

10 / Non-coherent transport

10.1. Why does an atom emit light?

10.2. Examples

10.3. Inflow and outflow

10.4. Supplementary notes: Phonons

In Chapter 9, we have discussed a quantum mechanical model that describes the flow of electrons *coherently* through a channel. All dissipative/ phase-breaking processes were assumed to be limited to the contacts where they act to keep the electrons in local equilibrium. In practice, such processes are present in the channel as well and their role becomes increasingly significant as the channel gets longer. Indeed prior to the advent of mesoscopic physics, the role of contacts was assumed to be minor and quantum transport theory was essentially focused on the effect of such processes. By contrast, we have taken a “bottom-up” view of the subject and now that we understand how to model a small coherent device, we are ready to discuss dissipative/phase-breaking processes.

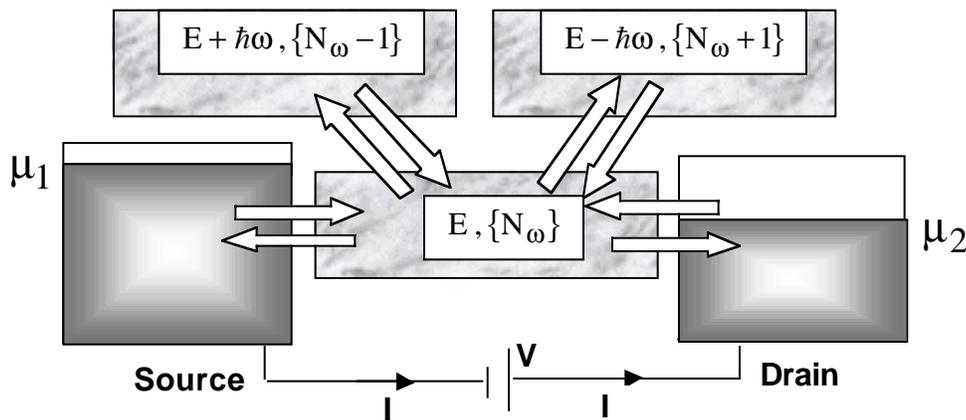


Fig.10.1. Phase-breaking introduces a coupling to neighboring configurations having one more or one less number of excitations $\{N_\omega\}$ than the original.

Phase-breaking processes arise from the interaction of one electron with the surrounding bath of photons, phonons and other electrons. Compared to the coherent processes that we have discussed so far, the essential difference is that phase-breaking processes involve a

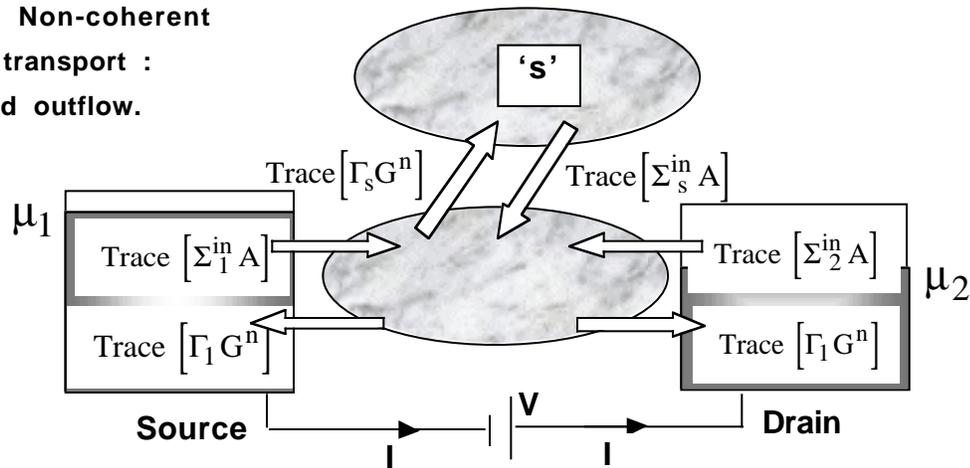
change in the “surroundings”. In coherent interactions, the background is rigid and the electron interacts elastically with it, somewhat like a ping pong ball bouncing off a truck. The motion of the truck is insignificant. In reality, the background is not quite as rigid as a truck and is set in “motion” by the passage of an electron and this excitation of the background is described in terms of phonons, photons etc. This is in general a difficult problem with no exact solutions and what we will be describing here is the lowest order approximation, sometimes called the self-consistent Born approximation, which usually provides an adequate description. Within this approximation, these interactions can essentially be viewed as a coupling of the channel from the “standard” configuration with $\{N_\omega\}$ phonons/photons (in different modes with different frequencies $\{\omega\}$) to a neighboring configuration with one less (absorption) or one more (emission) phonon/photon as depicted in Fig.10.1.

This coupling to neighboring configurations results in an outflow of electrons from our particular subspace and a subsequent return or inflow back into this subspace. A general model for quantum transport needs to include this inflow and outflow into the coherent transport model from Chapter 9, through an additional terminal ‘s’ described by the additional terms Σ_s^{in} and Σ_s (see Fig.10.2). My objective in this Chapter is to explain how these additional terms are calculated. We have seen that for the regular contacts, the inscattering is related to the broadening:

$$\Sigma_1^{\text{in}} = \Gamma_1 f_1 \quad \text{and} \quad \Sigma_2^{\text{in}} = \Gamma_2 f_2$$

However, for the scattering terminal both Σ_s^{in} and Σ_s have to be determined separately since there is no Fermi function f_s describing the scattering “terminal” and hence no simple connection between Σ_s^{in} and Σ_s (or Γ_s), unlike the contacts. Of course, one could adopt a phenomenological point of view and treat the third terminal like another contact whose chemical potential μ_s is adjusted to ensure zero current at this terminal. That would be in the spirit of the “Buttiker probe” discussed in Chapter 9 and could well be adequate for many applications. However, I will describe microscopic (rather than phenomenological) models for Σ_s^{in} and Σ_s that can be used to benchmark any phenomenological models that the reader may choose to use. They can also use these models as a starting point to include more sophisticated scattering mechanisms as needed.

Fig.10.2. Non-coherent quantum transport : Inflow and outflow.



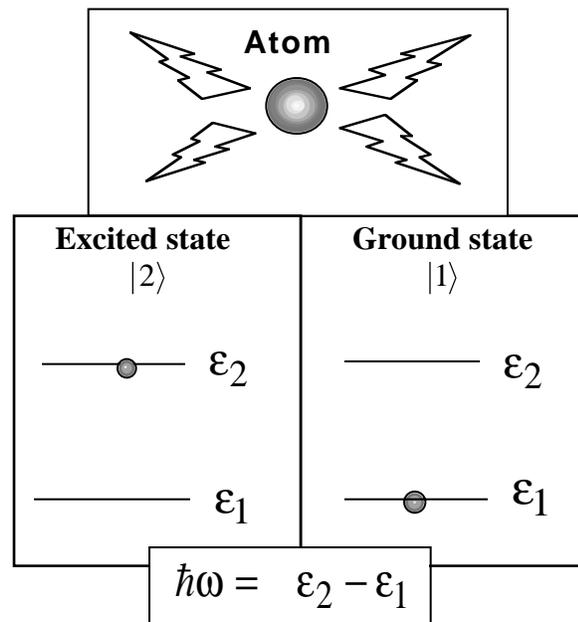
The inflow and outflow associated with dissipative processes involves subtle conceptual issues beyond what we have encountered so far with coherent transport. A fully satisfactory description requires the advanced formalism described in the Appendix, but in this Chapter I will try to derive the basic results and convey the subtleties without the use of this formalism. In the next Chapter I will summarize the complete set of equations for dissipative quantum transport and illustrate their use with a few interesting examples.

We will start in Section 10.1 by explaining two viewpoints that one could use to model the interaction of electrons with its surroundings, say the electromagnetic vibrations or photons. One viewpoint is based on the one-particle picture where we visualize the electron as being affected by its surroundings through a scattering potential U_s . However, as we will see, in order to explain the known equilibrium properties it is necessary to endow this potential U_s with rather special properties that make it difficult to include in the Schrodinger equation. Instead we could adopt a viewpoint whereby we view the electron and photons together as one giant system described by a giant multiparticle Schrodinger equation. This viewpoint leads to a more satisfactory description of the interaction, but at the expense of conceptual complexity. In general it is important to be able to switch between these viewpoints so as to combine the simplicity of the one-particle picture with the rigor of the multiparticle approach. I will illustrate the basic principle in Section 10.2 using a few simple examples before discussing the general expressions for inflow and outflow in Section 10.3.

10.1. Why does an atom emit light?

We started this book by noting that the first great success of the Schrodinger equation was to explain the observed optical spectrum of the Hydrogen atom. It was found that the light emitted by a hot vapor of hydrogen atoms consisted of discrete frequencies $\omega = 2\pi\nu$ that were related to the energy eigenvalues from the Schrodinger equation : $\hbar\omega = \epsilon_n - \epsilon_m$. This is explained by saying that if an electron is placed in an excited state $|2\rangle$, it relaxes to the ground state $|1\rangle$ and the difference in energy is radiated in the form of light or photons (Fig.10.1.1). Interestingly, however, this behavior does not really follow from the Schrodinger equation, unless we add something to it.

Fig.10.1.1. If an electron is placed in an excited state $|2\rangle$, it will lose energy by radiating light and relax to the ground state $|1\rangle$. However, this behavior does not follow from the Schrodinger equation, unless we modify it appropriately.



To see this let us write the time-dependent Schrodinger equation (Eq.(1.1.8)) in the form of a matrix equation

$$i\hbar \frac{d}{dt} \{\psi\} = [H] \{\psi\} \quad (10.1.1)$$

using a suitable set of basis functions. If we use the eigenfunctions of $[H]$ as our basis then this equation has the form:

$$i\hbar \frac{d}{dt} \begin{Bmatrix} \Psi_1 \\ \Psi_2 \\ \dots \\ \dots \end{Bmatrix} = \begin{bmatrix} \varepsilon_1 & 0 & 0 & \dots \\ 0 & \varepsilon_2 & 0 & \dots \\ 0 & 0 & \varepsilon_3 & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \begin{Bmatrix} \Psi_1 \\ \Psi_2 \\ \dots \\ \dots \end{Bmatrix}$$

which decouples neatly into a set of independent equations:

$$i\hbar \frac{d}{dt} \{\Psi_n\} = [\varepsilon_n] \{\Psi_n\} \quad (10.1.2)$$

one for each energy eigenvalue ε_n . It is easy to write down the solution to Eq.(10.1.2) for a given set of initial conditions at $t = 0$:

$$\Psi_n(t) = \Psi_n(0) \exp(-i\varepsilon_n t / \hbar) \quad (10.1.3a)$$

This means that the probability P_n for finding an electron in state ‘n’ does not change with time:

$$P_n(t) = |\Psi_n(t)|^2 = |\Psi_n(0)|^2 = P_n(0) \quad (10.1.3b)$$

According to the Schrodinger equation, an electron placed in an excited state would stay there for ever! Whatever it is that causes the excited state to relax is clearly not a part of Eq.(10.1.1) or (10.1.2).

So what is missing? There are two ways to answer this question. Let us describe these one by one.

One-particle viewpoint: This viewpoint says that the electrons feel a random external potential U^S due to the photons in the surrounding “box” which causes it to relax to the ground state. This potential gives rise to off-diagonal terms in the Hamiltonian which couple the different states together.

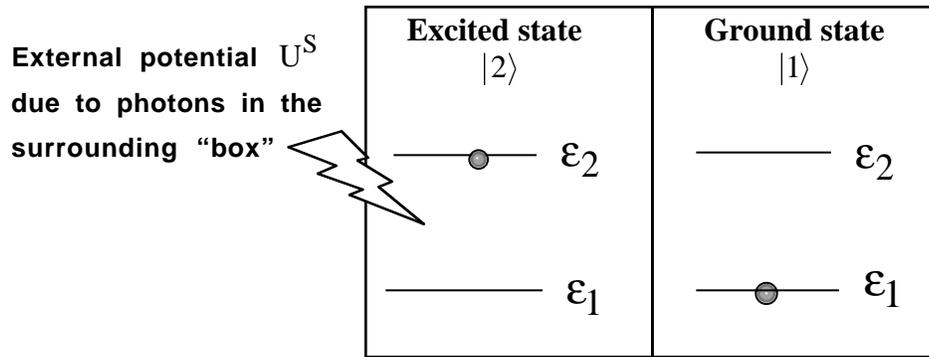


Fig.10.1.2. In the one-particle viewpoint the electrons are said to feel an external potential U^S due to the photons in the surrounding "box" which causes it to relax from $|2\rangle$ to $|1\rangle$.

With just two states we could write

$$i\hbar \frac{d}{dt} \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} = \begin{bmatrix} \epsilon_1 & U_{12}^S \\ U_{21}^S & \epsilon_2 \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} \quad (10.1.4)$$

Without getting into any details it is clear that if the electron is initially in state $|2\rangle$, the term U_{12}^S will tend to drive it to state $|1\rangle$. But this viewpoint is not really satisfactory. Firstly, one could ask why there should be any external potential U^S at zero temperature when all thermal excitations are frozen out. The answer usually is that even at zero temperature there is some noise present in the environment, and these so-called zero point fluctuations tickle the electron into relaxing from $|2\rangle$ to $|1\rangle$. But that begs the second question: why do these zero point fluctuations not provide any transitions from $|1\rangle$ to $|2\rangle$? Somehow we need to postulate a scattering potential for which (note that $\epsilon_2 > \epsilon_1$)

$$U_{21}^S = 0 \quad \text{but} \quad U_{12}^S \neq 0$$

at zero temperature.

For non-zero temperatures, U_{21}^S need not be zero, but it will still have to be much smaller than U_{12}^S , so as to stimulate a greater rate $S(2 \rightarrow 1)$ of transitions from 2 to 1 than from 1 to 2. For example, we could write

$$S(2 \rightarrow 1) = K_{2 \rightarrow 1} f_2 (1 - f_1) \quad , \text{ and } \quad S(1 \rightarrow 2) = K_{1 \rightarrow 2} f_1 (1 - f_2)$$

where $f_1 (1 - f_2)$ is the probability for the system to be in state $|1\rangle$ (level '1' occupied with level '2' empty) and $f_2 (1 - f_1)$ is the probability for it to be in state $|2\rangle$ (level '2' occupied with level '1' empty). At equilibrium the two rates must be equal, which requires that

$$\frac{K_{1 \rightarrow 2}}{K_{2 \rightarrow 1}} = \frac{f_2 (1 - f_1)}{f_1 (1 - f_2)} = \frac{(1 - f_1) / f_1}{(1 - f_2) / f_2} \quad (10.1.5)$$

But at equilibrium, the occupation factors f_1 and f_2 are given by the Fermi function:

$$f_n = \frac{1}{1 + \exp((\epsilon_n - \mu) / k_B T)} \quad \rightarrow \quad \frac{1 - f_n}{f_n} = \exp\left(\frac{\epsilon_n - \mu}{k_B T}\right)$$

Hence from Eq.(10.1.5),

$$\left(\frac{K_{1 \rightarrow 2}}{K_{2 \rightarrow 1}}\right)_{\text{equilibrium}} = \exp\left(-\frac{\epsilon_2 - \epsilon_1}{k_B T}\right) \quad (10.1.6)$$

Clearly at equilibrium, $K_{2 \rightarrow 1} \gg K_{1 \rightarrow 2}$, as long as the energy difference $(\epsilon_2 - \epsilon_1) \gg k_B T$.

Early in the twentieth century, Einstein argued that if the number of photons with energy $\hbar\omega$ present in the box is N then the rate of downward transitions is proportional to $(N+1)$ while the rate of upward transitions is proportional to N :

$$\begin{aligned} K(1 \rightarrow 2) &= \alpha N && \textit{photon absorption} \\ K(2 \rightarrow 1) &= \alpha(N+1) && \textit{photon emission} \end{aligned} \quad (10.1.7)$$

This ensures that at equilibrium, Eq.(10.1.6) is satisfied since the number of photons is given by the Bose-Einstein factor

$$[N]_{\text{equilibrium}} = \frac{1}{\exp(\hbar\omega/k_B T) - 1}$$

(10.1.8)

and it is easy to check that

$$\left(\frac{K_{1 \rightarrow 2}}{K_{2 \rightarrow 1}} \right)_{\text{equilibrium}} = \left(\frac{N}{N+1} \right)_{\text{equilibrium}} = \exp\left(-\frac{\hbar\omega}{k_B T} \right)$$

(10.1.9)

Since $\hbar\omega = \varepsilon_2 - \varepsilon_1$, Eqs.(10.1.9) and (10.1.6) are consistent.

What is not clear is why the external potential should stimulate a greater rate of downward transitions ($2 \rightarrow 1$) than upward transitions ($1 \rightarrow 2$), but clearly this must be the case if we are to rationalize the fact that at equilibrium, lower energy states are more likely to be occupied than higher energy states as predicted by the Fermi function. But there is really no straightforward procedure for incorporating this effect into the Schrodinger equation with an appropriate choice of the scattering potential U^S . Any Hermitian operator U^S will have $U_{12}^S = U_{21}^S$ and thus provide equal rates of upward and downward transitions.

Many-particle viewpoint: This brings us to the other viewpoint which provides a natural explanation for the difference between upward and downward transition rates, but is conceptually more complicated. In this viewpoint we picture the electron + photon as one big many-particle system whose dynamics is described by an equation that formally looks just like the Schrodinger equation (Eq.(10.1.1))

$$i\hbar \frac{d}{dt} \{\Psi\} = [H] \{\Psi\} \quad (10.1.10)$$

However, $\{\Psi\}$ now represents a statevector in a multiparticle Hilbert space which includes both the electron and the photon systems. The basis functions in this multiparticle space can be written as a product of the electronic and photonic subspaces (see Fig.10.1.3):

$$|n, N\rangle = |n\rangle \otimes |N\rangle$$

electron photon

just as the basis functions in a 2-dimensional problem can be written as the product of the basis states of two 1-dimensional problems:

$$|k_x, k_y\rangle = |k_x\rangle \otimes |k_y\rangle \sim \exp(ik_x x) \exp(ik_y y)$$

x- y-

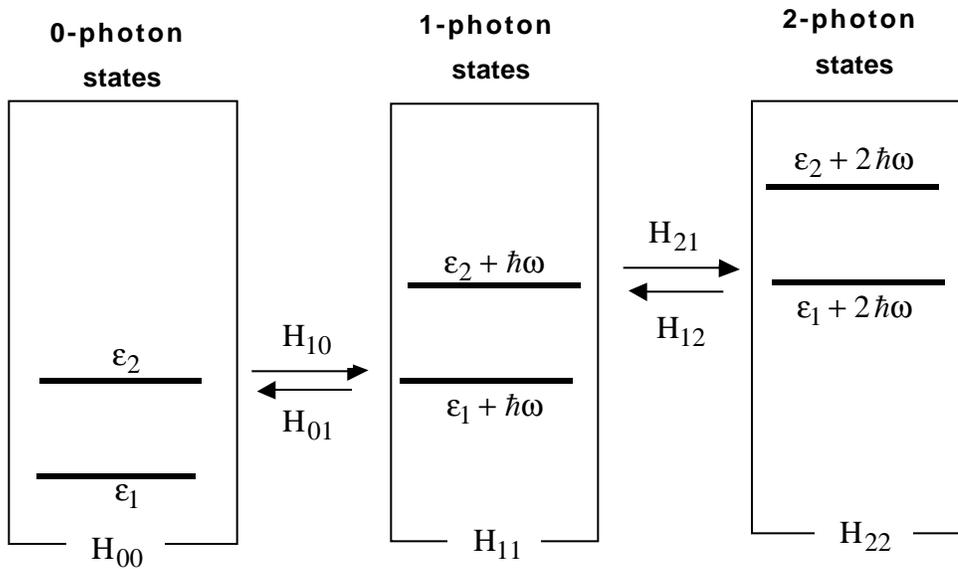


FIG.10.1.3. In the multiparticle viewpoint, the electron-photon coupling causes transitions between $|2, N\rangle$ and $|1, N-1\rangle$ which are degenerate states of the composite system.

We can write Eq.(10.1.10) in the form of a matrix equation:

$$i\hbar \frac{d}{dt} \begin{Bmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \end{Bmatrix} = \begin{bmatrix} H_{00} & H_{01} & 0 & \cdots \\ H_{10} & H_{11} & H_{12} & \cdots \\ 0 & H_{21} & H_{22} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \begin{Bmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \end{Bmatrix}$$

where $\{\Psi_N\}$ represents the N-photon component of the wavefunction. If the electronic subspace is spanned by two states $|1\rangle$ and $|2\rangle$ as shown in Fig.10.1.4 then $\{\Psi_N\}$ is a (2x1)

column vector $\{\Psi_N\} = \begin{Bmatrix} \Psi_{1,N} \\ \Psi_{2,N} \end{Bmatrix}$ and the matrices H_{NM} are each (2x2) matrices given by

$$H_{NN} = \begin{bmatrix} \epsilon_1 + N\hbar\omega & 0 \\ 0 & \epsilon_2 + N\hbar\omega \end{bmatrix} \quad (10.1.11)$$

$$H_{N,N+1} = \begin{bmatrix} 0 & K\sqrt{N+1} \\ K^*\sqrt{N+1} & 0 \end{bmatrix}, \quad H_{N+1,N} = H_{N,N+1}^\dagger$$

Broadening: The point is that if we consider the N-photon subspace, it is like an open system that is connected to the (N+1)- and (N-1)-photon subspaces, just as a device is connected to the source and drain contacts. In chapter 7, we saw that the effect of the source or drain contact could be represented by a self-energy matrix

$$\Sigma = \tau g \tau^\dagger \quad (\text{same as Eq.(7.2.7)})$$

whose imaginary (more precisely anti-Hermitian) part represents the broadening

$$\Gamma \equiv i[\Sigma - \Sigma^\dagger] = \tau a \tau^\dagger$$

$a \equiv i[g - g^\dagger]$ being the spectral function of the isolated reservoir. We could use the same relation to calculate the self-energy function that describes the effect of the rest of the photon reservoir on the N-photon subspace, which we view as the “channel”. Actually the details are somewhat more complicated because (unlike coherent interactions) we have to account for the exclusion principle. For the moment, however, let us calculate the broadening (or the outflow) assuming all other states to be “empty” so that there is no exclusion principle to worry about. Also, to keep things simple, let us focus just on the diagonal element of the broadening;

$$\begin{aligned} [\Gamma_{mn}(E)]_{N,N} &= [H_{nm}]_{N,N+1} [a_{mm}]_{N+1,N+1} [H_{mn}]_{N+1,N} \\ &+ [H_{nm}]_{N,N-1} [a_{mm}]_{N-1,N-1} [H_{mn}]_{N-1,N} \end{aligned}$$

Assuming that the coupling from one photon subspace to the next is weak, we can approximate the spectral functions ‘a’ with their unperturbed values:

$$[\Gamma_{mn}(E)]_{N,N} = \left| K_{mn}^{\text{em}} \right|^2 (N+1) 2\pi \delta(E - \epsilon_m - (N+1)\hbar\omega) \\ + \left| K_{mn}^{\text{ab}} \right|^2 N 2\pi \delta(E - \epsilon_m - (N-1)\hbar\omega)$$

where $K_{mn}^{\text{em}} \equiv [H_{mn}]_{N+1,N}$ (10.1.12a)

and $K_{mn}^{\text{ab}} \equiv [H_{mn}]_{N-1,N}$ (10.1.12b)

Again with weak coupling between photon subspaces we can assume that the state $|n,N\rangle$ remains an approximate eigenstate with an energy $\epsilon_n + N\hbar\omega$, so that we can evaluate the broadening at $E = \epsilon_n + N\hbar\omega$:

$$\Gamma_{nn} = 2\pi \left| K_{mn}^{\text{em}} \right|^2 (N+1) \delta(\epsilon_n - \epsilon_m - \hbar\omega) \quad (\text{emission}) \\ + 2\pi \left| K_{mn}^{\text{ab}} \right|^2 N \delta(\epsilon_n - \epsilon_m + \hbar\omega) \quad (\text{absorption}) \quad (10.1.13)$$

The first term arises from the coupling of the N-photon subspace to the (N+1)-photon subspace indicating that it represents a **photon emission** process. Indeed it is peaked for photon energies $\hbar\omega$ for which $\epsilon_n - \hbar\omega = \epsilon_m$, suggesting that we view it as a process in which an electron in state ‘n’ transitions to state ‘m’ and emits the balance of the energy as a photon. The second term in Eq.(10.1.12) arises from the coupling of the N-photon subspace to the (N-1)-photon subspace indicating that it represents a **photon absorption** process. Indeed it is peaked for photon energies $\hbar\omega$ for which $\epsilon_n + \hbar\omega = \epsilon_m$, suggesting that we view it as a process in which an electron in state ‘n’ transitions to state ‘m’ and absorbs the balance of the energy from a photon.

Coupling constants: How do we write down the coupling constants ‘K’ appearing in Eq.(10.1.12)? This is where it helps to invoke the one-electron viewpoint (Fig.10.1.2). The

entire problem then amounts to writing down the “potential” U_S that an electron feels due to one photon or phonon occupying a particular mode with a frequency ω in the form:

$$U_S(\vec{r}, t) = U^{ab}(\vec{r}) \exp(-i\omega t) + U^{em}(\vec{r}) \exp(+i\omega t)$$

where $U^{ab}(\vec{r}) = U^{em}(\vec{r})^*$ (10.1.14)

Once we have identified this “interaction potential”, the coupling constants for emission and absorption can be evaluated simply from the matrix elements of U^{em} and U^{ab} :

$$K_{mn}^{em} = \int d\mathbf{r} \phi_m^*(\mathbf{r}) U^{em} \phi_n(\mathbf{r}) \equiv \langle m | U^{em} | n \rangle$$

and $K_{mn}^{ab} = \int d\mathbf{r} \phi_m^*(\mathbf{r}) U^{ab} \phi_n(\mathbf{r}) \equiv \langle m | U^{ab} | n \rangle$ (10.1.15)

where ϕ_m and ϕ_n are the wavefunctions for levels ‘m’ and ‘n’ respectively.

Electron-phonon coupling: In the supplementary section (Section 10.4), I have tried to elaborate on the meaning of phonons. But for the moment we could simply view it as representing the vibrations of the lattice of atoms, just as photons represent electromagnetic vibrations. To write down the interaction potential for phonons, we need to write down the atomic displacement or the strain due to the presence of a single phonon in a mode with frequency ω and then multiply it by the change, D in the electronic energy per unit displacement or strain. The quantity D is called the deformation potential and is known experimentally for most bulk materials of interest and one could possibly use the same parameters unless dealing with very small structures. Indeed relatively little work has been done on phonon modes in nanostructures and it is common to assume plane wave modes labeled by a wavevector $\vec{\beta}$, which is appropriate for bulk materials. The presence of a (longitudinal) phonon in such a plane wave mode gives rise to a strain (ρ is the mass density and Ω is the normalization volume)

$$S = \beta \sqrt{2\hbar/\rho\omega\Omega} \cos(\vec{\beta}\cdot\vec{r} - \omega(\beta)t) \quad (10.1.16)$$

so that the interaction potentials in Eq.(10.1.14) are given by

$$U_{\vec{\beta}}^{\text{ab}}(\vec{r}) \equiv (U_{\vec{\beta}}/2) \exp(i\vec{\beta}\cdot\vec{r}) \quad \text{and} \quad U_{\vec{\beta}}^{\text{em}}(\vec{r}) = U_{\vec{\beta}}^{\text{ab}}(\vec{r})^*$$

$$\text{where } U_{\vec{\beta}} = D\beta \sqrt{2\hbar/\rho\omega\Omega} \quad (10.1.17)$$

Electron-photon coupling: The basic principle for writing down the electron-photon coupling coefficient is similar: we need to write down the interaction potential that an electron feels due to the presence of a single photon in a particular mode. However, the details are complicated by the fact that the effect of an electromagnetic field enters the Schrodinger equation through the vector potential (which we discussed very briefly in the supplementary notes in Chapter 5) rather than a scalar potential.

First, we write down the electric field due to a single photon in mode $(\vec{\beta}, \hat{v})$ in the form

$$\vec{E} = \hat{v} E_0 \sin(\vec{\beta}\cdot\vec{r} - \omega(\beta)t)$$

whose amplitude E_0 is evaluated by equating the associated energy to $\hbar\omega$ (Ω :volume of “box”):

$$\epsilon E_0^2 \Omega / 2 = \hbar\omega \rightarrow |E_0| = \sqrt{2\hbar\omega/\epsilon\Omega}$$

The corresponding vector potential \vec{A} is written down, noting that for electromagnetic waves, $\vec{E} = -\partial\vec{A}/\partial t$:

$$\vec{A} = \hat{v} A_0 \cos(\vec{\beta}\cdot\vec{r} - \omega(\beta)t) \quad \text{with} \quad |A_0| = \sqrt{2\hbar/\omega\epsilon\Omega} \quad (10.1.18)$$

Next we separate the vector potential due to one photon into two parts (cf. Eq.(10.1.14)):

$$\vec{A}(\vec{r}, t) = \vec{A}^{\text{ab}}(\vec{r}) \exp(-i\omega(\beta)t) + \vec{A}^{\text{em}}(\vec{r}) \exp(+i\omega(\beta)t) \quad (10.1.19)$$

$$\text{where } \vec{A}_{\text{abs}}(\vec{r}) \equiv \hat{v} (A_0/2) \exp(i\vec{\beta}\cdot\vec{r}) \quad \text{and} \quad \vec{A}_{\text{em}}(\vec{r}) = \vec{A}_{\text{abs}}(\vec{r})^*$$

The coupling coefficient for absorption processes is given by the matrix element for $(q/m) \vec{A}^{\text{ab}}(\vec{r}) \cdot \vec{p}$, while the coupling coefficient for emission processes is given by the matrix element for $(q/m) \vec{A}^{\text{em}}(\vec{r}) \cdot \vec{p}$ so that ($\vec{p} \equiv -i\hbar\vec{\nabla}$)

$$K_{mn}(\vec{\beta}, \hat{v}) = (qA_0/2m) \langle m | \exp(i\vec{\beta} \cdot \vec{r}) \vec{p} \cdot \hat{v} | n \rangle \quad \textit{Absorption} \quad (10.1.20a)$$

$$K_{mn}(\vec{\beta}, \hat{v}) = (qA_0/2m) \langle m | \exp(-i\vec{\beta} \cdot \vec{r}) \vec{p} \cdot \hat{v} | n \rangle \quad \textit{Emission} \quad (10.1.20b)$$

Note that the ‘m’ appearing in the denominator stands for mass and is different from the index ‘m’ we are using to catalog basis functions.

Eqs.(10.1.20a, b) require a slightly extended justification since we have not had much occasion to deal with the vector potential. We know that the scalar potential $\phi(\vec{r})$ enters the Schrodinger equation additively:

$$p^2/2m \rightarrow (p^2/2m) - q\phi(\vec{r})$$

and if the photon could be represented by scalar potentials the coupling coefficients would simply be given by the matrix elements of $(-q)\phi_{\text{abs}}(\vec{r})$ and $(-q)\phi_{\text{em}}(\vec{r})$ for absorption and emission respectively as we did in writing down the electron-phonon coupling. But photons require a vector potential which enters the Schrodinger equation as

$$p^2/2m \rightarrow (\vec{p} + q\vec{A}) \cdot (\vec{p} + q\vec{A})/2m$$

so that the change due to the photon is given by

$$(q/2m)(\vec{A} \cdot \vec{p} + \vec{p} \cdot \vec{A}) + (q^2/2m)\vec{A} \cdot \vec{A} \approx (q/2m)(\vec{A} \cdot \vec{p} + \vec{p} \cdot \vec{A})$$

assuming that the vector potential is small enough that the quadratic term is negligible. Finally we note that for any scalar function $\phi(\vec{r})$

$$\vec{p} \cdot (\vec{A} \phi) = \vec{A} \cdot (\vec{p} \phi) + \phi (\vec{p} \cdot \vec{A})$$

so that we can write $(q/2m)(\vec{A} \cdot \vec{p} + \vec{p} \cdot \vec{A}) = (q/m)\vec{A} \cdot \vec{p}$

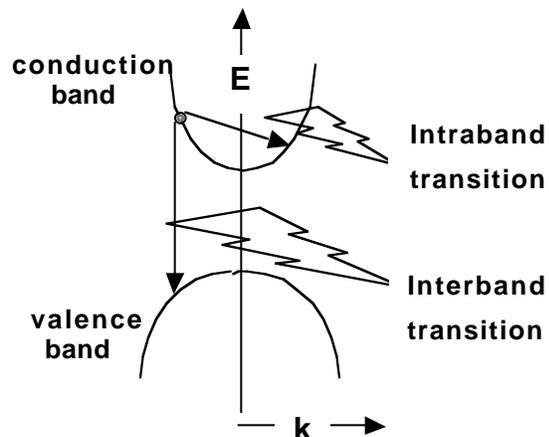
as long as $\vec{p} \cdot \vec{A} = 0$. It can be checked that this is indeed true of the photon vector potential given in Eq.(10.1.19) because of the transverse nature of electromagnetic waves which requires that the wavevector $\vec{\beta}$ and the polarization \hat{v} be orthogonal to each other: $\vec{\beta} \cdot \hat{v} = 0$.

This allows us to obtain the coupling coefficient from the matrix element for $(q/m)\vec{A}(\vec{r})\cdot\vec{p}$ using $\vec{A}\rightarrow\vec{A}^{\text{ab}}(\vec{r})$ for absorption processes and $\vec{A}\rightarrow\vec{A}^{\text{em}}(\vec{r})$ for emission processes.

10.2. Examples

In this section, I will go through a few examples to illustrate the basic approach for describing incoherent interactions discussed in the last section. I will take up the more general case of inflow and outflow in Section 10.3, but in this section I will assume all other states to be “empty” so that there is no exclusion principle to worry about and I will calculate the broadening (or the outflow) which can be identified with \hbar/τ , τ being the lifetime of the state. This will include the (1) photo-induced (radiative) lifetime due to atomic transitions, (2) radiative lifetime due to interband transitions in semiconductors, and (3) phonon-induced (non-radiative) lifetime due to intraband transitions in semiconductors (Fig.10.2.1). The basic approach is to write down the interaction potential (cf. Eq.(10.1.14)), evaluate the coupling constants (cf. Eq.(10.1.15)) and obtain the broadening and hence the lifetime from Eq.(10.1.13).

Fig.10.2.1. Electronic transitions in semiconductors can be classified as interband and intraband. The former is associated primarily with electron-photon interactions while the latter is associated primarily with electron-phonon interactions.



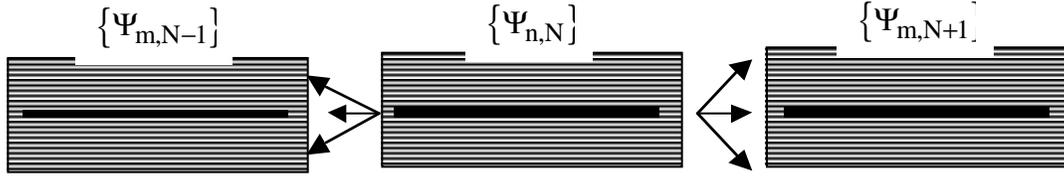
10.2.1. Atomic transitions

From Eq.(10.1.13) it is apparent that the broadening is large when the argument of the delta function vanishes. How large it is at that point depends on the value of 0^+ (see Section 7.4) that we choose to broaden each reservoir state with, As we have seen in Chapter 7, the precise value of 0^+ usually does not matter as long as the system is coupled to a continuous distribution of reservoir states. That is true in this case, because we usually do not have a

single photon mode with energy $\hbar\omega$. Instead we have a continuous distribution of photons with different wavevectors $\vec{\beta}$ with energies given by

$$\hbar\omega(\vec{\beta}) = \hbar\bar{c}\beta \quad (10.2.1)$$

where \bar{c} is the velocity of light in the solid. Consequently the states in a particular subspace do not look discrete as shown in Fig.10.1.3, but more like this:



The broadening is obtained from Eq.(10.1.13) after summing over all modes $\vec{\beta}$ and the two allowed polarizations \hat{v} for each $\vec{\beta}$:

$$\begin{aligned} \Gamma_{mn} = & \sum_{\vec{\beta}, \hat{v}} 2\pi \left| K_{mn}(\vec{\beta}, \hat{v}) \right|^2 (N_{\vec{\beta}, \hat{v}} + 1) \delta(\epsilon_n - \epsilon_m - \hbar\omega(\beta)) \\ & + \sum_{\vec{\beta}, \hat{v}} 2\pi \left| K_{mn}(\vec{\beta}, \hat{v}) \right|^2 N_{\vec{\beta}, \hat{v}} \delta(\epsilon_n - \epsilon_m + \hbar\omega(\beta)) \end{aligned} \quad (10.2.2)$$

If the photon reservoir is in equilibrium then the number of photons in mode $\vec{\beta}$ and polarization \hat{v} is given by the Bose-Einstein factor (Eq.(10.1.8)):

$$N_{\vec{\beta}, \hat{v}} = \frac{1}{\exp(\hbar\omega(\beta) / k_B T) - 1} \quad (10.2.3)$$

If we consider transitions involving energies far in excess of $k_B T$, then we can set $N_{\vec{\beta}, \hat{v}}$ equal to zero, so that the broadening (which is proportional to the inverse radiative lifetime τ_r) is given by

$$\Gamma_{mn} = \left(\frac{\hbar}{\tau_r} \right)_n = \sum_{\vec{\beta}, \hat{v}} 2\pi \left| K_{mn}(\vec{\beta}, \hat{v}) \right|^2 \delta(\epsilon_n - \epsilon_m - \hbar\omega_{\beta}) \quad (10.2.4a)$$

which is evaluated by converting the summation into an integral assuming periodic boundary conditions for the photon modes. We follow the same prescription that we have used in the past for electronic states, namely,

$$\sum_{\vec{\beta}} \rightarrow \frac{\Omega}{8\pi^3} \int_0^{\infty} d\beta \beta^2 \int_0^{+\pi} d\theta \sin\theta \int_0^{2\pi} d\phi \quad , \Omega : \text{Volume of "box"}$$

to obtain

$$\Gamma_{mn} = \frac{\Omega}{8\pi^3} \sum_{\hat{v}} \int_0^{\infty} d\beta \beta^2 \int_{-\pi}^{+\pi} d\theta \sin\theta \int_0^{2\pi} d\phi 2\pi \left| K_{mn}(\vec{\beta}, \hat{v}) \right|^2 \delta(\epsilon_n - \epsilon_m - \hbar\omega_{\beta}) \quad (10.2.4b)$$

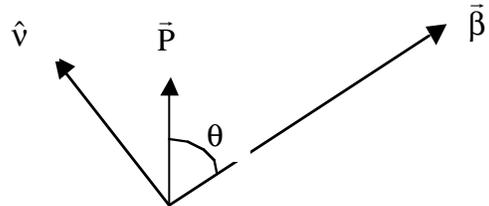
To proceed further, we need to insert the electron-photon coupling coefficients, K from Eqs.(10.1.20).

For atomic wavefunctions that are localized to extremely short dimensions (much shorter than an optical wavelength) we can neglect the factor $\exp [i\vec{\beta} \cdot \vec{r}]$ and write from Eq.(10.1.19a or b)

$$K_{mn}(\vec{\beta}, \hat{v}) = \frac{q}{m} \sqrt{\frac{\hbar}{2\epsilon\omega\Omega}} P \sin\theta \quad \text{where } \vec{P} \equiv \langle m | \vec{p} | n \rangle \quad (10.2.5)$$

and θ is the complement of the angle between the and the polarization of the photon (Fig.10.1.4).

Fig.10.2.2 Emission of photon with wavevector $\vec{\beta}$ and polarization \hat{v} by an atomic transition with an equivalent dipole moment \vec{P} .



Using Eq.(10.2.5) and (10.2.1) we can find the radiative lifetime from Eq.(10.2.4)

$$\Gamma = \frac{\Omega}{8\pi^3} \int_0^\infty \frac{d\omega \omega^2}{\bar{c}^3} \int_{-\pi}^{\pi} d\theta \sin^3 \theta \int_0^{2\pi} d\phi \frac{q^2 \hbar}{2m^2 \epsilon \omega \Omega} P^2 2\pi \delta(\epsilon_n - \epsilon_m - \hbar\omega)$$

so that

$$\frac{1}{\tau_r} = \frac{\Gamma}{\hbar} = \frac{q^2}{4\pi\epsilon\hbar\bar{c}} \frac{2(\epsilon_n - \epsilon_m)}{3\hbar m \bar{c}^2} \frac{2P^2}{m} \quad (10.2.6)$$

Note that the answer is obtained without having to worry about the precise height of the delta function (which is determined by the value of 0^+ as we discussed in Section 7.4). But if the photon modes do not form a quasi-continuous spectrum (as in small nanostructures) then it is conceivable that there will be reversible effects that are affected by the precise values of 0^+ .

Analogy with a classical dipole antenna: We could calculate the amount of power radiated per electron (note that $\hbar\omega = \epsilon_n - \epsilon_m$)

$$W = \frac{\hbar\omega}{\tau} = \frac{q^2}{4\pi\epsilon\hbar\bar{c}} \frac{2(\epsilon_n - \epsilon_m)^2}{3\hbar m \bar{c}^2} \frac{2P^2}{m} = \frac{\omega^2}{12\pi\epsilon\bar{c}^3} \left(\frac{2qP}{m} \right)^2 \quad (10.2.7)$$

It is interesting to note that the power radiated from a classical dipole antenna of length ‘d’ carrying a current $I \cos \omega t$ is given by

$$W = \frac{\omega^2}{12\pi\epsilon\bar{c}^3} (Id)^2$$

suggesting that an atomic radiator behaves like a classical dipole with

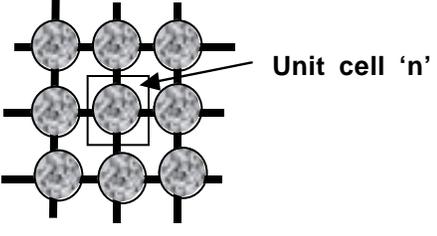
$$\begin{array}{l} \bar{I} d \\ \text{antenna} \end{array} = \begin{array}{l} 2q\bar{P}/m \\ \text{atomic radiator} \end{array} = (2q/m) \langle m | \bar{p} | n \rangle \quad (10.2.8)$$

Indeed it is not just the total power, even the polarization and angular distribution of the radiation is the same for a classical antenna and the atomic radiator. The light is polarized in

the plane containing the direction of observation and \vec{P} and its strength is proportional to $\sim \sin^2 \theta$, θ being the angle between the direction of observation and the dipole as shown in Fig.10.2.2.

10.2.2. Interband transitions in semiconductors:

The basic rule stated in Eqs.(10.2.4a,b) for the coupling coefficients can be applied to delocalized electronic states too, but we can no longer neglect the factor $\exp[i\vec{\beta} \cdot \vec{r}]$ as we did when going to Eq.(10.2.5). For example, in semiconductors (see Fig.10.2.1), the conduction ('c') and valence ('v') band electronic states are typically spread out over the entire solid consisting of many unit cells:

$$\begin{array}{ll}
 \text{Conduction} & \frac{1}{\sqrt{N}} \sum_n |c\rangle_n \exp(i\vec{k}_c \cdot \vec{r}_n) \\
 \text{band} & \\
 \\
 \text{Valence} & \frac{1}{\sqrt{N}} \sum_n |v\rangle_n \exp(i\vec{k}_v \cdot \vec{r}_n) \\
 \text{Band} &
 \end{array}$$


where $|c\rangle_n$ and $|v\rangle_n$ are the atomic parts of the conduction and valence band wavefunctions in unit cell 'n'. These functions depend on the wavevector \vec{k}_c or \vec{k}_v , but are the same in each unit cell, except for the spatial shift. This allows us to write the coupling elements for absorption and emission from Eq.(10.1.19) in the form

$$\langle v | \vec{p} \cdot \hat{v} | c \rangle \sum_n \frac{1}{N} \exp(i[\vec{k}_c \pm \vec{\beta} - \vec{k}_v] \cdot \vec{r}_n) \quad \begin{array}{l} \text{upper sign for absorption} \\ \text{lower sign for emission} \end{array}$$

where $\langle \dots \rangle$ denotes an integral over a unit cell, and we have neglected the variation of the factor $\exp[i\vec{\beta} \cdot \vec{r}]$ across a unit cell. This leads to non-zero values only if

$$\vec{k}_v = \vec{k}_c \pm \vec{\beta} \quad (10.2.9)$$

Eq.(10.2.9) can be viewed as a rule for momentum conservation, if we identify $\hbar\vec{k}$ as the electron momentum and $\hbar\vec{\beta}$ as the photon momentum. The final electronic momentum $\hbar\vec{k}_v$ is equal to the initial electronic momentum $\hbar\vec{k}_c$ plus or minus the photon momentum $\hbar\vec{\beta}$ depending on whether the photon is absorbed or emitted. The photon wavevector is typically very small compared to the electronic wavevector, so that radiative transitions are nearly “vertical” with $\vec{k}_v = \vec{k}_c \pm \vec{\beta} \approx \vec{k}_c$. This is easy to see if we note that the range of ‘k’ extends over a Brillouin zone which is $\sim 2\pi$ divided by an atomic distance, while the photon wavevector is equal to 2π divided by the optical wavelength which is thousands of atomic distances.

Assuming that the momentum conservation rule in Eq.(10.1.24) is satisfied, we can write the coupling coefficients from Eq.(10.1.19) as

$$K_{mn}(\vec{\beta}, \hat{v}) = \frac{q}{m} \sqrt{\frac{\hbar}{2\epsilon\omega\Omega}} P \sin\theta \quad \text{where } \vec{P} \equiv \langle v | \vec{p} | c \rangle \quad (10.2.10)$$

showing that “vertical” radiative transitions in semiconductors can be understood in much the same way as atomic transitions (see Eq.(10.1.20)) using the atomic parts of the conduction and valence band wavefunctions. For example, if we put the numbers characteristic of conduction – valence band transitions in a typical semiconductor like GaAs into Eq.(10.2.10), $\epsilon_n - \epsilon_m = 1.5$ eV, $2P^2/m = 20$ eV, $\epsilon_r = 10$, we obtain $\tau_r = 0.7$ nsec. for the radiative lifetime.

Polarization and angular distribution: We know that the electronic states at the bottom of the conduction band near the Γ -point are isotropic or s-type denoted by $|S\rangle$. If the states at the top of the valence band were purely p_x , p_y and p_z types denoted by $|X\rangle, |Y\rangle, |Z\rangle$, then we could view the system as being composed of three independent antennas with their dipoles pointing along x-, y- and z- directions since

$$\langle s | \vec{p} | X \rangle = \hat{x} P, \langle s | \vec{p} | Y \rangle = \hat{y} P \text{ and } \langle s | \vec{p} | Z \rangle = \hat{z} P$$

The resulting radiation can then be shown to be unpolarized and isotropic. In reality, however, the top of the valence band is composed of light hole and heavy hole bands which are

mixtures of up- and down-spin states and the equivalent dipole moments for each of the conduction-valence band pairs can be written as shown in Table 10.2.1.

We thus have eight independent antennas, one corresponding to each conduction band-valence band pair. If the C- state is occupied, then the first row of four antennas is active. If we look at the radiation coming out in the z- direction then we will see the radiation from the C-HH and C- $\overline{\text{LH}}$ transitions. The C-HH transition will emit right circularly polarized (RCP) light which will be three times as strong as the left circularly polarized (LCP) light from the C- $\overline{\text{LH}}$ transition. If the $\overline{\text{C}}$ state is also occupied then the $\overline{\text{C}}$ -HH transition would yield three times as much LCP light as the RCP light from the $\overline{\text{C}}$ -LH transition. Overall there would be just as much LCP as RCP light. But if only the C state is occupied then there would be thrice as much RCP light as LCP light. Indeed the degree of circular polarization of the emission is often used as a measure of the degree of spin polarization that has been achieved in a given experiment.

Table 10.2.1. Optical matrix elements for conduction-valence band transitions

	HH	$\overline{\text{HH}}$	LH	$\overline{\text{LH}}$
	$\left\{ \begin{array}{c} \frac{ \text{X}\rangle + i \text{Y}\rangle}{\sqrt{2}} \\ 0 \end{array} \right\}$	$\left\{ \begin{array}{c} 0 \\ \frac{ \text{X}\rangle - i \text{Y}\rangle}{\sqrt{2}} \end{array} \right\}$	$\left\{ \begin{array}{c} -\sqrt{\frac{2}{3}} \text{Z}\rangle \\ \frac{ \text{X}\rangle + i \text{Y}\rangle}{\sqrt{6}} \end{array} \right\}$	$\left\{ \begin{array}{c} \frac{ \text{X}\rangle - i \text{Y}\rangle}{\sqrt{6}} \\ \sqrt{\frac{2}{3}} \text{Z}\rangle \end{array} \right\}$
C $\left\{ \begin{array}{c} S\rangle \\ 0 \end{array} \right\}$	$\frac{\hat{x} + i\hat{y}}{\sqrt{2}} \text{P}$	0	$-\sqrt{\frac{2}{3}} \hat{z} \text{P}$	$\frac{\hat{x} - i\hat{y}}{\sqrt{6}} \text{P}$
$\overline{\text{C}}$ $\left\{ \begin{array}{c} 0 \\ S\rangle \end{array} \right\}$	0	$\frac{\hat{x} - i\hat{y}}{\sqrt{2}} \text{P}$	$\frac{\hat{x} + i\hat{y}}{\sqrt{6}} \text{P}$	$\sqrt{\frac{2}{3}} \hat{z} \text{P}$

10.2.3. Intraband transitions in semiconductors

We have just discussed the radiation of light due to interband transitions in semiconductors (see Fig.10.2.1). But what about intraband transitions? Can they lead to the emission of light ? We will show that the simultaneous momentum and energy conservation requirements prevent any radiation of light unless the electron velocity exceeds the velocity of

light: $\hbar k/m > \bar{c}$. This is impossible in vacuum, but could happen in a solid and such Cerenkov radiation of light by fast-moving electrons has indeed been observed. However, this is usually not very relevant to the operation of solid-state devices because typical electronic velocities are about a thousandth of the speed of light. What is more relevant is the Cerenkov emission of acoustic waves or phonons which are five orders of magnitude slower than light. Electron velocities are typically well in excess of the phonon velocity leading to extensive Cerenkov emission (and absorption) of phonons, somewhat like the sonic booms generated by supersonic jets.

Criteria for Cerenkov emission: For intraband transitions, both the final and initial states have the same atomic wavefunctions and for clarity, I will not write them down explicitly. Instead I will write the initial and final states in the form of plane waves as if we are dealing with electrons in vacuum:

$$|\vec{k}\rangle \equiv (1/\sqrt{\Omega}) \exp(i\vec{k}\cdot\vec{r}) \quad \text{and} \quad |\vec{k}_f\rangle \equiv (1/\sqrt{\Omega}) \exp(i\vec{k}_f\cdot\vec{r}) \quad (10.2.11)$$

From Eq.(10.1.19) we find that the radiative coupling constant is equal to

$$K(\vec{k}_f, \vec{k}, \vec{\beta}, \hat{v}) = (qA_0/2m) \hbar \vec{k} \cdot \hat{v} \quad (10.2.12)$$

$$\text{if} \quad \vec{k}_f = \vec{k} - \vec{\beta} \quad \vec{k}_f = \vec{k} + \vec{\beta} \quad (10.2.13)$$

Emission **Absorption**

and is zero otherwise. As I have mentioned before, Eq.(10.2.12) is interpreted as a condition for momentum conservation (Fig.10.2.1). Energy conservation, on the other hand, is enforced by the delta function in Eq.(10.1.16)

$$\varepsilon(\vec{k}_f) = \varepsilon(\vec{k}) - \hbar\omega(\vec{\beta}) \quad \varepsilon(\vec{k}_f) = \varepsilon(\vec{k}) + \hbar\omega(\vec{\beta}) \quad (10.2.14)$$

Emission **Absorption**

From Eqs.(10.2.13) and (10.2.14) we obtain for **emission** processes

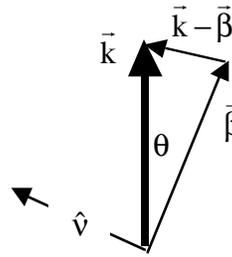
$$\varepsilon(\vec{k}_f) - \varepsilon(\vec{k}) + \hbar\omega(\vec{\beta}) = 0 = \frac{\hbar^2}{2m} \left([\vec{k} - \vec{\beta}] \cdot [\vec{k} - \vec{\beta}] - k^2 \right) + \hbar c \beta$$

so that,
$$\frac{\hbar^2}{2m} (-2k\beta \cos\theta + \beta^2) + \hbar\bar{c}\beta = 0$$

which yields
$$\cos\theta = \frac{\bar{c}}{\hbar k/m} + \frac{\beta}{2k} \quad (10.2.15)$$

The point is that, since $\cos\theta$ must be smaller than one, Cerenkov emission cannot take place unless the electron velocity $\hbar k/m$ exceeds the velocity of light \bar{c} . This is impossible in vacuum, but could happen in a solid and such Cerenkov radiation of light by fast-moving electrons has indeed been observed. The emitted light forms a cone around the electronic wavevector \vec{k} with a maximum angle $\theta_{\max} = \cos^{-1}(m\bar{c}/\hbar k)$.

Fig.10.2.3. Cerenkov emission: Initial state \vec{k} , photon wavevector $\vec{\beta}$ and final state $\vec{k}-\vec{\beta}$. The photon polarization is along \hat{v} .



Cerenkov emission of acoustic phonons: As I have stated before, the Cerenkov emission of light is not very relevant to the operation of solid state devices. But the emission (and absorption) of sound waves or acoustic phonons is quite relevant. Acoustic waves are five orders of magnitude slower than light and the velocity of electrons routinely exceeds the sound velocity. Since acoustic phonons typically have energies less than $k_B T$ they are usually present in copious numbers at equilibrium:

$$N_{\vec{\beta}} = (\exp(\hbar\omega(\beta)/k_B T) - 1)^{-1} \cong k_B T / \hbar\omega(\beta) \quad (\text{acoustic phonons})$$

Both terms in Eq.(10.1.13) now contribute to the broadening or inverse lifetime : Cerenkov absorption ('ab') is just as important as Cerenkov emission ('em'):

$$(\Gamma)_{\vec{k}, \text{em}} = \sum_{\vec{\beta}} 2\pi \frac{k_B T}{\hbar\omega(\beta)} \left| K(\vec{\beta}) \right|^2 \delta(\varepsilon(\vec{k}) - \varepsilon(\vec{k}-\vec{\beta}) - \hbar\omega(\vec{\beta})) \quad (10.2.16a)$$

$$(\Gamma)_{\vec{k}, ab} = \sum_{\vec{\beta}} 2\pi \frac{k_B T}{\hbar \omega(\vec{\beta})} \left| K(\vec{\beta}) \right|^2 \delta(\epsilon(\vec{k}) - \epsilon(\vec{k} + \vec{\beta}) + \hbar \omega(\vec{\beta}))$$

(10.2.16b)

The coupling element $K(\vec{\beta})$ is proportional to the potential that an electron feels due to the presence of a single phonon as discussed earlier (see Eq.(10.1.18)). Without getting into a detailed evaluation of Eqs.(10.2.16a,b), it is easy to relate the angle of emission θ to the magnitude of the phonon wavevector β by setting the arguments of the delta functions to zero and proceeding as we did in deriving Eq.(10.2.15):

$$\begin{aligned} \cos \theta &= \frac{c_s}{\hbar k/m} + \frac{\beta}{2k} && \text{(emission)} \\ \cos \theta &= \frac{c_s}{\hbar k/m} - \frac{\beta}{2k} && \text{(absorption)} \end{aligned} \quad (10.2.17)$$

where c_s is the velocity of sound waves: $\omega = c_s \beta$. The detailed evaluation of the electron lifetime due to acoustic phonon emission and absorption from Eq.(10.2.16) is described in Exercise 10.1.

Cerenkov emission of optical phonons: In addition to acoustic phonons, there are optical phonons (see supplementary notes) whose frequency is nearly constant $\omega = \omega_0$, where the phonon energy $\hbar \omega_0$ is typically a few tens of millielectron volts, so that the number of such phonons present at equilibrium at room temperature is of order one:

$$N_{\vec{\beta}} = (\exp(\hbar \omega_0 / k_B T) - 1)^{-1} \equiv N_0 \quad \text{(optical phonons)}$$

From Eq.(10.1.13) we now obtain for the emission and absorption rates

$$(\Gamma)_{\vec{k}, em} = (N_0 + 1) \sum_{\vec{\beta}} 2\pi \left| K(\vec{\beta}) \right|^2 \delta(\epsilon(\vec{k}) - \epsilon(\vec{k} - \vec{\beta}) - \hbar \omega_0) \quad (10.2.18a)$$

$$(\Gamma)_{\vec{k}, ab} = N_0 \sum_{\vec{\beta}} 2\pi \left| K(\vec{\beta}) \right|^2 \delta(\epsilon(\vec{k}) - \epsilon(\vec{k} + \vec{\beta}) + \hbar \omega_0) \quad (10.2.18b)$$

which can be evaluated as described in Exercise 10.2.

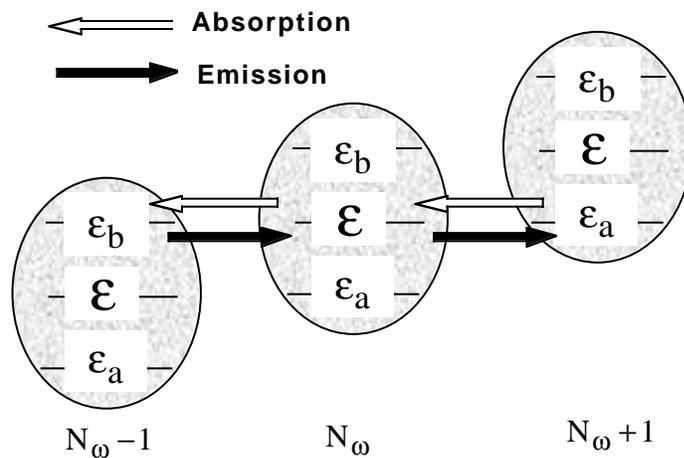
10.3. Inflow and outflow

Let me now explain how we can use the concepts developed in this Chapter to write down the new terms Σ_s^{in} and Σ_s appearing in Fig.10.2.

Discrete levels: To start with consider the inflow and outflow into a specific energy level ϵ due to transitions from levels ‘a’ and ‘b’ one above it and one below it, separated by an energy of $\hbar\omega$: $\epsilon_b - \epsilon = \epsilon - \epsilon_a = \hbar\omega$. We have seen in Section 10.1 that the rate constant (K^{ab}) for absorption processes is proportional to the number of phonons present (N_ω) while the rate constant (K^{em}) for emission processes is proportional to $(N_\omega + 1)$. To start with, assume the temperature is very low compared to $\hbar\omega$, so that $N_\omega \ll 1$ and we need only worry about emission. Using N , N_a and N_b to denote the number of electrons in each of these levels we can write for the level ϵ

$$\text{Inflow} = K^{\text{em}} (1 - N) N_b \quad \text{and} \quad \text{Outflow} = K^{\text{em}} N (1 - N_a)$$

Fig.10.3.1. An idealized device with three levels used to write down the inflow and outflow terms due to the absorption and emission of photons and phonons.



Now we can write the inflow term as a difference between two terms

$$\text{Inflow} = K^{\text{em}} N_b - K^{\text{em}} N N_b$$

where the second term represents the part of the inflow that is blocked by the exclusion principle. A non-obvious result that comes out of the advanced formalism (see Appendix,

Section A.3) is that this part of the inflow is not really blocked. Rather the outflow is increased by this amount ($K^{em} N N_b$):

$$\text{Inflow} = K^{em} N_b \quad \text{and} \quad \text{Outflow} = K^{em} N (1 - N_a + N_b) \quad (10.3.1a)$$

The difference between inflow and outflow is not changed from what we had guessed earlier. But the distinction is not academic, since the outflow (not the difference) determines the broadening of the level. We can compare this with the inflow and outflow between a contact and a discrete level that we discussed earlier (see Fig.8.1):

$$\text{Inflow} = \gamma f \quad \text{and} \quad \text{Outflow} = \gamma N \quad (10.3.1b)$$

The inflow looks similar with K^{em} playing the role of γ , but the outflow involves an extra factor $(1 - N_a + N_b)$ that reduces to one if $N_a = N_b$, but not in general. Eq.(10.3.1b) was earlier generalized to the form (see Fig.8.3)

$$\text{Inflow} = \text{Trace} [\Gamma A] f = \text{Trace} [\Sigma^{in} A] \quad \text{and} \quad \text{Outflow} = \text{Trace} [\Gamma G^n]$$

Similarly in the present case we can generalize Eq.(10.3.1a) to

$$\text{Inflow} = \text{Trace} [\Sigma_s^{in} A] \quad \text{and} \quad \text{Outflow} = \text{Trace} [\Gamma_s G^n] \quad (10.3.2)$$

where the expressions for Σ_s^{in} and Γ_s can be discovered heuristically by analogy. Let us do this one by one.

Inflow for continuous distribution of states: For regular contacts we saw in Chapter 8 that the inscattering function is given by

$$\Sigma^{in}(E) = [\tau A \tau^+] f = [\tau G^n \tau^+]$$

where $[G^n] = [A] f$ is the correlation function in the contact: The contact correlation function at energy E causes inscattering into the device at an energy E . Now for emission processes, the device correlation function at $E + \hbar\omega$ causes inscattering into the device at energy E , suggesting that we write

$$\Sigma_s^{\text{in}}(E) = \sum_{\bar{\beta}} (N_{\bar{\beta}} + 1) [U_{\bar{\beta}}^{\text{em}} G^n(E + \hbar\omega(\bar{\beta})) (U_{\bar{\beta}}^{\text{em}})^+]$$

where U^{em} is the emission component of the interaction potential (see Eq.(10.1.18)).

Writing out the matrix multiplication in detail we have

$$\begin{aligned} \Sigma_s^{\text{in}}(p,q;E) &= \sum_{p',q',\bar{\beta}} (N_{\bar{\beta}} + 1) U_{\bar{\beta}}^{\text{em}}(p,p') G^n(p',q';E + \hbar\omega(\bar{\beta})) U_{\bar{\beta}}^{\text{em}}(q,q')^* \\ &= \int_0^{\infty} d(\hbar\omega) \sum_{p',q'} D^{\text{em}}(p,p';q,q';\hbar\omega) G^n(p',q';E + \hbar\omega) \end{aligned} \quad (10.3.3)$$

$$\text{where } D^{\text{em}}(p,p';q,q';\hbar\omega) \equiv \sum_{\bar{\beta}} (N_{\bar{\beta}} + 1) \delta(\hbar\omega - \hbar\omega(\bar{\beta})) U_{\bar{\beta}}^{\text{em}}(p,p') U_{\bar{\beta}}^{\text{em}}(q,q')^* \quad (10.3.4)$$

In real space representation, this simplifies somewhat since the matrix representation of the potential U^{em} is diagonal so that the only non-zero elements of D^{em} are given by

$$\begin{aligned} D^{\text{em}}(r,r';\hbar\omega) &\equiv D^{\text{em}}(r,r;r',r';\hbar\omega) \\ &= \sum_{\beta} (N_{\beta} + 1) \delta(\hbar\omega - \hbar\omega(\beta)) U_{\beta}^{\text{em}}(r) U_{\beta}^{\text{em}}(r')^* \end{aligned}$$

and the inscattering function is given by an *element by element matrix multiplication* of D with the correlation function.

$$\Sigma_s^{\text{in}}(r,r';E) = \int_0^{\infty} d(\hbar\omega) D^{\text{em}}(r,r';\hbar\omega) G^n(r,r';E + \hbar\omega) \quad (10.3.5)$$

If we include absorption processes we obtain

$$\Sigma_s^{\text{in}}(r,r';E) = \int_0^{\infty} d(\hbar\omega) \left(\begin{array}{l} D^{\text{em}}(r,r';\hbar\omega) G^n(r,r';E + \hbar\omega) \\ + D^{\text{ab}}(r,r';\hbar\omega) G^n(r,r';E - \hbar\omega) \end{array} \right)$$

where the absorption term is given by an expression similar to the emission term with N instead of $(N+1)$:

$$D^{\text{em}}(r,r';\hbar\omega) = \sum_{\beta} (N_{\beta} + 1) \delta(\hbar\omega - \hbar\omega(\vec{\beta})) U_{\beta}^{\text{em}}(r) U_{\beta}^{\text{em}}(r')^* \quad (10.3.7a)$$

$$D^{\text{ab}}(r,r';\hbar\omega) = \sum_{\beta} N_{\beta} \delta(\hbar\omega - \hbar\omega(\vec{\beta})) U_{\beta}^{\text{ab}}(r) U_{\beta}^{\text{ab}}(r')^* \quad (10.3.7b)$$

We can define a single “phonon spectral function” (as seen by the electron system through the interaction potential)

$$D_0(r,r';\hbar\omega) = \sum_{\beta} \delta(\hbar\omega - \hbar\omega(\vec{\beta})) U_{\beta}^{\text{em}}(r) U_{\beta}^{\text{em}}(r')^* \quad (10.3.8)$$

such that the emission and absorption functions are given by

$$D^{\text{em}}(r,r';\hbar\omega) \equiv (N_{\omega} + 1) D_0(r,r';\hbar\omega) \quad (10.3.9a)$$

$$\text{and } D^{\text{ab}}(r,r';\hbar\omega) \equiv N_{\omega} D_0(r,r';\hbar\omega) \quad (10.3.9b)$$

Denoting the element-by element matrix multiplication with a ‘•’ we can write

$$\Sigma_s^{\text{in}}(E) = \int_0^{\infty} d(\hbar\omega) D_0(\hbar\omega) \bullet \left(\begin{array}{l} (N_{\omega} + 1) G^{\text{n}}(E + \hbar\omega) \\ + N_{\omega} G^{\text{n}}(E - \hbar\omega) \end{array} \right) \quad (10.3.10)$$

Outflow for continuous distribution of states: For the outflow term, in extrapolating from the discrete version in Eq.(10.3.1) to a continuous version we replace

$$N_b \quad \text{with} \quad G^{\text{n}}(E + \hbar\omega)$$

$$\text{and } 1 - N_a \quad \text{with} \quad G^{\text{p}}(E - \hbar\omega)$$

$$\text{to obtain } \Gamma_s(E) = \int d(\hbar\omega) D^{\text{em}}(\hbar\omega) \bullet \left[G^{\text{p}}(E - \hbar\omega) + G^{\text{n}}(E + \hbar\omega) \right]$$

where I have defined a new quantity $G^P \equiv A - G^n$ that tells us the number of empty states or holes, just as G^n tells us the number of filled states or electrons. The sum of the two is equal to the spectral function A which represents the density of states. We can extend this result as before (cf. (10.3.5) \rightarrow (10.3.10)) to include absorption terms as before to yield

$$\Gamma_s(E) = \int d(\hbar\omega) D_0(\hbar\omega) \bullet \left(\begin{array}{l} (N_\omega + 1) [G^P(E - \hbar\omega) + G^n(E + \hbar\omega)] \\ + N_\omega [G^n(E - \hbar\omega) + G^P(E + \hbar\omega)] \end{array} \right) \quad (10.3.11)$$

Eqs.(10.3.10)-(10.3.11) are the expressions for the scattering functions that we are looking for. The self-energy function Σ_s can be written as $\text{Real}(\Sigma_s) + i \Gamma_s/2$ where the real part can be obtained from the Hilbert transform of the imaginary part given in Eq.(10.3.11) as explained in Section 8.4.

Migdal's "theorem" : If the electronic distribution can be described by an equilibrium Fermi function

$$G^n(E') \equiv f(E') A(E') \quad \text{and} \quad G^P(E') \equiv (1-f(E')) A(E')$$

then

$$\Gamma_s(E) = \int d(\hbar\omega) \int dE' D_0(\hbar\omega) \bullet A(E') \left(\begin{array}{l} (N_\omega + 1 - f(E')) \delta(E - E' - \hbar\omega) \\ + (N_\omega + f(E')) \delta(E - E' + \hbar\omega) \end{array} \right)$$

which is the expression commonly found in the literature on electron-phonon scattering in metals where it is referred to as Migdal's "theorem" [10.3b]. Close to equilibrium, a separate equation for the inscattering function $\Sigma_s^{\text{in}}(E)$ is not needed, since it is simply equal to $f(E)\Gamma_s(E)$, just like an ordinary contact.

Nearly elastic processes: Note that the expressions simplify considerably for low energy scattering processes ($\hbar\omega \rightarrow 0$) for which we can set $E + \hbar\omega \approx E \approx E - \hbar\omega$:

$$\Sigma_s^{\text{in}}(E) = \int_0^{\infty} d(\hbar\omega) (D^{\text{em}}(\hbar\omega) + D^{\text{ab}}(\hbar\omega)) \bullet G^n(E) \quad (10.3.9)$$

$$\Gamma_s(E) = \int_0^{\infty} d(\hbar\omega) (D^{\text{em}}(\hbar\omega) + D^{\text{ab}}(\hbar\omega)) \bullet A(E) \quad (10.3.10)$$

Indeed, in this case the real part of the self-energy Σ_s does not require a separate Hilbert transform. We can simply write

$$\Sigma_s(E) = \int_0^{\infty} d(\hbar\omega) (D^{\text{em}}(\hbar\omega) + D^{\text{ab}}(\hbar\omega)) \bullet G(E) \quad (10.3.11)$$

since $\text{Real}(\Sigma_s)$ is related to Γ_s in exactly the same way as $\text{Real}(G)$ is related to A , namely through a Hilbert transform.

10.4. Supplementary notes: Phonons

As I have mentioned before, phonons represent the vibrations of the lattice just as photons represent electromagnetic vibrations. In this section I will try to elaborate on this statement and clarify what I mean. At low temperatures, the atoms that comprise a molecule or a solid are frozen in their positions on the lattice and this frozen atomic potential is used in calculating the energy levels for the electrons, starting from the Schrodinger equation. As the temperature is raised these vibrations increase in amplitude and exchange energy with the electrons through the “electron-phonon interaction”. To understand how we describe these vibrations, let us start with a simple example, namely a Hydrogen molecule.

Fig.10.4.1. A Hydrogen molecule can be viewed as two masses connected by a spring.



As we discussed in Chapter 3, we could describe the vibrations of this molecule in terms of a mass and spring system (Fig.10.4.1). The mass, M is just that of the two hydrogen atoms,

while the spring constant, K is equal to the second derivative of the potential energy with respect to the interatomic distance. We know from freshman physics that such a system behaves like an oscillator with a resonant frequency $\omega = \sqrt{K/M}$. Experimentalists have measured this frequency to be approximately $\omega = 2\pi (10^{14} / \text{sec})$. Knowing M we could calculate K and compare against theory, but that is a different story. The question we wish to address is the following. As we raise the temperature we expect the molecule to vibrate with increasing amplitude due to the thermal energy that it takes up from the surroundings. At very high temperatures the vibrations could become so violent that the molecule dissociates. But we are assuming that the temperature is way below that so that the amplitude of this vibration is much smaller than the bond length, a . What is this amplitude as a function of the temperature?

To make our discussion quantitative, let us define a variable $u(t)$ that measures the distance between the two atoms, relative to the equilibrium value of “ u_0 ”. We expect the atoms to oscillate with a frequency ω such that

$$u(t) = A \cos(\omega t + \phi)$$

It is convenient to define a complex amplitude $\tilde{u} = (A/2) \exp[i\phi]$ and write

$$u(t) = \tilde{u} \exp[-i\omega t] + \tilde{u}^* \exp[+i\omega t] \quad (10.4.1)$$

The kinetic energy associated with this vibration is written as

$$\text{KE} = \frac{M}{2} \left(\frac{du}{dt} \right)^2 = \frac{M\omega^2 A^2}{2} \sin^2(\omega t + \phi)$$

while the potential energy is given by (note that $K = M\omega^2$)

$$\text{PE} = \frac{K}{2} u^2 = \frac{M\omega^2 A^2}{2} \cos^2(\omega t + \phi)$$

so that the total energy is independent of time as we might expect:

$$E = \text{KE} + \text{PE} = M\omega^2 A^2 / 2 = 2M\omega^2 |\tilde{u}|^2 \quad (10.4.2)$$

Classical physics believed that the energy E could have any value. Early in this century, Planck showed that the experimentally observed radiation spectra could be explained by postulating that the energy of electromagnetic oscillators is quantized in units of $\hbar\omega$. It is now believed that the energy of all harmonic oscillators occur only in integer multiples of $\hbar\omega$ as shown in Fig.10.4.1 ($n = 0, 1, 2, \dots$):

$$E = 2M\omega^2 |\tilde{u}|^2 = n\hbar\omega \rightarrow |\tilde{u}| = \sqrt{n\hbar/2M\omega} \quad (10.4.3)$$

Using Eq.(10.4.3) we can rewrite Eq.(10.4.1) as

$$u(t) = \sqrt{\frac{\hbar}{2M\omega}} \left(a \exp[-i\omega t] + a^* \exp[+i\omega t] \right) \quad (10.4.4)$$

where $|a|^2 = n = 0, 1, 2, \dots$

Since the energy of the oscillator is an integer multiple of $\hbar\omega$, we can alternatively visualize it as a single energy level of energy $\hbar\omega$ into which we can put an integer number $\nu = 0, 1, 2, \dots$ of particles called phonons (for electromagnetic oscillators the particles are called photons). If the oscillator is in a state with an energy $4\hbar\omega$ we say that four phonons are present. Vibrations too thus acquire a particulate character like electrons. The difference is that electrons are Fermi particles, obeying the exclusion principle. Consequently the number of particles n_k that we can put into a given state 'k' is either zero or one. Phonons on the other hand are Bose particles that do not have any exclusion principle. Any number of phonons can occupy a state. The greater the number of particles ν , the greater the energy of the vibrations and hence the greater the amplitude of the oscillation 'a' in Eq.(10.3.4). For a coherent vibrations, the amplitudes 'a' are complex numbers with well-defined phases, but for thermal vibrations, there is no definite phase.

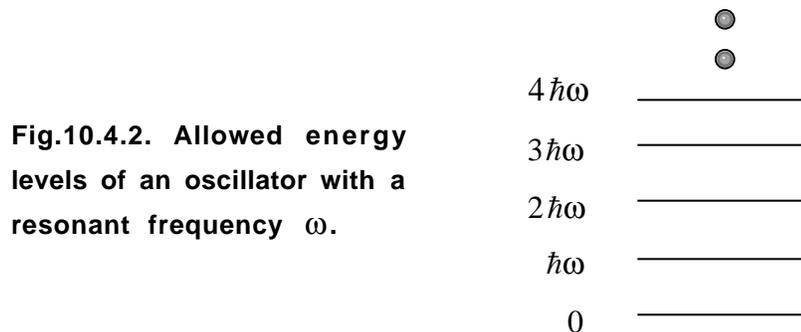


Fig.10.4.2. Allowed energy levels of an oscillator with a resonant frequency ω .

What is the average number of phonons at a given temperature? For electrons we know that the number of particles n_k in a state 'k' can be either 0 or 1 and that the average value at equilibrium is given by the Fermi function (Eq.(1.1.1)). For phonons, the number of particles ν for a particular vibrational mode can be any positive number and the average value $\langle n \rangle$ at equilibrium is given by the Bose function:

$$\langle n \rangle = \frac{1}{\exp(\hbar\omega/k_B T) - 1} \quad (10.4.5)$$

I will not discuss the physical basis for this function (we did not discuss the Fermi function either) – in the last chapter I will try to explain how both the Bose and Fermi functions follow from a more general principle.

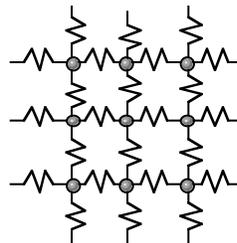
So what is the rms amplitude of vibration at a temperature T? From Eq.(10.4.3)

$$\langle |\tilde{u}|^2 \rangle = \langle n \rangle \hbar / 2M\omega$$

showing that the vibration amplitude is proportional to the number of phonons and thus can be expected to increase with temperature. At temperatures far below the melting point, this amplitude should be a small fraction of the equilibrium bond length.

Phonons: We argued in Chapter 4 that a hydrogen molecule could be visualized as two masses connected by a spring whose equilibrium length is equal to the hydrogen-hydrogen bond length. Extending the same argument we could visualize a solid lattice as a periodic array of masses connected by springs (Fig.10.4.3).

Fig.10.4.3. A crystal lattice as a mass and spring system.



How do we describe the vibrations of such a mass and spring array? One could equate the total force exerted by the springs on an individual mass to its mass times its acceleration and write

down an infinite set of equations, one for each mass. This sounds like a complicated insoluble (non quantum mechanical) problem, but we will show that it can be tackled in much the same way that we tackled the bandstructure problem in Chapter 5.

1-D solid: For simplicity, let us consider a one-dimensional array of atoms represented by a mass and spring system (Fig.10.4.4a). Assuming that u_m is the displacement of the m th atom from its equilibrium position in the lattice, the force exerted on the m th atom by the spring on the left is $K(u_m - u_{m-1})$, while that exerted by the spring on the right is $K(u_m - u_{m+1})$. From Newton's Law,

$$M \frac{d^2 u_m}{dt^2} = K [u_{m+1} - 2u_m + u_{m-1}] \quad (10.4.6)$$

where M is the mass of the atom. Assuming sinusoidal vibrations with frequency ω , $u_m = \tilde{u}_m \exp(-i\omega t)$ we can write

$$M \omega^2 \tilde{u}_m = K [2\tilde{u}_m - \tilde{u}_{m-1} - \tilde{u}_{m+1}]$$

which can be written in the form of a matrix equation:

$$\omega^2 \{\tilde{u}\} = [\Omega] \{\tilde{u}\} \quad (10.4.7)$$

where $\omega_0 \equiv \sqrt{K/M}$,

and	$\Omega =$	1	2	N-1	N
		1	$2\omega_0^2$	$-\omega_0^2$		0	$-\omega_0^2$
		2	$-\omega_0^2$	$2\omega_0^2$		0	0
					
		N-1	0	0		$2\omega_0^2$	$-\omega_0^2$
		N	$-\omega_0^2$	0		$-\omega_0^2$	$2\omega_0^2$

Here we have used periodic boundary conditions, that is, we have assumed the solid to be in the form of a ring with atom 'N' connected back to atom '1'. Note that this matrix has exactly the same form as the Hamiltonian matrix for a one-dimensional solid (Eq.(5.1.1)).

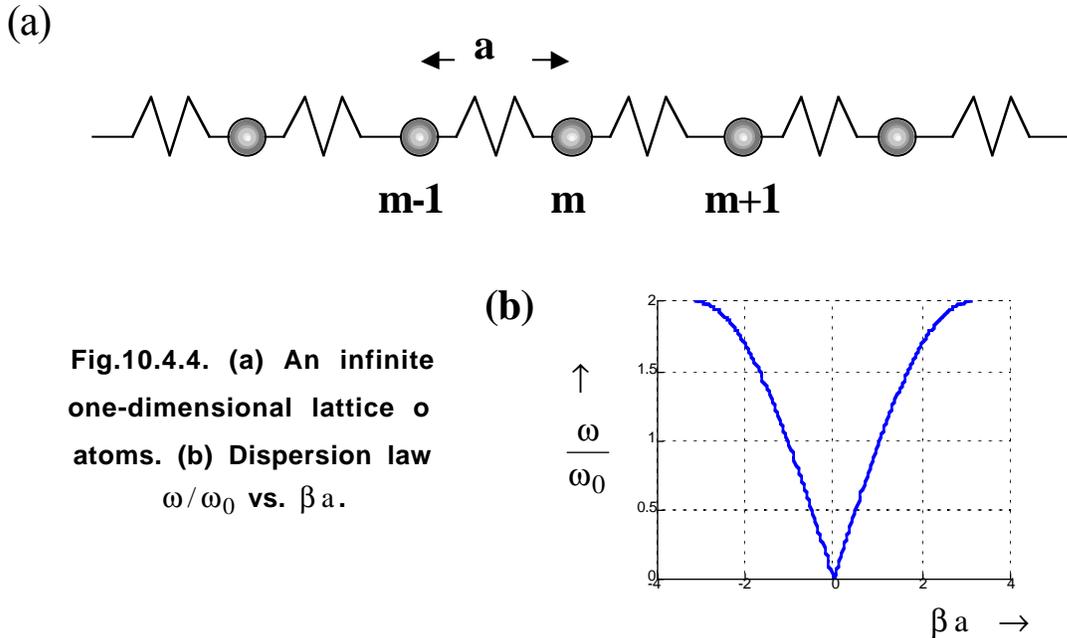


Fig.10.4.4. (a) An infinite one-dimensional lattice of atoms. (b) Dispersion law ω/ω_0 vs. βa .

The similarity is of course purely mathematical. Eqs.(5.1.1) and (10.4.2) describe very different physics: the former describes the quantum mechanics of electrons in a periodic lattice, while the latter describes the classical dynamics of a periodic mass and spring system. But since the matrix $[H]$ in Eq.(5.1.1) has exactly the same form as the matrix $[\Omega]$ in Eq.(10.3.2) they can be diagonalized in exactly the same way to obtain (cf. Eq.(5.1.2)):

$$\omega^2 = 2\omega_0^2 (1 - \cos\beta a) \quad \text{where } \beta a = n.2\pi/N \quad (10.4.8)$$

The values of βa run from $-\pi$ to $+\pi$ and are spaced by $2\pi/N$, just like the values of ‘ ka ’ in Fig.5.1.2. The eigen-displacements \tilde{u}_m corresponding to a given eigenmode β are given by

$$\sum_{\beta} \tilde{u}_{\beta} \exp [i\beta ma] = \sum_{\beta} u_{\beta} \exp [i\beta ma - \omega(\beta)t]$$

The actual instantaneous values of the displacement are obtained by taking the real parts of these phasor amplitudes (just as we do with voltages and currents in ac circuits):

$$\begin{bmatrix} \omega_1^2 + \omega_2^2 & \omega_1^2 + \omega_2^2 e^{-i\beta a} \\ \omega_1^2 + \omega_2^2 e^{+i\beta a} & \omega_1^2 + \omega_2^2 \end{bmatrix} \begin{Bmatrix} u_1(t) \\ u_2(t) \end{Bmatrix} = \omega^2(\beta) \begin{Bmatrix} u_1(t) \\ u_2(t) \end{Bmatrix} \quad (10.4.11)$$

Setting the determinant to zero

$$\begin{bmatrix} \omega_1^2 + \omega_2^2 - \omega^2 & \omega_1^2 + \omega_2^2 e^{-i\beta a} \\ \omega_1^2 + \omega_2^2 e^{+i\beta a} & \omega_1^2 + \omega_2^2 - \omega^2 \end{bmatrix} = 0$$

we obtain the dispersion relation

$$\omega^2(\beta) = \omega_1^2 + \omega_2^2 \pm (\omega_1^4 + \omega_2^4 + 2\omega_1^2\omega_2^2 \cos\beta a)^{1/2} \quad (10.4.12)$$

Like Eq.(5.1.10), Eq.(10.4.12) leads to two branches in the phonon spectrum as shown in Fig.10.4.5b (cf. Fig.5.1.5). The lower branch is called the acoustic phonon branch since it corresponds to ordinary acoustic waves at low frequencies. The displacement of both atoms in a unit cell (Ga and As) have the same sign for the acoustic branch. By contrast their displacements have opposite signs for the optical branch. The name “optical” comes from the fact that these vibrations can be excited by an incident electromagnetic radiation whose electric field sets the Ga and the As atoms moving in opposite directions, since one is negatively charged and one is positively charged.

(a)

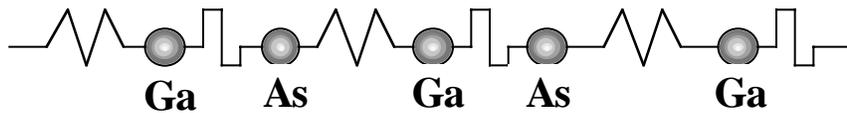
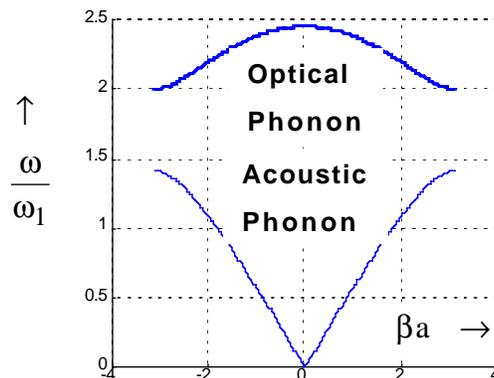


Fig.10.4.5. (a) Snapshot of a GaAs lattice viewed along the (111) direction

(b) Dispersion law ω/ω_1 vs. βa showing acoustic and optical phonons assuming $\omega_2 = \sqrt{2} \omega_1$.

(b)



It is easy to see why ω increases with β for the acoustic branch, but is nearly constant for the optical branch. We know that the resonant frequency of a mass and spring system increases as the spring gets stiffer. An acoustic mode with a small β results in very little stretching of the springs because all the atoms tend to move together. So the springs appear less stiff for smaller β leading to a lower frequency ω . But with optical modes, the distortion of the springs is nearly independent of β . Even if β is zero the Ga and As atoms move against each other distorting the springs significantly. The frequency ω thus changes very little with β .

Three-dimensional solids: Finally we note that in real three-dimensional solids, the displacement is actually a vector with three components: u_x, u_y, u_z for each of the two atoms in a unit cell. This leads to six branches in the dispersion curves, three acoustic and three optical. One of the three is a longitudinal mode with a displacement along the vector β , while the other two are transverse modes with displacements perpendicular to β . We thus have a longitudinal acoustic (LA) mode, two transverse acoustic (TA) modes, one longitudinal optical (LO) mode and two transverse optical (TO) modes. The overall displacement at a point (\vec{r}, t) can be written in the form (\vec{r} denotes the position vector of the different points of the lattice)

$$\begin{aligned} \{\vec{u}(\vec{r}, t)\} = & \sum_{v, \beta} \{u_{v, \beta}\} \exp [i(\vec{\beta} \cdot \vec{r} - \omega_v(\beta)t)] \\ & + \{u_{v, \beta}\}^* \exp [-i(\vec{\beta} \cdot \vec{r} - \omega_v(\beta)t)] \end{aligned} \quad (10.4.13)$$

Here the index v runs over the six branches of the dispersion curve (LA, TA etc) and $\{u_{v, \vec{\beta}}\}$ are the (6×1) eigenvectors of the (6×6) eigenvalue equation obtained by generalizing Eq.(10.4.9) to include three components for each of the two displacement vectors. We could write the displacements as (2×1) eigenvectors one for each the three polarizations \hat{v} :

$$\begin{aligned} \{\vec{u}(\vec{r}, t)\}_v = & \hat{v} \sum_{\beta} \{u_{\beta}\}_v \exp [i(\vec{\beta} \cdot \vec{r} - \omega_v(\beta)t)] \\ & + \{u_{\beta}\}_v^* \exp [-i(\vec{\beta} \cdot \vec{r} - \omega_v(\beta)t)] \end{aligned} \quad (10.4.14)$$

The two components represent the displacements of the two atoms in a unit cell. Following the same arguments as in Eq.(10.4.4) we can write

$$\left\{ u_{\vec{\beta}} \right\}_{\nu} = \hat{\nu} \sqrt{\frac{\hbar}{2\rho\Omega\omega}} a_{\nu, \vec{\beta}} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \quad (10.4.15)$$

where $(u_1 \quad u_2)$ is equal to $(1 \quad 1)/\sqrt{2}$ for acoustic phonons and to $(1 \quad -1)/\sqrt{2}$ for optical phonons. The square of the amplitude is the number of phonons occupying the mode, whose average value is given by the Bose-Einstein factor:

$$\left| a_{\nu, \vec{\beta}} \right|^2 = n_{\nu, \vec{\beta}}, \quad \langle n_{\nu, \vec{\beta}} \rangle = \frac{1}{\exp(\hbar\omega_{\nu}(\vec{\beta})/k_B T) - 1} \quad (10.4.16)$$

From Eqs.(10.4.14) – (10.4.16), the mean squared displacement of an atom due to phonons can be written as

$$\langle u^2 \rangle = \sum_{\vec{\beta}} \frac{\hbar}{2\rho\omega\Omega} \frac{1}{e^{\hbar\omega/k_B T} - 1} \quad (10.4.17)$$

Strain due to a single phonon: Finally let us obtain the result we stated earlier in Eq.(10.2.7). The longitudinal strain is defined as the divergence of the displacement:

$$S = \vec{\nabla} \cdot \vec{u} = \sum_{\vec{\beta}} \vec{\beta} \cdot \hat{\nu} \sqrt{\frac{\hbar}{2\rho\omega\Omega}} \left(a_{\vec{\beta}, \hat{\nu}} \exp [i(\vec{\beta} \cdot \vec{r} - \omega_{\nu}(\vec{\beta})t)] + a_{\vec{\beta}, \hat{\nu}}^* \exp [-i(\vec{\beta} \cdot \vec{r} - \omega_{\nu}(\vec{\beta})t)] \right)$$

For a single phonon with wavevector $\vec{\beta}$ and polarization $\hat{\nu}$, we can set $a_{\vec{\beta}, \hat{\nu}} = 1$, so that

$$S = (\hat{\nu} \cdot \vec{\beta}) \sqrt{2\hbar/\rho\omega\Omega} \cos(\vec{\beta} \cdot \vec{r} - \omega(\vec{\beta})t)$$

as stated in Eq.(10.2.8).

Exercises

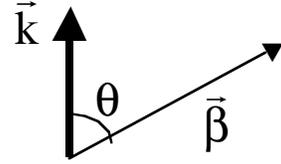
E.10.1. Assume that the electron velocity $\hbar k / m \gg$ sound velocity c_s .

(a) Evaluate Eqs.(10.2.6a,b) by (1) converting the summation into an integral, (2) expressing the argument of the delta function in the form

$$\delta \left(\frac{\hbar^2 k \beta}{m} \left[\cos \theta - \frac{\bar{c}}{\hbar k / m} \pm \frac{\beta}{2k} \right] \right)$$

(3) performing the integral over $\cos \theta$ to get rid of the delta function and set a finite range to the limits of the integral over $\beta : \beta_{\min} < \beta < \beta_{\max}$, and finally (4) performing the integral over β . Show that the lifetime due to acoustic phonon absorption and emission is given by

$$\frac{1}{\tau(k)} = \frac{m D^2 k_B T}{\pi \hbar^3 \rho c_s^2} k$$



(b) What is the angular distribution of the emitted phonons?

E.10.2. Consider an electron in a state \vec{k} in a parabolic band with mass m having an energy E that exceeds the optical phonon energy $\hbar \omega_0$. Equating the argument of the delta function in Eq.(10.2.9) to zero, obtain an expression relating the magnitude of the wavevector β of an *emitted* optical phonon to the angle θ at which it is emitted (measured from \vec{k}). What is the range of values of θ outside which no optical phonons are emitted ?

E.10.3. The mean squared displacement of an atom due to phonons is given in Eq.(10.4.17):

$$\langle u^2 \rangle = \sum_{\vec{\beta}} \frac{\hbar}{2\rho\omega\Omega} \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

Convert the summation into an integral using periodic boundary conditions and evaluate the integral numerically to plot $\sqrt{\langle u^2 \rangle}$ vs. T over the range $0 \text{ K} < T < 1000 \text{ K}$. Assume acoustic phonons with $\omega_{\beta} = c_s \beta$ ($c_s = 5 \times 10^3 \text{ m/sec}$) and $\rho = 5 \times 10^3 \text{ Kg/m}^3$