} + \hbar\mathbf{k}') u_{v\mathbf{k}'}(\mathbf{r}) = \frac{\sum_l e^{i(\mathbf{k}_p + \mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}_l}}{V} \int_{\Omega} d^3r u_{c\mathbf{k}}^*(\mathbf{r}) \mathbf{e} \cdot (\mathbf{p} + \hbar\mathbf{k}') u_{v\mathbf{k}'}(\mathbf{r}) \\ &= \frac{N}{V} \delta_{\mathbf{k}_p + \mathbf{k}' - \mathbf{k}, \mathbf{K}} \int_{\Omega} d^3r u_{c\mathbf{k}}^*(\mathbf{r}) \mathbf{e} \cdot (\mathbf{p} + \hbar\mathbf{k}') u_{v\mathbf{k}'}(\mathbf{r}). \end{aligned} \quad (4.61)$$

Here, l is the label of lattice points, V, Ω are the volumes of the system and the unit cell respectively. \mathbf{K} is a reciprocal lattice vector, \mathbf{k}_p a photon wavenumber, N the total number of the lattice points, $N\Omega = V$.

In eq.(4.61) we implicitly consider a direct excitation of an electron by the electromagnetic field of a photon. Such a transition is called a **direct transition**. The necessary condition for the momentum conservation in a fundamental absorption is $\mathbf{k}_p + \mathbf{k}' - \mathbf{k} = \mathbf{K}$, though practically from common values of band gaps, effective masses and lattice constants, it turns to be $\mathbf{K} = \mathbf{0}$. Also within the dipole transition approximation, \mathbf{k}_p can be ignored and we can put

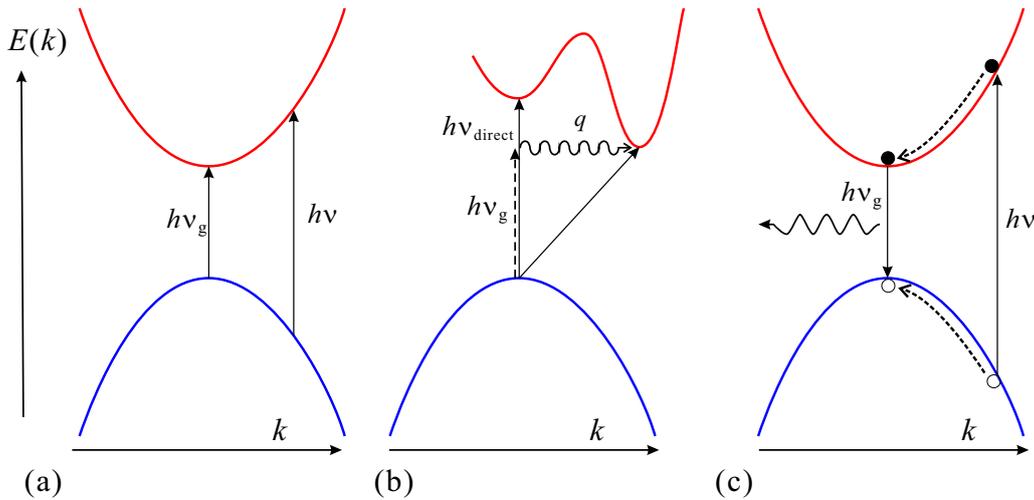


Fig. 4.2 Illustrations of optical response due to the interband transition of an electron. (a) Optical absorption with direct interband transition. (b) Optical absorption with indirect interband transition. (c) Photoluminescence, in which optically excited electron-hole pair recombine for the light emission.

$\mathbf{k} = \mathbf{k}'$. $u_{c\mathbf{k}}(\mathbf{r})$, $u_{v\mathbf{k}}(\mathbf{r})$ belong to different eigenvalues hence the term of $\hbar\mathbf{k}'$ in (4.61) vanishes giving

$$M = \int_{\Omega} \frac{d^3r}{\Omega} u_{c\mathbf{k}}^*(\mathbf{r}) \mathbf{e} \cdot \mathbf{p} u_{v\mathbf{k}}(\mathbf{r}). \quad (4.62)$$

From (4.59) and (4.62), we assume \mathbf{k} -dependence of M is weak and obtain the expression for the absorption coefficient for direct transition as

$$\alpha_{\text{da}} = \frac{\pi e^2}{\bar{n}\epsilon_0\omega cm_0^2} |M|^2 \sum_{\mathbf{k}} \delta(E_c(\mathbf{k}) - E_v(\mathbf{k}) - \hbar\omega). \quad (4.63)$$

The summation part on \mathbf{k} is called **joint density of states**. Let us write it as $J_{cv}(\hbar\omega)$ and $E_c(\mathbf{k}) - E_v(\mathbf{k})$ as $E_{cv}(\mathbf{k})$, and turn the summation on \mathbf{k} in an integral form to get

$$J_{cv}(\hbar\omega) = \sum_{\mathbf{k}} \delta(E_{cv}(\mathbf{k}) - \hbar\omega) = 2 \int \frac{d^3k}{(2\pi)^3} \delta(E_{cv}(\mathbf{k}) - \hbar\omega). \quad (4.64)$$

We transform the integral in \mathbf{k} -space into that on the infinitesimal area dS on an equi-energy surface and on the energy E_{cv} . By writing the k -component perpendicular to the equi-energy surface as k_{\perp} , the integration can be transformed into

$$\begin{aligned} d^3k &= dS dk_{\perp} = dS \frac{dk_{\perp}}{dE_{cv}} dE_{cv} = dS |\nabla_{\mathbf{k}} E_{cv}|^{-1} dE_{cv}, \\ \therefore J_{cv}(\hbar\omega) &= \frac{2}{(2\pi)^3} \int \frac{dS}{|\nabla_{\mathbf{k}} E_{cv}(\mathbf{k})|_{E_{cv}=\hbar\omega}}. \end{aligned} \quad (4.65)$$

From the above we see that we have absorption anomalies around the points where the integrand of (4.65) vanishes. Let us consider the case of a direct gap semiconductor as illustrated in Fig. ??(a), and assume $E_{cv} = E_g$, $\nabla_{\mathbf{k}} E_{cv} = \mathbf{0}$ at $\mathbf{k} = \mathbf{k}_0$. In the expansion of E_{cv} around \mathbf{k}_0 , the first order term is zero and taking the second order term we get

$$E_{cv}(\mathbf{k}) = E_g + \sum_i \frac{\hbar^2}{2\xi_i} (k_i - k_{i0})^2. \quad (4.66)$$

For simplicity let $\xi_i > 0 (i = 1, 2, 3)$. With variable translation $(\hbar/(2\xi_i)^{1/2})(k_i - k_{i0}) = s_i$,

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

We also consider the integration in s -space with that on equi-energy surfaces and on the energy. Because $|\nabla_{\mathbf{s}} E_{cv}| = 2s$,

$$J_{cv} = \frac{2}{(2\pi)^3} \frac{\sqrt{8\xi_1\xi_2\xi_3}}{\hbar^3} \int \frac{dS}{2s} = \frac{1}{2\pi^2} \frac{\sqrt{8\xi_1\xi_2\xi_3}}{\hbar^3} \sqrt{\hbar\omega - E_g} = \frac{\sqrt{2}}{\pi^2} \frac{m_r^{3/2}}{\hbar^3} \sqrt{\hbar\omega - E_g}. \quad (4.67)$$

The calculation in the last line is for a direct gap semiconductor as illustrated in Fig. ??(a), based on the assumption of isotropic effective mass at the band edge, *i.e.*, $\forall i \quad \xi_i = m_r$. From $m_r^{-1} = m_e^{*-1} + m_h^{*-1}$ this is the reduced mass for an electron-hole pair. After all, (4.67) is the density of states in a three dimensional \mathbf{k} space, that is just a re-calculation of the density of states in a three dimensional system (2.14). In this case, from the expression of the absorption coefficient in a direct transition (4.63),

$$\alpha(\hbar\omega) = \frac{e^2(2m_r)^{3/2} |M|^2}{2\pi\epsilon_0 m_0^2 \bar{n}\omega c \hbar^3} \sqrt{\hbar\omega - E_g}, \quad (4.68)$$

is obtained. The factor in the left hand side other than the joint density of states

$$f_{vc} = \frac{2|M|^2}{m_0\hbar\omega}, \quad (4.69)$$

in which $|M|^2/\omega$ is representing the strength of the transition. The dimensionless quantity f_{vc} is called **oscillator strength**.

Appendix 4A: Rate of stimulated emission, spontaneous emission

Here we consider many identical two-level systems with states ($|a\rangle, |b\rangle$). They are placed in the electromagnetic field with the energy density spectrum $U(\omega)$, where ω is the angular frequency. There is no direction interaction between the two-level systems while they are in equilibrium with the electromagnetic field, which is in thermal equilibrium, *i.e.* has the energy distribution of Planck law of radiation, and the momentum distributes isotopically. The rate of optical absorption (frequency per unit time) for $\omega \sim \omega_0$ is obtained from (4.37) as

$$|\langle b|\mathcal{H}'|a\rangle| = |E_0\mathbf{e}_p \cdot \langle b|(-e)\hat{\mathbf{r}}|a\rangle| = |E_0\mathbf{e}_p \cdot \boldsymbol{\mu}_{ba}|, \quad (4A.1)$$

where $E_0 = \omega A_0$ is the amplitude of the oscillation in electric field. From(4.43), the absorption probability is proportional to the square of the above, hence to $E_0^2 \propto U$. In the form of equation the absorption rate W_{ba} is written as

$$W_{ba} = B_{ba}U(\omega), \quad (4A.2)$$

with B_{ba} a coefficient. We write the emission rate as the sum of the rate for spontaneous emission, which is independent of U and the rate for the stimulated emission, which is proportional to U .

$$W_{ab} = A + B_{ab}U(\omega). \quad (4A.3)$$

As seen in Sec.4.1.4, the optical absorption and the stimulated emission are in the relation of reversed process,

$$B_{ba} = B_{ab} \equiv B. \quad (4A.4)$$

We write $E_b - E_a = \hbar\omega$, and let the numbers of the two-level systems in the states a, b as N_a, N_b respectively. Then

$$N_b = N_a \exp\left(-\frac{\hbar\omega}{k_B T}\right). \quad (4A.5)$$

Because the system is in equilibrium, the event frequencies of emissions and absorption should be the same, *i.e.*

$$BUN_a = (A + BU)N_b. \quad (4A.6)$$

These leads to the following expression for $U(\omega)$.

$$U(\omega) = \frac{A}{B} \frac{1}{\exp(\hbar\omega/k_B T) - 1}. \quad (4A.7)$$

We request this to be equivalent to the Planck law of radiation

$$U(\omega) = \frac{\hbar\omega^3}{\pi^2 c^3} \frac{1}{\exp(\hbar\omega/k_B T) - 1}, \quad (4A.8)$$

and obtain

$$\frac{A}{B} = \frac{\hbar\omega^3}{\pi^2 c^3}. \quad (4A.9)$$

These coefficient A, B are called **Einstein A coefficient, B coefficient** respectively.

In the discussion of transition probability (4.43), we have considered photons with single energy $\hbar\omega$. Now we consider a finite width $\delta\omega$ of the energy distribution around ω_0 with the photon density (4A.8). We write the electric field amplitude for ω_0 as E_0 , then the energy density is $\epsilon_0 E_0^2/2$ ^{*2}.

$$\epsilon_0 \frac{E_0^2}{2} = \int_{\omega_0 - \delta\omega/2}^{\omega_0 + \delta\omega/2} U(\omega) d\omega. \quad (4A.10)$$

^{*2} From (??), the energy of oscillating electromagnetic field is $\langle (\epsilon_0 E^2 + B^2/\mu_0)/2 \rangle = \epsilon_0 \langle (E^2) \rangle$, and then the time average gives $\epsilon_0 E_0^2/2$.

And taking the directional average, we obtain

$$\langle |\boldsymbol{\mu}_{ab} \cdot \mathbf{e}_p|^2 \rangle = \langle \mu_{12}^2 \cos^2 \theta \rangle = \frac{\mu_{12}^2}{3}. \quad (4A.11)$$

The the transition probability (4.43) can be approximated as

$$|c_b(t)|^2 \simeq \frac{|\boldsymbol{\mu}_{ab}|^2}{3\hbar^2} \frac{1}{\epsilon_0} \int_{\omega_0 - \delta\omega/2}^{\omega_0 + \delta\omega/2} U(\omega) \frac{\sin^2[(\omega - \omega_0)t/2]}{(\omega - \omega_0)^2} d\omega \approx \frac{\pi\mu_{ab}^2}{3\epsilon_0\hbar^2} U(\omega_0)t. \quad (4A.12)$$

We replace the integral over the period $\delta\omega$ with the infinite integration. And we applied the identity $\lim_{\lambda \rightarrow \infty} \sin^2 \lambda x / \lambda x^2 = \pi\delta(x)$. The transition probability is obtained as $|c_b(t)|^2/t$. Then the discussion leads to the expression of B coefficient as

$$B = \frac{\pi\mu_{ab}^2}{3\epsilon_0\hbar^2} = \frac{\pi e^2}{6\epsilon_0 m \hbar \omega_0} f_{ba}. \quad (4A.13)$$

If we use the frequency spectrum $\rho(\nu)$ ($2\pi\nu = \omega$) instead of the angular frequency spectrum $U(\omega)$, the expression needs correction of 2π , of course.

References

- [1] N. F. Mott, “Metal-Insulator Transitions” (CRC Press, 1990); 和訳 「金属と非金属の物理」 小野嘉之, 大槻東巳 (丸善, 1996).
- [2] 小野嘉之 「金属絶縁体転移」 (朝倉書店, 2002).
- [3] 大槻東巳 「不規則電子系の金属-絶縁体転移」 (現代物理最前線 (2) 共立出版, 2000).
- [4] 米沢富美子 「金属-非金属転移の物理」 (朝倉書店, 2012).
- [5] D. Stauffer and A. Aharony, “Introduction to Percolation Theory” (2nd ed., Taylor & Francis, 2018); 和訳 「パーコレーションの基本原理」 小田垣 孝 (吉岡書店, 2001).
- [6] M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. **70**, 1039 (1998).
- [7] D. C. Reynolds, “Excitons: Their Properties and Uses” (Academic Press, 1981).
- [8] 本格的に学ぶには例えば, R. Loudon, “The Quantum Theory of Light” (3rd ed., Oxford, 2000); P. Meystre and M. Sargent III, “Elements of Quantum Optics” (Springer, 1990); 松岡正浩 「量子光学」 (裳華房, 2000) など.
- [9] J. H. Jeans, Phil. Mag. **10**, 91 (1905).
- [10] 太田浩一 「マクスウェル理論の基礎」 (東京大学出版会, 2002).
- [11] 霜田光一 「レーザー物理入門」