

Introduction to Quantum Well Theory and Intersubband Transitions

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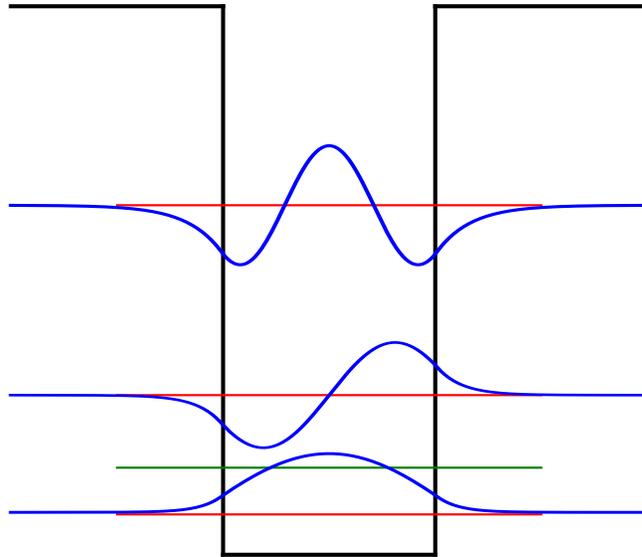


Figure 1: A typical diagram of a Quantum Well (for the conduction band). The black lines show the potential well due to the changes in conduction band energy between the different materials. The red lines show the allowed energy levels for an electron within the well. The blue lines show the (envelope) wavefunctions of the electrons for each energy level (and the green line shows the Fermi level which indicates how many electrons have been put into the quantum well). Plotting the wavefunctions at each energy level is just a convenient convention for understanding the system.

1 Introduction

In the study of quantum mechanics, the finite potential well is one of the first problems to be studied as it demonstrates the new behaviours that arise due to the electron wavefunction[1]. However, it is also possible to construct similar potential wells in real semiconductor structures. We find in both cases that an electron's energy can only take certain values that we call energy levels. A *quantum well* is one such semiconductor nanostructure[2, 3, 4, 5]; it is a nanometre thick layer of semiconductor sandwiched between layers of a different but compatible semiconductor. If the semiconductors are chosen correctly then we have created a structure that can trap electrons within this thin layer.

This article will give a very basic introduction to quantum well energy levels and their intersubband transitions. It should be accompanied by a small script written in python called pyQW which can calculate the electron states, Fermi levels and transitions for finite potential wells (in the absence of more advanced effects such as non-parabolicity or Poisson effects), moreover this case can even be solved analytically whereas anything more advanced must rely on numerical methods.

2 Designing Semiconductor Quantum Wells

In order to create a quantum well, we need to use semiconductors that have compatible lattice constants[2, 4, 3]. Otherwise, we would not be able to create a clean interface between the different layers as stresses would form between the incompatible layers which would damage the interface. For the material family GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$, the lattice constant is almost independent of the aluminium percentage which is one reason that these materials have been exploited so much for creating semiconductor structures. In fact, when using other materials, there are often small stresses present in quantum well structures and this affects their properties and bandstructure but I will ignore this complication here.

We also need to know the size of the potential steps that form between the different bands of the layers; surprisingly, this is difficult to model and so we usually have to rely on values that have been

reported in the literature.

3 Wavefunction calculations

As we would expect, an electron moving within a semiconductor crystal is affected by the lattice of atoms that surround it. We find the electron's mass and energy vary for different velocities (and directions) within the crystal and we describe these relationships as the bandstructure of the material. To understand bandstructure, we would need to learn about Bloch states, crystal types, Brillouin zones and Fermi levels but instead I'm going to take the useful approximation that electrons at the bottom of the semiconductor conduction band behave like free electrons except that they have a different effective mass[6, 7]. This is a good approximation for the material GaAs which will be the focus of my calculations.

To model a quantum well, it is assumed that the well layer and the barrier layers have the same bandstructure as they would if they were bulk samples and at the interfaces, there are abrupt steps in the conduction and valence band potentials[8, 3]. For directions within the plane of the layers, the electronic bandstructure is similar to that of a bulk material. The electron wavefunctions will have complexities due to the crystal lattice that they are moving within but we can actually ignore that component (as a first approximation) and concern ourselves only with the wavefunction at the scale of the structure, this is called the envelope wavefunction. So the envelope function ($f_j(z)$) is the j^{th} solution to Schrodinger's equation using the 1D potential $V(z)$; where $V(z)$ is the average potential of each material's conduction band edge. The equation to solve is given by

$$\left[\hat{p}_z \left(\frac{1}{2m^*(z)} \hat{p}_z \right) + V(z) \right] f_j(z) = (E_j - \varepsilon) f_j(z) \quad (1)$$

where \hat{p}_z is the z component of the momentum operator ($= -i\hbar \frac{\delta}{\delta z}$) and $m^*(z)$ is the effective mass of the charge carrier in each material. E_j is the energy of the QW subband and ε is the energy that the charge carrier would have for a bulk sample of the quantum well material i.e. GaAs at $\mathbf{k} = 0$. At the interfaces between the materials the wavefunctions must satisfy

$$f_A = f_B \quad (2)$$

$$\frac{1}{m_A^*} \frac{df_A}{dz} = \frac{1}{m_B^*} \frac{df_B}{dz} \quad (3)$$

where the subscripts A and B denote different layers of the well.

3.1 Solutions for a symmetric finite well

For the very simple potential shown in fig.1, we can find analytical solutions. In other cases, solutions need to be found numerically.

Consider a well of width d and depth V that is centred about the origin of the z axis.

Inside the well

$$f_{QW} = A \sin(kz) + B \cos(kz) \quad (4)$$

where $k = \sqrt{2m_w^* E} / \hbar$. In the barriers

$$f_{lhs} = Ge^{\alpha z} \quad (5)$$

$$f_{rhs} = He^{-\alpha z} \quad (6)$$

where $\alpha = \sqrt{2m_b^* (V - E)} / \hbar$.

There are odd and even solutions.

- Even solutions - $A = 0, G = H$ and $\tan\left(\frac{kd}{2}\right) = \alpha m_w^* / km_b^*$
- Odd solutions - $B = 0, G = -H$ and $\tan\left(\frac{kd}{2}\right) = -km_b^* / \alpha m_w^*$

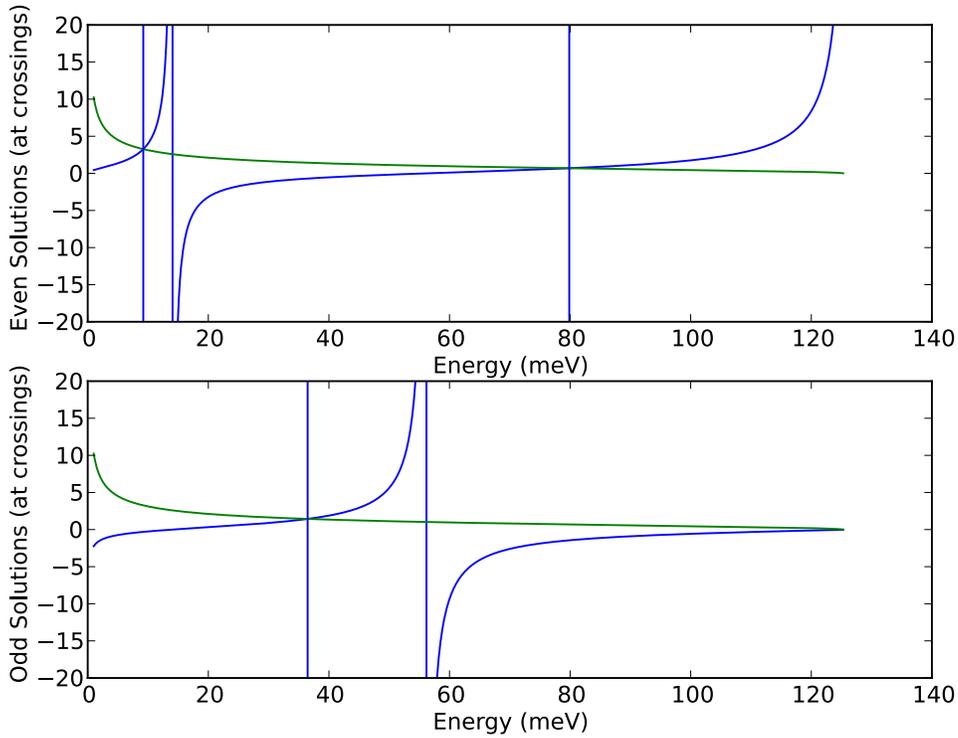


Figure 2: Graphical solution for finding a finite potential well's energy levels. Solutions exist where the blue and green curves meet.

The k values need to be found numerically which is trivially done in modern computing environments such as python or matlab. We can also find the solutions graphically by plotting both sides of the equation and seeing the points where they meet.

There is also a neat trick that allows us to have one equation that gives both the odd and even solutions. Using

$$\tan(\theta) = \frac{\tan\left(\frac{\theta}{2}\right)}{1 - \tan^2\left(\frac{\theta}{2}\right)}$$

we can easily show that

$$\left(\frac{km_b^*}{\alpha m_w^*} - \frac{\alpha m_w^*}{km_b^*}\right) \tan(kL) = 2 \quad (7)$$

in both cases!

In order to find the wavefunctions, we need to connect the amplitudes of the different parts and then normalise the wavefunction over all space (just so that the total probability of the electron existing *somewhere* is 100%!). I find that

- Even

$$A = \left(\frac{d}{2} + \frac{\sin(kd)}{2k} + \frac{\cos^2\left(\frac{kd}{2}\right)}{\alpha}\right)^{-1/2} \quad (8)$$

$$H = A \cos\left(\frac{kd}{2}\right) \exp\left(\frac{\alpha d}{2}\right) \quad (9)$$

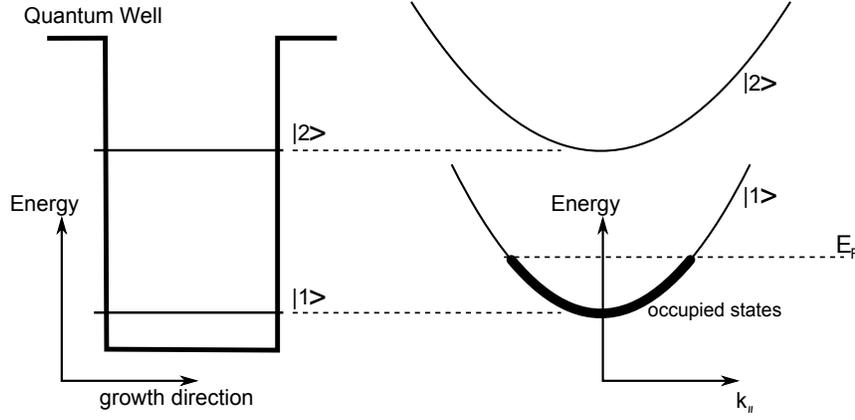


Figure 3: Shows how electrons fill up the levels of a quantum well. The quantum well states are quantised in the growth direction by its potential barriers but in the plane of the well they are subbands with parabolic dispersions with respect to the crystal momentum (k_{\parallel}). The lower subband is occupied up to the Fermi level E_F . The two subbands only have the same dispersion curves to first approximation, the figure illustrates that they are different.

- Odd

$$B = \left(\frac{d}{2} - \frac{\sin(kd)}{2k} + \frac{\sin^2\left(\frac{kd}{2}\right)}{\alpha} \right)^{-1/2} \quad (10)$$

$$H = A \sin\left(\frac{kd}{2}\right) \exp\left(\frac{\alpha d}{2}\right) \quad (11)$$

4 Fermi level

If we put a number of electrons into our structure, they will fill up the available states of the quantum well in order of increasing energy. The density of states for each level in a quantum well comes from its 2d motion within the layer. We find that the 2d density of states is

$$g_{2d} = \frac{m^*}{\pi \hbar^2} \quad (12)$$

which is (interestingly) independent of energy. We can now find the Fermi level for the well and a known doping density using

$$N = \int_0^{\infty} g(E) f(E, E_F) dE \quad (13)$$

where N is the number of electrons, E_F is the Fermi level and the Fermi-Dirac distribution is

$$f(E, E_F) = \left(1 + \exp\left(\frac{E - E_F}{k_B T}\right) \right)^{-1} \quad (14)$$

At 0K, the Fermi-Dirac distribution looks like a step function and we can derive

$$E_F = \frac{N/g_{2d} + \sum_i^n E_i}{n} \quad (15)$$

where E_i are the energy levels of the quantum well and n is the number of the levels occupied. The population of each level is

$$N_i = g_{2d} \cdot (E_F - E_i) \quad (16)$$

At higher temperatures, we have to integrate the Fermi-Dirac distribution, which yields

$$N = g_{2d} k_B T \sum_i^n \ln \left(\exp \left(\frac{E_F - E_i}{k_B T} \right) + 1 \right) \quad (17)$$

which we solve numerically to find the Fermi energy. We can find the population density of each level then using

$$N_i = g_{2d} k_B T \ln \left(\exp \left(\frac{E_F - E_i}{k_B T} \right) + 1 \right) \quad (18)$$

5 AlGaAs/GaAs material constants

Finding material values that you trust for your modelling is actually harder than might be expected. I've found that every research group will generally have numbers that they prefer to use for their modelling based on literature, experience and their particular modelling programs.

Here are some numbers to start with from the literature and taken from [9, 10]

Effective mass

- GaAs $0.067m_e$
- $\text{Al}_x\text{Ga}_{1-x}\text{As}$ $0.063+0.083x m_e$ ($x<0.45$)

Does effective mass change with temperature?

From Vurgaftman[10]

- GaAs $0.067m_e@4\text{ K}, 0.0635m_e@300\text{ K}$
- $\text{Al}_x\text{Ga}_{1-x}\text{As}$ $0.067+0.0838x m_e$ ($x<0.45$) @4 K (?)

conduction band offset

$\text{Al}_x\text{Ga}_{1-x}\text{As}$ - GaAs

- $x<0.41$ $\Delta E_c = 0.79x$ (eV)
- $x>0.41$ $\Delta E_c = 0.475 - 0.335x + 0.143x^2$ (eV)

What is temperature dependence of the offset?

from Vurgaftman[10]

- $x<0.41$ $\Delta E_c = 0.83x$ (eV)

6 More Advanced Modelling

The theory given in the previous sections can only approximately predict the energy levels of a real quantum well. For instance, in most semi-conductor materials, we can not assume that conduction electrons behave exactly like free electrons which just have a different effective mass. Normally the energy/momentum dependence is more complicated; this can be handled very approximately by adding a *non-parabolicity* term to the equations, or by using one of various k.p models to describe the electronic bandstructure of the quantum well more accurately. This leads to more accurate predictions for the energy levels, particularly the higher energy states. Also, to model the valence band levels this type of modelling is essential[3, 4].

In addition, the presence of electrons and donor atoms in a real structure create additional fields which affect the effective potential that an electron will observe. The next section outlines the calculation necessary to account for the coulombic potentials. Those are the most important but there is also an

exchange-correlation interaction between the electrons which can be described by an effective field[11, 12].

There are also strain effects due to the interplay between the different layers of materials that make of the QWs. When the system is grown, the atoms are persuaded to fit into the lattice spacings defined by the substrate even if this is smaller or larger than normal for the new layer's material and this strain affects the bandstructure of the layer[4, 3].

Finally, it is normally assumed that the interfaces are perfectly sharp between the different layers but in some material systems, the boundary can blur out which changes the predicted states[4].

These are just a few of the effects that can complicate or enrich real QW devices. Also real devices, might need to worry about current flow which is a different problem again.

6.1 Poisson Effects

When we have many charges in a structure, their potentials will affect the effective potential seen by each charge and so alter the resultant states. If we are to find a solution that makes sense, this process of self-interaction requires that a system is self-consistently solved for the states and potential and typically this requires that we iterate our calculations towards a stable solution. This effect is alternately known as a Poisson, a Hartree or a Coulomb effect/field/correction[4].

The effective potential seen by an electron is given by the bandstructure, the electric potential of the donor atoms and the electric potential due to the free electrons.

$$V_{eff}(z) = V_{BS} - e\Phi_{Donors} - e\Phi_{elec} \quad (19)$$

The electric potential is given by the solution to Poisson's equation

$$\Phi_{Donors} + \Phi_{elec} = \frac{-e}{\epsilon_0\epsilon} \int_{-\infty}^z \int_{-\infty}^{z'} (n(z'') - N_D(z'')) dz'' dz' \quad (20)$$

but this can be rewritten as a single integral (clue: find the integration of the Heaviside step function)

$$\Phi_{Donors} + \Phi_{elec} = \frac{-e}{\epsilon_0\epsilon} \int_{-\infty}^z (z - z') (n(z') - N_D(z')) dz' \quad (21)$$

where the distribution of electrons is given by

$$n(z') = \sum_i n_i |\xi_i(z')|^2 \quad (22)$$

where n_i is normally given by the Fermi-Dirac distribution

$$n_i = \frac{m_i^* kT}{\pi \hbar^2} \ln \left(1 + \exp \left(\frac{E_F - E_i}{kT} \right) \right) \quad (23)$$

where E_F is the Fermi Energy and m_i^* is the effective mass of the subband.

Note that $V_H = -e\Phi_{Donors} - e\Phi_{elec}$ is normally called the Hartree potential because this way of reducing the multielectron system down to a single electron model plus an effective potential is known as the Hartree approach. It's also an example of mean field theory.

In the case of a periodic structure, the limits change and there is an additional term

$$V_{Donors} + V_{elec} = \frac{e^2}{\epsilon_0\epsilon} \int_0^z (z - z') (n(z') - N_D(z')) dz' + \frac{e^2}{\epsilon_0\epsilon} \frac{z}{L} \int_0^L z' (n(z') - N_D(z')) dz' \quad (24)$$

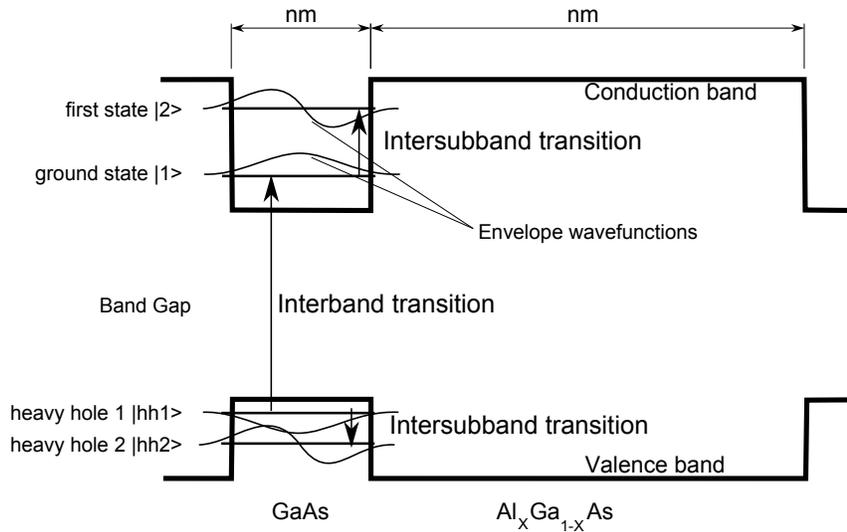


Figure 4: Illustration of a quantum well structure and some of the different optical transitions possible.

7 Optical Transitions

7.1 Introduction

Quantum wells are important semiconductor devices that are used in many ways. They have strong optical transitions and moreover, transitions that we are able to tune in energy (by changing the well thickness as well as other parameters); hence quantum well structures are found in many leds, detectors and lasers (such as those in our dvd players or driving optical signals across the internet backbone). However, those devices rely on optical transitions between the conduction and the valence band, these are called interband transitions (see fig.4). There are also optical transitions between the different electron levels within the quantum well, these are the intersubband transitions. These transitions have a smaller energy gap and so they interact with light in the mid- to far- infrared part of the spectrum and they are used increasingly for detectors and lasers in this region of the spectrum after years of research (see QWIPs and QCLs).

Here I will just give some formulae for calculating intersubband absorptions (ISBTs); anyone interested in a more detailed approach can read the following sections (or go to [3, 11, 13, 8, 5]). Firstly, ISBTs only interact with the electric field component perpendicular to the plane of the QW. It can be shown that the absorption of such a layer is given by

$$\alpha' \approx -\Im \left[\frac{\epsilon_b}{\epsilon_{zz}} \right] \frac{n\omega \sin^2 \theta}{c \cos \theta} L \quad (25)$$

where $\Im [\]$ selects the imaginary component of its contents, ϵ_b is the background dielectric constant, ϵ_{zz} is the dielectric constant of the ISBT, n is the background refractive index, ω is (natural) frequency, c is speed of light, θ is the angle of incidence of the light passing through the QW (wrt it's normal) and L is the thickness of the layer. For a QW, we can calculate that the effective dielectric constant averaged over the thickness of a single quantum well period (L_{SQWP}) is given by

$$\frac{1}{\epsilon_{zz}} = \frac{1}{\epsilon_b} \left\{ 1 - \frac{L_{ij}^{eff}}{L_{SQWP}} \frac{\omega_{p_{ij}}^2 f_{ij}}{\tilde{\omega}_{ij}^2 + \omega_{p_{ij}}^2 - \omega^2 - 2i\gamma_{ij}\omega} \right\} \quad (26)$$

where ω_{ij} is the transition frequency, $\omega_{p_{ij}}$ is the transition's plasma frequency, f_{ij} is the transition's oscillator strength, γ_{ij} is the transition's broadening and L_{ij}^{eff} is the effective thickness of the transition¹. To

¹The accompanying program pyQW calculates most of these values (except for broadening which is left as arbitrary).

calculate these terms, we use

$$f_{ij} = \frac{2m^* \omega_{ij} \mu_{ij}^2}{\hbar e^2} \quad (27)$$

$$\omega_p^2 = \frac{n'_{ij} e^2}{m^* \epsilon_r \epsilon_0 L_{ij}^{eff}} \quad (28)$$

$$L_{ij}^{eff} = \frac{\hbar}{2S_{ij} m^* \omega_{ij}} \quad (29)$$

where μ_{ij} is the dipole matrix element of the transition and n'_{ij} is the 2-dimensional population difference density. More details can be found in the proceeding sections.

The imaginary part of a Lorentz oscillator is approximately a Lorentzian, so our final absorption (for a single transition) is given by

$$\alpha' \approx \frac{n\omega}{2\omega'_0 c} \frac{\sin^2 \theta}{\cos \theta} \left(L_{ij}^{eff} \omega_{p_{ij}}^2 \right) f_{ij} \frac{\gamma_{ij}}{(\omega'_{ij} - \omega)^2 + \gamma_{ij}^2} \quad (30)$$

where $\omega_{ij}^{\prime 2} = \omega_{p_{ij}}^2 f_{ij} + \omega_{ij}^2 - \gamma_{ij}^2$.

The effect of multiple transitions can be approximated by summing the inverses of dielectrics of the different oscillators together (although the most accurate approach recalculates the plasma frequencies taking into account couplings between the different transitions which won't be covered here) ie.

$$\frac{1}{\epsilon_{zz}} = \frac{1}{\epsilon_b} \left\{ 1 - \sum_{i,j} \frac{L_{ij}^{eff}}{L_{SQWP}} \frac{\omega_{p_{ij}}^2 f_{ij}}{\tilde{\omega}_{ij}^2 + \omega_{p_{ij}}^2 - \omega^2 - 2i\gamma_{ij}\omega} \right\} \quad (31)$$

7.2 Basic Derivation

We know from quantum theories of interactions that in order to calculate the strength of an optical transitions, we need to calculate its matrix element[1, 5].

$$\langle \Phi_m | \hat{H}' | \Phi_n \rangle \equiv \iiint \Phi_m^* \Delta \hat{H} \Phi_n \, d\mathbf{r} \quad (32)$$

The strongest type of optical transitions arise from the electric dipole interaction where

$$\Delta \hat{H} = e\mathbf{E} \cdot \hat{\mathbf{r}} \quad (33)$$

e is the electron charge, \mathbf{E} is the electric field and $\hat{\mathbf{r}}$ is the position operator. This gives us the dipole matrix element

$$\mu_{mn} = |\langle \Phi_m | e\hat{\mathbf{r}} | \Phi_n \rangle|$$

For the particular case of quantum well intersubband transitions, the dipole matrix element can be simplified to

$$\mu_{12} = e \langle f_2(z) | z | f_1(z) \rangle \quad (34)$$

where we have assigned the cross-section of the QW to be along the z-axis (which we also call the growth direction due to the way that these structures are made). In this equation, e is the electron charge, $f_j(z)$ are the envelope wavefunctions of the quantum well states (eg. as shown in fig.1 and fig.4) and z is the position operator along the z-axis. There is also an implicit assumption that we are coupling electron states with the same crystal momentum within the plane of the QW (see fig.3).

Although eqn.34 is conveniently simple, some effects require the derivation to be repeated using more accurate wavefunctions; these wavefunctions can be found using the $\mathbf{k} \cdot \mathbf{p}$ method. for example, this equation work well for conduction band ISBTs but less so, in the case of valence band ISBTs.

Importantly eqn.34 finds that transitions only occur if the electric field is polarized along the QW's growth direction (along z). Therefore ISBTs are an anisotropic phenomena; this has important implications for their experimental observation since light crossing the QWs at normal incidence won't interact with the ISBTs.

If we want to know the rate of excitation of carriers then we can use Fermi's golden rule to find the rate for normal conditions (i.e. systems where the light intensity is not too high or the system is not strongly coupled). The derivation of Fermi's golden rule is summarised in appendix C. If we had an absorbing volume, we would use

$$\frac{\delta I}{\delta z} = -n_{12}R_{12}\hbar\omega_{12} = -\alpha_{12}I \quad (35)$$

where R_{12} is the rate of excitation given by Fermi's golden rule, n_{12} is the population difference density between the levels and I is the optical intensity (irradiance) given by

$$I = \frac{nc\epsilon_0}{2}|\mathbf{E}|^2 \quad (36)$$

But our transition is confined to an almost 2-dimensional layer and so we define

$$\frac{\Delta I}{I} = -\alpha'_{12} \quad (37)$$

where now the absorption is per unit area. We find that the optical absorption (per quantum well) is

$$\alpha'_{12} = \frac{n'_{12}\mu_{12}^2\pi\omega_{12}}{nc\epsilon_0\hbar}L(\omega_{12} - \omega)\frac{\sin^2\theta}{\cos\theta} \quad (38)$$

where n'_{12} is the population difference density per unit area between the levels, ω_{12} is the (natural) frequency difference, n is the refractive index, $L(\cdot)$ is the normalised profile of the absorption and the rest are fundamental coefficients. The $\sin^2\theta$ term arises from the angle between the electric field vector and the anisotropic intersubband transition. The $\cos\theta$ term accounts for the difference between an unit area of the incident light and an unit area of the quantum well.

It is usual to define two new variables, the oscillator strength f_{01} and the plasma frequency ω_p . The oscillator strength is a unitless parameter that is commonly used in spectroscopic studies while the plasma frequency comes from the Drude model of the dielectric properties of a plasma and has units of natural frequency². Definitions may vary slightly but they are defined here as

$$f_{01} = \frac{2m^*\omega_{12}\mu_{12}^2}{\hbar e^2} \quad (39)$$

$$\omega_p^2 = \frac{n_{12}e^2}{m^*\epsilon_r\epsilon_0} \quad (40)$$

For the plasma frequency we need to define a 3-dimensional charge density to use this definition and so we say that

$$n_{12} = \frac{n'_{12}}{L_{12}^{eff}} \quad (41)$$

where L_{12}^{eff} is the effective thickness of the transition (as yet undefined). The intersubband absorption can now be written as

$$\alpha'_{12} = \frac{n\omega_p^2 f_{01}\pi}{2c}L(\omega_{12} - \omega)L_{12}^{eff}\frac{\sin^2\theta}{\cos\theta} \quad (42)$$

This might seem like a step backwards from eqn.38, we've introduced a new parameter to no advantage. However, when we want to model a real structure, it becomes useful to assign the transition a thickness and a dielectric constant so that we can model how the overall structure behaves. I will show how to do this in a later section and we will also see that this derivation has also missed an effect known as the depolarisation shift which is due to interactions between the electrons occupying the QW states.

²Natural frequency is 2π times real frequency. Forgetting which one you are using can get you into trouble!

7.3 Dipole Matrix Elements for the Finite Potential Well

First, we note that each state in the potential well has a parity property, each state is either even or odd in parity. Transitions can only occur between states of different parity. For a transition from odd parity to even parity, we have

$$\delta_{ij} = 1$$

for even to odd parity, we have

$$\delta_{ij} = -1$$

For our finite potential well system, we can calculate the dipole matrix elements analytically:

$$z_{ij} = A_i A_j (\text{well} + \text{barrier}) \quad (43)$$

$$\text{well} = \left(\frac{\sin(k_{tot}a)}{k_{tot}^2} - \frac{a \cos(k_{tot}a)}{k_{tot}} \right) + \delta_{ij} \left(\frac{\sin(\Delta ka)}{\Delta k^2} - \frac{a \cos(\Delta ka)}{\Delta k} \right) \quad (44)$$

$$\text{barrier} = (\sin(k_{tot}a) + \delta_{ij} \sin(\Delta ka)) \frac{(a + \kappa_{tot})}{\kappa_{tot}} \quad (45)$$

where $k_{tot} = k_i - k_j$, $\Delta k = k_i + k_j$, $\kappa_{tot} = \kappa_i + \kappa_j$, $a = d/2$ where d is the width of the well. The wavevectors in the layer and barrier can be calculated for the wavefunctions

$$k_i = \sqrt{2m_w^* E_i} / \hbar \quad (46)$$

$$\kappa_i = \sqrt{2m_b^* (V - E_i)} / \hbar \quad (47)$$

m_w^* is the effective mass of the well layer, m_b^* is the effective mass of barrier layer, E_i is the energy of the level (Joules) and V is the potential barrier (Joules).

Finally, the coefficients are calculated. For even parity, we use

$$A_i = \left(a + \frac{\sin(k_i d)}{2k_i} + \frac{\cos^2(k_i a)}{\kappa_i} \right)^{-\frac{1}{2}} \quad (48)$$

For odd parity, we use

$$A_i = \left(a - \frac{\sin(k_i d)}{2k_i} + \frac{\sin^2(k_i a)}{\kappa_i} \right)^{-\frac{1}{2}} \quad (49)$$

7.4 Collective Effects - Classical

It is often useful to calculate an effective dielectric constant for the transitions when we do more advanced modelling. A useful model is that of the Lorentz oscillator

$$\varepsilon_r(\omega) = \varepsilon_b \left(1 + \frac{\omega_p^2 f}{\omega_0^2 - \omega^2 - 2i\gamma\omega} \right) \quad (50)$$

where ε_b is the background dielectric constant, ω_p is called the plasma frequency (eqn.40), ω_0 is the frequency of the transition, γ is the broadening of the transition and f is the oscillator strength (eqn.39). In the classical model $f = 1$ but quantum mechanics yields values both more and less than unity.

In the above model, we see a simple linear dependence upon the density of the oscillators (via the plasma frequency) but for a dense medium of oscillators, we need to adjust the model to account for their mutual interactions via the electric fields that the oscillators produce. The effect of these local field correction leads to the Clausius-Mossotti relation (also known as the Lorentz-Lorenz relation).

$$N\chi_0 = 3 \frac{\varepsilon_r - 1}{\varepsilon_r + 2} \quad (51)$$

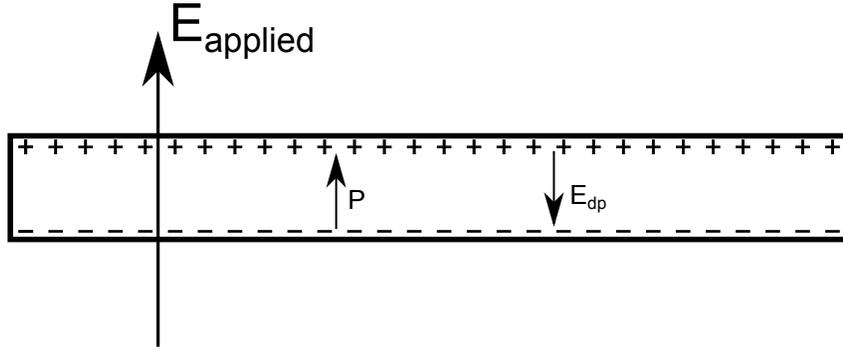


Figure 5: Shows the effect of an electric field applied across a thin dielectric layer. The layer is polarised (P) and this creates a depolarisation field E_{dp} due to the layer's surface charges.

where N is the density of oscillators and χ_0 is the susceptibility of a single oscillator³. Our quantum well transitions don't use the above relation but there is a Coulomb interaction between the free charges present in the levels. We can see this in two different approaches.

Qualitative Approach In the first approach, we consider the effect of an applied electric field across a thin layer of dielectric; we can take this static approach because the layer is much thinner than the wavelength of the light. The applied field polarizes the layer leading to surface charge densities which creates an extra opposing electric field within the layer. We have that the polarisation of the layer is given by

$$\mathbf{P} = \epsilon_0(\epsilon_{layer} - 1)\mathbf{E}_{local} \quad (52)$$

and the induced electric field inside the layer (\mathbf{E}_{dp}) is given by

$$\mathbf{E}_{dp} = -\frac{\mathbf{P}}{\epsilon_0} \quad (53)$$

So the electric field inside the layer is given by

$$\mathbf{E}_{local} = \mathbf{E}_{applied} + \mathbf{E}_{dp} \quad (54)$$

leading to

$$\mathbf{E}_{local} = \frac{\mathbf{E}_{applied}}{\epsilon_{layer}} \quad (55)$$

Now if we define our dielectric constant wrt the applied electric field, we have that

$$\mathbf{D} = \epsilon_0\epsilon_r\mathbf{E}_{applied} = \epsilon_0\mathbf{E}_{applied} + \mathbf{P} \quad (56)$$

and can find that

$$\epsilon_r = 1 + \frac{\epsilon_{layer} - 1}{\epsilon_{layer}} = 2 - \frac{1}{\epsilon_{layer}} \quad (57)$$

The absorption coefficient of a medium can be calculated from

$$\alpha \approx \frac{\omega \Im[\epsilon_r]}{cn_b} \quad (58)$$

where $\Im[\]$ means take the imaginary component and n_b is the background refractive index. Although note that this approximation breaks down in the case of strong absorption. In this case, the dielectric component becomes

$$\alpha \approx \frac{\omega}{cn_b} \Im \left[\frac{-1}{\epsilon_{layer}} \right] \quad (59)$$

³ $\chi_0 = \frac{e^2}{m^*\epsilon_0} \frac{f}{\omega_0^2 - \omega^2 - 2i\gamma\omega}$

For absorption of a plane wave incident at an angle to the plane, the total absorption of the layer becomes

$$\alpha' \approx \frac{\omega}{cn_b} \Im \left[\frac{-1}{\epsilon_{layer}} \right] \frac{\sin^2 \theta}{\cos \theta} L \quad (60)$$

where $\sin^2 \theta$ accounts for the anisotropic absorption and $L/\cos \theta$ is the effective thickness of the layer. This approach offers some insight but I find that it becomes very confusing when trying to consider the details of the derivation. Also, it does not account for a background dielectric constant and the anisotropic properties of the transition are largely added by hand.

Analytical Approach Instead, in the second approach, we can reach the above equation by starting with the equation for an etalon adjusted for an anisotropic absorbing material (which interacts only with electric field perpendicular to the plane of the film just like the ISBT) and then making assumptions about the layer's thickness and simplifying to

$$\alpha' \approx -\Im \left[\frac{\epsilon_b}{\epsilon_{zz}} \right] \frac{n\omega}{c} \frac{\sin^2 \theta}{\cos \theta} L \quad (61)$$

The derivation is given in appendix A. Interestingly, the absorption is proportional to the *inverse* of the dielectric constant. For a Lorentz oscillator, this leads to

$$\Im \left[\frac{\epsilon_b}{\epsilon_{zz}} \right] = \Im \left[1 - \frac{\omega_p^2 f}{\omega_p^2 f + \omega_0^2 - \omega^2 - 2i\gamma\omega} \right] \quad (62)$$

$$\approx \frac{\omega_p^2 f}{2\omega_0'} \left(\frac{\gamma}{(\omega_0' - \omega)^2 + \gamma^2} \right) \quad (63)$$

where $\omega_0'^2 = \omega_p^2 f + \omega_0^2 - \gamma^2$. We see that our absorption peak has been shifted to a higher frequency (assuming that γ is quite small). This is known as the 'depolarisation shift' due to its origins in the depolarisation field of the layer and such an effect is observed in measurements.

So we have found that consideration of the optics of the thin film geometry has led to a shift in the absorption peak. This was not predicted by the initial derivation of the optical absorption shown in sec.7.2. However, there is a remaining problem since we are not sure what thickness to apply to the intersubband transition (eqn.41). This thickness affects the plasma frequency of the transition and hence the size of the depolarisation shift. Although, we might initially guess that the thickness is the same as the quantum well layer L_{QW} , this is not really the case. In fact, we need to perform a quantum mechanical derivation in order to find this thickness and the most accurate form of the dielectric constant.

7.5 Collective Effects - Quantum

The concept in the following derivation[11, 3] is that we calculate the effect that an optical interaction has on the quantum well charge distribution in the QW. Consider that if a static electric field is applied to the QW system, this will change the envelope wavefunctions and the energies of the allowed states; the dynamic electric field of a light wave will have a corresponding dynamical effect on the QW states. We also saw in sec.6.1 that similarly the charges inside a QW affect the states that they occupy through their electric fields, in a self-interaction of the charges on their own states. In the static case, we usually solve the problem self-consistently to get the final energies and wavefunctions whereas in the dynamic situation (well, in this derivation), we are going to use time-dependent perturbation theory. We will call this the dynamic Hartree effect.

The matrix element for the optical interaction becomes

$$\langle i | eDz - e \Delta \Phi(z) | j \rangle \quad (64)$$

where $\Delta\Phi(z)$ is the effective (oscillating) change to the QW potential due to the presence of the light wave. We will label this matrix element as M_{ij} . We can calculate the change in potential using

$$\Delta\Phi(z) = \frac{-e}{\epsilon_0\epsilon} \int_{-\infty}^z \int_{-\infty}^{z'} \Delta n(z'') dz'' dz' \quad (65)$$

where $\Delta n(z'')$ is the (oscillating) change in the charge distribution. Starting from the equation for the charge density

$$n(z) = \sum_i n_i |\xi_i(z')|^2 \quad (66)$$

where ξ_i is the wavefunction and n_i is the population density of the i^{th} level. We can use time perturbation theory (see Appendix D) to get

$$n(z, t) = n(z) + \Delta n(z) \cos \omega t + \dots \quad (67)$$

$$\Delta n(z) = - \sum_i n_i \sum_m \frac{2}{\hbar} \xi_i(z') \xi_m(z') M_{mi} \left(\frac{\omega_{mi}}{\omega_{mi}^2 - \omega^2} \right) \quad (68)$$

where ω_{ij} is the frequency between the levels i and j . We can now write that

$$M_{ij} = eDz_{ij} + \frac{e^2}{\epsilon_0\epsilon} (-2) \sum_n n_n \sum_m \left\{ S_{ijmn} M_{mn} \frac{\hbar\omega_{mn}}{(\hbar\omega_{mn})^2 - (\hbar\omega)^2} \right\} \quad (69)$$

where $z_{ij} = \langle i | z | j \rangle$ and

$$S_{ijmn} = - \frac{1}{\hbar\omega_{ij}} \frac{1}{\hbar\omega_{mn}} \left(-\frac{\hbar^2}{2m^*} \right)^2 \int_0^\infty \left(\frac{d\xi_i}{dz} \xi_j - \xi_i \frac{d\xi_j}{dz} \right) \left(\frac{d\xi_m}{dz} \xi_n - \xi_m \frac{d\xi_n}{dz} \right) dz \quad (70)$$

See Appendix E and Appendix F to see the derivation of S_{ijmn} . In order to calculate the effective properties of the QW intersubband transitions, we calculate the conductivity of the transitions (which can easily be related to the equivalent dielectric constant), defined as

$$\sigma_{zz} = \frac{1}{D} \int_0^\infty j(z) dz \quad (71)$$

we use the continuity equation

$$\frac{\partial j_z}{\partial z} + \frac{\partial \tilde{n}}{\partial t} = 0 \quad (72)$$

where \tilde{n} is the charge density (while n is the carrier density). This leads to

$$\sigma_{zz}(\omega) = (-i\omega) \frac{2e}{D} \sum_n \left[n_n \sum_m \left\{ M_{mn} \left(\frac{\hbar\omega_{mn}}{\hbar^2\omega_{mn}^2 - \hbar^2\omega^2} \right) z_{mn} \right\} \right] \quad (73)$$

see Appendix G for the details. Let's assume now that there are only 2 levels in our summations, our matrix element becomes

$$M_{ij} = + \frac{e^2}{\epsilon_0\epsilon} (-2) \Delta n_{ij} S_{ijij} M_{ij} \frac{\hbar\omega_{ij}}{(\hbar\omega_{ij})^2 - (\hbar\omega)^2} \quad (74)$$

where Δn_{ij} is the difference in population density between the two levels. So the conductivity becomes

$$\sigma_{zz}(\omega) = (-i\omega) \frac{2e}{D} \Delta n_{ij} M_{ij} \left(\frac{\hbar\omega_{ij}}{\hbar^2\omega_{ij}^2 - \hbar^2\omega^2} \right) z_{ij} \quad (75)$$

$$= (-i\omega) 2e^2 \Delta n_{ij} z_{ij}^2 \left(\frac{\hbar\omega_{ij}}{\hbar^2\omega_{ij}^2 + \frac{e^2}{\epsilon_0\epsilon} 2\Delta n_{ij} S_{ijij} \hbar\omega_{ij} - \hbar^2\omega^2} \right) \quad (76)$$

It is usual now to use our definitions for the oscillator strength and plasma frequency

$$f_{ij} = \frac{2m^* \omega_{ij} z_{ij}^2}{\hbar} \quad (77)$$

$$\omega_{p_{ij}}^2 = \frac{\Delta n_{ij} e^2}{m^* \epsilon_r \epsilon_0 L_{ij}^{eff}} \quad (78)$$

$$L_{ij}^{eff} = \frac{\hbar}{2S_{ij} m^* \omega_{ij}} \quad (79)$$

so we have

$$\sigma_{zz}(\omega) = (-i\omega) \epsilon_r \epsilon_0 L_{ij}^{eff} \left(\frac{f_{ij} \omega_{p_{ij}}^2}{\omega_{ij}^2 + \omega_{p_{ij}}^2 - \omega^2} \right) \quad (80)$$

We finally calculate the effective dielectric constant for the quantum structure using an effective medium (appendix B)

$$\frac{1}{\epsilon_{zz}} = \frac{(1-f)}{\epsilon_b} + \frac{f}{\epsilon_w} - \frac{i\tilde{\sigma}_{zz}^{(2D)}(\omega)}{\epsilon_0 \epsilon_w^2 \omega L_{SQW}} \quad (81)$$

where ϵ_w is the dielectric constant for the well layers, ϵ_b is the dielectric constant for the barrier layers, f is the fraction of the whole structure which is the well layers and L_{SQW} is the thickness of one period of the structure (note that a normal quantum well sample typically has many repeats of the quantum well in order to increase absorption/emission etc). So, if we assume that the dielectric constants of the different layers are about the same, we finally have

$$\frac{1}{\epsilon_{zz}} = \frac{1}{\epsilon_w} \left(1 - \frac{L_{ij}^{eff}}{L_{SQW}} \frac{f_{ij} \omega_{p_{ij}}^2}{\omega_{ij}^2 + \omega_{p_{ij}}^2 - \omega^2} \right) \quad (82)$$

to which we would add a broadening term γ_{ij} by hand.

$$\frac{1}{\epsilon_{zz}} = \frac{1}{\epsilon_w} \left(1 - \frac{L_{ij}^{eff}}{L_{SQW}} \frac{f_{ij} \omega_{p_{ij}}^2}{\omega_{ij}^2 + \omega_{p_{ij}}^2 - \omega^2 - 2i\gamma_{ij}\omega} \right) \quad (83)$$

8 Bibliography

References

- [1] Alastair Rae. *Quantum Mechanics*. IOP Publishing, 3ed. edition, 1998.
- [2] Simon M. Sze Kwok K. Ng. *Semiconductor Devices: Physics and Technology*. Wiley-Blackwell, 3rd edition, 2006.
- [3] H.C. Liu. *Intersubband Transitions in Quantum Wells: Physics and Device Applications II*, volume vol.65 of *Semiconductors and Semimetals*. academic press, 2000.
- [4] Paul Harrison. *Quantum Wells, Wires and Dots: Theoretical and Computational Physics of Semiconductor Nanostructures*. Wiley, 2011.
- [5] E. Rosencher and B. Vinter. *Optoelectronics*. Cambridge University Press, 2002.
- [6] John Singleton. *Band theory and electronic properties of solids*. Oxford University Press Oxford, UK, 2001.

- [7] Neil W Ashcroft and N David Mermin. *Solid State Physics*. Brooks Cole, 1976.
- [8] Gerald Bastard. *Wave Mechanics Applied to Semiconductor Heterostructures*. Editions de Physique, 1990.
- [9] Electronic archive: New semiconductor materials. characteristics and properties. <http://www.ioffe.ru/SVA/NSM/Semicond/>.
- [10] I Vurgaftman, JR Meyer, and LR Ram-Mohan. Band parameters for iii-v compound semiconductors and their alloys. *Journal of applied physics*, 89(11):5815–5875, 2001.
- [11] Tsuneya Ando. Intersubband optical absorption in space-charge layers on semiconductor surfaces. *Z. Physik B*, 26:263–272, 1977.
- [12] Tsuneya Ando. Electronic properties of two-dimensional systems. *Reviews of Modern Physics*, 54(2), 1982.
- [13] M. Zaluzny C. Nalewajko. Coupling of infrared radiation to intersubband transitions in multiple quantum wells: The effective-medium approach. *Physical Review B*, 59(20), 1999.
- [14] Max Born and Emil Wolf. *Principles of optics: electromagnetic theory of propagation, interference and diffraction of light*. Cambridge university press, 1999.

A Transmission through a slab of a particular case of uniaxial material

For studying intersubband absorption in quantum wells, we have a lossy uniaxial material with optical axis along the growth direction. Therefore we are interested in studying (and calculating) the transmission of an extra-ordinary wave through a uniaxial layer.

Surprisingly, the standard equation for an etalon can be used for this type of anisotropic layer although the definitions of its components are adjusted. This can be derived from the transfer matrix formalism given in [13].

$$t = \frac{t_{01}t_{12}e^{i\delta_1}}{1 + r_{01}r_{12}e^{2i\delta_1}} \quad (84)$$

where we use for a TM (p) polarised wave:

$$t_{01} = \frac{2\varepsilon_{xx}k_z^{(0)}}{\varepsilon_{xx}k_z^{(0)} + \varepsilon'_0k_z^{(1)}} \frac{n_0}{n_1} \quad (85)$$

$$r_{01} = \frac{\varepsilon_{xx}k_z^{(0)} - \varepsilon'_0k_z^{(1)}}{\varepsilon_{xx}k_z^{(0)} + \varepsilon'_0k_z^{(1)}} \quad (86)$$

$$t_{12} = \frac{2\varepsilon_2k_z^{(1)}}{\varepsilon_2k_z^{(1)} + \varepsilon_{xx}k_z^{(2)}} \frac{n_1}{n_2} \quad (87)$$

$$r_{12} = \frac{\varepsilon_2k_z^{(1)} - \varepsilon_{xx}k_z^{(2)}}{\varepsilon_2k_z^{(1)} + \varepsilon_{xx}k_z^{(2)}} \quad (88)$$

$$\delta_1 = k_z^{(1)}d_1 \quad (89)$$

where d_1 is the thickness of the layer and ε_{xx} is the dielectric constant of the layer for electric fields parallel to the interface. ε_2 is the dielectric constant of the second layer and ε'_0 is the dielectric constant of the zeroth layer (not the vacuum constant - sorry about the bad notation). n_x is the refractive index of the x th layer.

The k-vector components are calculated using

$$k_z^2 = \varepsilon_{xx}K^2 - \frac{\varepsilon_{xx}}{\varepsilon_{zz}}k_x^2 \quad (90)$$

where $K = \frac{\omega}{c}$ and k_x is constant across the layers.

$$k_x = k_0 \sin \theta_0 = \frac{n_0\omega}{c} \sin \theta \quad (91)$$

$$k_z^{(0)} = \frac{n_0\omega}{c} \cos \theta \quad (92)$$

where θ is the angle of incidence. Finally, in this case, we have

$$T = \left(\frac{k_z^{(f)}}{k_z^{(0)}} \right) |t|^2 \quad (93)$$

If $\varepsilon'_0 = \varepsilon_2 = \varepsilon_b$, this can be simplified down to

$$t_p = \left(\cos \delta_1 - i \sin \delta_1 \left(\frac{\varepsilon_{xx}^2 k_z^{(0)2} + \varepsilon_b^2 k_z^{(1)2}}{2\varepsilon_{xx}\varepsilon_b k_z^{(0)} k_z^{(1)}} \right) \right)^{-1}$$

Consider

$$\begin{aligned} \left(\frac{k_z^{(1)}}{k_z^{(0)}} \right)^2 &= \frac{\varepsilon_{xx} K^2 - \frac{\varepsilon_{xx}}{\varepsilon_{zz}} k_x^2}{\varepsilon_b K^2 - k_x^2} \\ &= \frac{\varepsilon_{xx} - \frac{\varepsilon_{xx}}{\varepsilon_{zz}} \varepsilon_b \sin^2 \theta}{\varepsilon_b - \varepsilon_b \sin^2 \theta} \\ &= \frac{\varepsilon_{xx}}{\varepsilon_b} \frac{1 - \frac{\varepsilon_b}{\varepsilon_{zz}} \sin^2 \theta}{\cos^2 \theta} \end{aligned}$$

Also

$$\frac{\varepsilon_{xx}^2 k_z^{(0)2} + \varepsilon_b^2 k_z^{(1)2}}{2\varepsilon_{xx}\varepsilon_b k_z^{(0)} k_z^{(1)}} = \frac{1}{2} \left(\frac{\varepsilon_{xx} k_z^{(0)}}{\varepsilon_b k_z^{(1)}} + \frac{\varepsilon_b k_z^{(1)}}{\varepsilon_{xx} k_z^{(0)}} \right)$$

For now put $\varepsilon_{xx} = \varepsilon_b$

$$\Rightarrow \frac{1}{2} \left(\frac{1 - \frac{\varepsilon_b}{\varepsilon_{zz}} \sin^2 \theta + \cos^2 \theta}{\sqrt{1 - \frac{\varepsilon_b}{\varepsilon_{zz}} \sin^2 \theta} \cos \theta} \right)$$

Now, we can often assume that $\delta_1 \ll 1$, we can also write

$$\delta_1 = \sqrt{\varepsilon_{xx}} K \left(1 - \frac{\varepsilon_b}{\varepsilon_{zz}} \sin^2 \theta \right)^{1/2} d$$

so that

$$t_p = \left(1 - in_0 K \frac{d}{2} \left(\frac{1 - \frac{\varepsilon_b}{\varepsilon_{zz}} \sin^2 \theta + \cos^2 \theta}{\cos \theta} \right) \right)^{-1}$$

(where we have continued to assume that $\sqrt{\varepsilon_{xx}} = n_0$). In this equation ε_{zz} is imaginary, so that

$$T_p = \left(\left| 1 - in_0 K \frac{d}{2} \left(\frac{1 - \frac{\varepsilon_b}{\varepsilon_{zz}} \sin^2 \theta + \cos^2 \theta}{\cos \theta} \right) \right|^2 \right)^{-1}$$

In this equation ε_{zz} is imaginary, so that complicates things slightly. Put

$$\frac{\varepsilon_b}{\varepsilon_{zz}} = z + iz'$$

to get

$$\begin{aligned} T_p &= \left(\left| 1 - n_0 K \frac{d}{2} \left(\frac{z' \sin^2 \theta}{\cos \theta} \right) - in_0 K \frac{d}{2} \left(\frac{1 - z \sin^2 \theta + \cos^2 \theta}{\cos \theta} \right) \right|^2 \right)^{-1} \\ T_p &= \left(\left\{ 1 - n_0 K \frac{d}{2} \left(\frac{z' \sin^2 \theta}{\cos \theta} \right) \right\}^2 + \left\{ n_0 K \frac{d}{2} \left(\frac{1 - z \sin^2 \theta + \cos^2 \theta}{\cos \theta} \right) \right\}^2 \right)^{-1} \end{aligned}$$

If we assume that $z = 1$, the second term becomes $\{n_0 K d \cos \theta\}^2$ and as before, we can assume that this is small. So that now we have

$$T_p = \left(1 - n_0 K \frac{d}{2} \left(\frac{z' \sin^2 \theta}{\cos \theta} \right) \right)^{-2}$$

expand this using

$$\frac{1}{(1+x)^2} \approx 1 - 2x + 3x^2 - 4x^3 \dots$$

$$T_p = 1 + 2n_0K \frac{d}{2} \left(\frac{z' \sin^2 \theta}{\cos \theta} \right) \dots$$

I assume that z' will turn out to be negative. So finally, we have

$$T_p = 1 + \Im \left[\frac{\epsilon_b}{\epsilon_{zz}} \right] n_0K \frac{\sin^2 \theta}{\cos \theta} d$$

B Effective Medium Theory for a Thin Films

When we have a body that is a composite of materials, as long as the sizes of the particles/structures are smaller than the wavelength of the light then we can use an effective dielectric to describe the bodies properties. For more information see the Maxwell-Garnett and Bruggeman theories.

It can be useful to replace a stack of dielectric layers with an effective dielectric constant. This is a kind of effective medium [14, 13]; Born and Wolf call this form birefringence as the resulting effective medium will be uniaxial even when all of the layers are dielectric.

For the electric field parallel to the interfaces, we get

$$\epsilon_{xx} = \sum_i f_i \epsilon_i$$

where f_i is the fractional volume/width of each layer and ϵ_i is its dielectric constant.

Whereas for electric field perpendicular to the interfaces (along the growth direction), the dielectric constant is given by

$$\frac{1}{\epsilon_{zz}} = \sum_i \frac{f_i}{\epsilon_i}$$

C Time-Dependent Perturbation Theory

A quick revision of time dependent quantum mechanics follows. First we have Schrodinger's equation

$$\hat{H}_0 \Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad (94)$$

If \hat{H}_0 has no time dependence then we can separate the variables to get

$$\hat{H}_0 \Phi = E \Phi \quad (95)$$

and

$$\Psi = \Phi \exp \left(-i \frac{E}{\hbar} t \right) \quad (96)$$

If we now include a time dependent term to the Hamiltonian, we get

$$(\hat{H}_0 + \hat{H}') \Psi' = i\hbar \frac{\partial \Psi'}{\partial t} \quad (97)$$

We can posit that the solution is described by

$$\Psi' = \sum_n c_n(t) \Phi_n \exp(-i\omega_n t) \quad (98)$$

where n numerates the possible solutions to the Hamiltonian. This leads to

$$\sum_n \hat{H}' (c_n(t) \Phi_n \exp(-i\omega_n t)) = i\hbar \sum_n \frac{\partial c_n(t)}{\partial t} \Phi_n \exp(-i\omega_n t) \quad (99)$$

If we assume that \hat{H}' includes no time derivatives then we get

$$\sum_n c_n(t) \exp(-i\omega_n t) \hat{H}' \Phi_n = i\hbar \sum_n \frac{\partial c_n(t)}{\partial t} \Phi_n \exp(-i\omega_n t) \quad (100)$$

Multiplying the equations by Φ_m^* and integrating over space gives us

$$\frac{\partial c_m(t)}{\partial t} = \frac{1}{i\hbar} \sum_n c_n(t) \langle \Phi_m | \hat{H}' | \Phi_n \rangle \exp(i\omega_{mn} t) \quad (101)$$

where $\omega_{mn} = \omega_m - \omega_n$.

Now, let us assume that the time dependent term is a perturbation to the system and that we really want to obtain an approximate solution to the problem, so we expand c_n with respect to the size of the perturbation i.e.

$$\hat{H}' \rightarrow \beta \hat{H}' \quad (102)$$

$$c_n(t) \rightarrow c_n^{(0)}(t) + \beta c_n^{(1)}(t) + \beta^2 c_n^{(2)}(t) + \dots \quad (103)$$

where each $c_n^{(i)}$ is a different function and not c_n raised to a power. This leads to

$$\frac{\partial c_m^{(0)}(t)}{\partial t} + \frac{\partial c_m^{(1)}(t)}{\partial t} \beta + \frac{\partial c_m^{(2)}(t)}{\partial t} \beta^2 + \dots = \frac{1}{i\hbar} \sum_n \left(c_n^{(0)}(t) + \beta c_n^{(1)}(t) + \beta^2 c_n^{(2)}(t) + \dots \right) \beta \langle \Phi_m | \hat{H}' | \Phi_n \rangle \exp(i\omega_{mn} t) \quad (104)$$

and matching up orders of β gives

$$c_m^{(0)}(t) = \text{constant} = c_m^{(0)} \quad (105)$$

$$\frac{\partial c_m^{(1)}(t)}{\partial t} = \frac{1}{i\hbar} \sum_n c_n^{(0)} \langle \Phi_m | \hat{H}' | \Phi_n \rangle \exp(i\omega_{mn} t) \quad (106)$$

...

This looks like Fermi's Golden rule but in fact our matrix term is still time dependent so we're not quite there. We haven't made too many assumptions about the form of the time dependent term in the Hamiltonian. Let's take the obvious case of a periodic interaction

$$\hat{H}' = \hat{H}'_0 \cos \omega t \quad (107)$$

We can also briefly go back to the non-perturbative equations, so that we get

$$\frac{\partial c_m(t)}{\partial t} = \frac{1}{i\hbar} \sum_n c_n(t) \langle \Phi_m | \hat{H}'_0 | \Phi_n \rangle \cos(\omega t) \exp(i\omega_{mn} t) \quad (108)$$

or

$$\frac{\partial c_m(t)}{\partial t} = \frac{1}{i\hbar} \sum_n c_n(t) \langle \Phi_m | \hat{H}'_0 | \Phi_n \rangle \frac{1}{2} (\exp(i(\omega_{mn} + \omega)t) + \exp(i(\omega_{mn} - \omega)t)) \quad (109)$$

For the perturbative case, we get

$$\frac{\partial c_m^{(1)}(t)}{\partial t} = \frac{1}{i\hbar} \sum_n c_n^{(0)} \langle \Phi_m | \hat{H}'_0 | \Phi_n \rangle \frac{1}{2} (\exp(i(\omega_{mn} + \omega)t) + \exp(i(\omega_{mn} - \omega)t)) \quad (110)$$

which we can solve to give

$$c_m^{(1)}(t) = \frac{1}{i\hbar} \sum_n c_n^{(0)} \langle \Phi_m | \hat{H}'_0 | \Phi_n \rangle \frac{1}{2} \left(\frac{\exp(i(\omega_{mn} + \omega)t) - 1}{i(\omega_{mn} + \omega)} + \frac{\exp(i(\omega_{mn} - \omega)t) - 1}{i(\omega_{mn} - \omega)} \right) \quad (111)$$

Normally, the first term is disregarded because it is small close to $\omega = \omega_{mn}$. This is known as the 'rotating wave approximation'. This leads to

$$c_m^{(1)}(t) = \frac{1}{i\hbar} \sum_n c_n^{(0)} \langle \Phi_m | \hat{H}'_0 | \Phi_n \rangle \frac{1}{2} \exp\left(\frac{i}{2}(\omega_{mn} - \omega)t\right) \left(\frac{\exp\left(\frac{i}{2}(\omega_{mn} - \omega)t\right) - \exp\left(-\frac{i}{2}(\omega_{mn} - \omega)t\right)}{i(\omega_{mn} - \omega)} \right) \quad (112)$$

$$c_m^{(1)}(t) = \frac{1}{i\hbar} \sum_n c_n^{(0)} \langle \Phi_m | \hat{H}'_0 | \Phi_n \rangle \exp\left(\frac{i}{2}(\omega_{mn} - \omega)t\right) \frac{\sin\left(\frac{1}{2}(\omega_{mn} - \omega)t\right)}{(\omega_{mn} - \omega)} \quad (113)$$

So that we get

$$\left| c_m^{(1)}(t) \right|^2 = \left(\frac{1}{\hbar} \sum_n c_n^{(0)} \langle \Phi_m | \hat{H}'_0 | \Phi_n \rangle \frac{\sin\left(\frac{1}{2}(\omega_{mn} - \omega)t\right)}{(\omega_{mn} - \omega)} \right)^2 \quad (114)$$

In the usual case, the wavefunction is initially only in one state. Also as t increases, the last part of the formula tends towards a delta function

$$\left| c_m^{(1)}(t) \right|^2 = \frac{1}{\hbar^2} |\langle \Phi_m | \hat{H}'_0 | \Phi_n \rangle|^2 \delta(\omega_{mn} - \omega) \frac{1}{4} t^2 \quad (115)$$

However, this isn't the form normally given. Typically, the linewidth of the transition or perturbation is introduced and the formula is integrated over frequency; this changes the final form to

$$\left| c_m^{(1)}(t) \right|^2 = \frac{1}{\hbar^2} |\langle \Phi_m | \hat{H}'_0 | \Phi_n \rangle|^2 \delta(\omega_{mn} - \omega) \frac{1}{2} \pi t \quad (116)$$

so that finally we get Fermi's Golden Rule

$$\frac{\left| c_m^{(1)}(t) \right|^2}{t} = \frac{\pi}{2\hbar} |\langle \Phi_m | \hat{H}'_0 | \Phi_n \rangle|^2 \delta(\omega_{mn} - \omega) \quad (117)$$

or

$$\frac{\left| c_m^{(1)}(t) \right|^2}{t} = \frac{\pi}{2\hbar^2} |\langle \Phi_m | \hat{H}'_0 | \Phi_n \rangle|^2 \delta(\omega_{mn} - \omega) g(\omega) g'(\omega_{mn}) \quad (118)$$

where $g(\omega)$ and $g'(\omega_{mn})$ are the density of states of the interaction and the interacting levels.

D Charge Perturbation

We start from

$$n(z) = \sum_i n_i |\xi_i(z')|^2 \quad (119)$$

The interaction changes our states to

$$n(z, t) = \sum_i n_i \left| \sum_m c_{im}(t) \xi_m(z') \exp(-i\omega_m t) \right|^2 \quad (120)$$

Taking a perturbative approach and assuming that we are dealing with a harmonic perturbation, we can expand $c_{im}(t)$

$$n(z, t) = \sum_i n_i \left| \sum_m \left\{ c_{mi}^{(0)} \xi_m(z') \exp(-i\omega_m t) + c_{mi}^{(1)}(t) \xi_m(z') \exp(-i\omega_m t) \right\} \right|^2 \quad (121)$$

but we require that $c_{ii}^{(0)} = 1$ (and all others equal 0) since that is where we started from.

$$n(z, t) = \sum_i n_i \left| \xi_i(z') \exp(-i\omega_i t) + \sum_m \left\{ c_{mi}^{(1)}(t) \xi_m(z') \exp(-i\omega_m t) \right\} \right|^2 \quad (122)$$

Expanding this gives

$$n(z, t) = \sum_i n_i |\xi_i(z')|^2 + \sum_i n_i \sum_m 2\Re \left[\xi_i^*(z') \exp(i\omega_i t) c_{mi}^{(1)}(t) \xi_m(z') \exp(-i\omega_m t) \right] + \dots \quad (123)$$

We also have a formula for $c_{im}^{(1)}(t)$

$$c_{mi}^{(1)}(t) = -\frac{1}{2\hbar} \langle \Phi_m | \hat{H}'_0 | \Phi_i \rangle \left(\frac{\exp(i(\omega_{mi} + \omega)t) - 1}{(\omega_{mi} + \omega)} + \frac{\exp(i(\omega_{mi} - \omega)t) - 1}{(\omega_{mi} - \omega)} \right) \quad (124)$$

putting $M_{mi} = \langle \Phi_m | \hat{H}'_0 | \Phi_i \rangle$ and combining the two terms in the bracket, gives

$$c_{mi}^{(1)}(t) = -\frac{1}{\hbar} M_{mi} \left(\frac{\omega_{mi} \exp(i\omega_{mi} t) \cos(\omega t) - \omega \exp(i\omega_{mi} t) \sin(\omega t) - \omega_{mi}}{\omega_{mi}^2 - \omega^2} \right) \quad (125)$$

So we can write

$$n(z, t) = \sum_i n_i |\xi_i(z')|^2 - \sum_i n_i \sum_m \frac{2}{\hbar} \Re \left[\xi_i^*(z') \xi_m(z') M_{mi} \left(\frac{\omega_{mi} \cos(\omega t) - \omega \sin(\omega t) - \omega_{mi} \exp(-i\omega_{mi} t)}{\omega_{mi}^2 - \omega^2} \right) \right] + \dots \quad (126)$$

assuming that ξ_i and M_{mi} are both real quantities, we get

$$n(z, t) = \sum_i n_i |\xi_i(z')|^2 - \sum_i n_i \sum_m \frac{2}{\hbar} \xi_i(z') \xi_m(z') M_{mi} \left(\frac{\omega_{mi} \cos(\omega t) - \omega \sin(\omega t) - \omega_{mi}}{\omega_{mi}^2 - \omega^2} \right) + \dots \quad (127)$$

The $\cos(\omega_{mi} t)$ is puzzling, it is present because we integrated over $t = 0 \rightarrow t$. Perhaps we can simply neglect this term? Something to do with steady state solutions? or integrating over linewidth of perturbation?

Now we can separate the terms into

$$n(z, t) = n(z) + \Delta n(z) \cos \omega t + \dots \quad (128)$$

where

$$\Delta n(z) = -\sum_i n_i \sum_m \frac{2}{\hbar} \xi_i(z') \xi_m(z') M_{mi} \left(\frac{\omega_{mi}}{\omega_{mi}^2 - \omega^2} \right) \quad (129)$$

E Collective Effect Matrix Element

$$M_{ij} = \langle i | eDz - e \Delta \Phi(z) | j \rangle \quad (130)$$

$$\Rightarrow M_{ij} = eDz_{ij} + \frac{e^2}{\varepsilon_0 \varepsilon} (-2) \int_{-\infty}^{\infty} \sum_n n_n \sum_m \left\{ \int_{-\infty}^z \int_{-\infty}^{z'} \frac{1}{\hbar} \xi_n(z') \xi_m(z') M_{mn} \left(\frac{\omega_{mi}}{\omega_{mi}^2 - \omega^2} \right) dz'' dz' \right\} \xi_i(z) \xi_j(z) dz \quad (131)$$

$$\Rightarrow M_{ij} = eDz_{ij} + \frac{e^2}{\varepsilon_0 \varepsilon} (-2) \sum_n n_n \sum_m \left\{ S_{ijnm} M_{mn} \left(\frac{\hbar \omega_{mi}}{(\hbar \omega_{mi})^2 - (\hbar \omega)^2} \right) \right\} \quad (132)$$

where

$$S_{ijnm} = \int_{-\infty}^{\infty} \xi_i(z) \xi_j(z) \left\{ \int_{-\infty}^z \int_{-\infty}^{z'} \xi_n(z') \xi_m(z') dz'' dz' \right\} dz \quad (133)$$

F Simplifying S_{nm}

$$S_{nm} = \int_0^{\infty} dz \xi_n(z) \xi_0(z) \int_0^z dz' \int_0^{z'} dz'' \xi_m(z'') \xi_0(z'') \quad (134)$$

By substituting the Heaviside step function for the limit of the middle integral ie.

$$\int_0^z dz' = \int_0^{\infty} H(z - z') dz' \quad (135)$$

we can swap the order of the integrals and rewrite the equation as

$$S_{nm} = \int_0^{\infty} dz' \int_{z'}^{\infty} dz \xi_n(z) \xi_0(z) \int_0^{z'} dz'' \xi_m(z'') \xi_0(z'') \quad (136)$$

Consider

$$\int_0^{z'} dz'' \xi_m(z'') \xi_0(z'') \quad (137)$$

We also know from Schrodinger's equation that

$$\xi_m(z) \equiv \frac{1}{\hbar\omega_m} \left[-\frac{\hbar^2}{2m_1} \frac{d^2}{dz^2} + V_{eff}(z) \right] \xi_m(z) \quad (138)$$

therefore we can integrate by parts, giving

$$\left[g \frac{d\xi_m(z'')}{dz''} \xi_0(z'') \right]_0^{z'} - g \int_0^{z'} dz'' \frac{d\xi_m(z'')}{dz''} \frac{d\xi_0(z'')}{dz''} + \frac{1}{\hbar\omega_m} \int_0^{z'} dz'' V_{eff}(z'') \xi_m(z'') \xi_0(z'') \quad (139)$$

where $g = \frac{1}{\hbar\omega_m} \left(-\frac{\hbar^2}{2m_1} \right)$.

And then we do it again

$$\begin{aligned} & \left[g \frac{d\xi_m(z'')}{dz''} \xi_0(z'') \right]_0^{z'} - \left[g \xi_m(z'') \frac{d\xi_0(z'')}{dz''} \right]_0^{z'} + \\ & \frac{1}{\hbar\omega_m} \left(-\frac{\hbar^2}{2m_1} \right) \int_0^{z'} dz'' \xi_m(z'') \frac{d^2 \xi_0(z'')}{dz''^2} + \frac{1}{\hbar\omega_m} \int_0^{z'} dz'' V_{eff}(z'') \xi_m(z'') \xi_0(z'') \end{aligned} \quad (140)$$

which simplifies to

$$g \left[\frac{d\xi_m(z'')}{dz''} \xi_0(z'') - \xi_m(z'') \frac{d\xi_0(z'')}{dz''} \right]_0^{z'} + \frac{\hbar\omega_0}{\hbar\omega_m} \int_0^{z'} dz'' \xi_m(z'') \xi_0(z'') \quad (141)$$

and therefore

$$\left(1 - \frac{\omega_0}{\omega_m} \right) \int_0^{z'} dz'' \xi_m(z'') \xi_0(z'') = g \left[\frac{d\xi_m(z'')}{dz''} \xi_0(z'') - \xi_m(z'') \frac{d\xi_0(z'')}{dz''} \right]_0^{z'} \quad (142)$$

and since we are considering confined wavefunctions then we can define $z'' = 0$ to be a position where $\xi_m(0) = \xi_n(0) = 0$.

$$\int_0^{z'} dz'' \xi_m(z'') \xi_0(z'') = \frac{g}{\left(1 - \frac{\omega_0}{\omega_m}\right)} \left(\frac{d\xi_m(z')}{dz'} \xi_0(z') - \xi_m(z') \frac{d\xi_0(z')}{dz'} \right) \quad (143)$$

$$\int_0^{z'} dz'' \xi_m(z'') \xi_0(z'') = \frac{1}{\hbar\omega_{m0}} \left(-\frac{\hbar^2}{2m_1} \right) \left(\frac{d\xi_m(z')}{dz'} \xi_0(z') - \xi_m(z') \frac{d\xi_0(z')}{dz'} \right) \quad (144)$$

We can do the same for the integral

$$\int_{z'}^{\infty} dz \xi_n(z) \xi_0(z)$$

This gives us

$$\int_{z'}^{\infty} dz \xi_n(z) \xi_0(z) = \frac{1}{\hbar\omega_{n0}} \left(-\frac{\hbar^2}{2m_1} \right) \left[\frac{d\xi_n(z')}{dz'} \xi_0(z') - \xi_n(z') \frac{d\xi_0(z')}{dz'} \right]_{z'}$$

Here we can use $\xi_m(\infty) = \xi_n(\infty) = 0$ and $g' = \frac{1}{\hbar\omega_n} \left(-\frac{\hbar^2}{2m_1} \right)$. We can now rewrite the total integral as

$$S_{nm} = -\frac{g}{\left(1 - \frac{\omega_0}{\omega_m}\right)} \frac{g'}{\left(1 - \frac{\omega_0}{\omega_n}\right)} \int_0^{\infty} dz' \left(\frac{d\xi_m(z')}{dz'} \xi_0(z') - \xi_m(z') \frac{d\xi_0(z')}{dz'} \right) \left(\frac{d\xi_n(z')}{dz'} \xi_0(z') - \xi_n(z') \frac{d\xi_0(z')}{dz'} \right) \quad (145)$$

or more simply

$$S_{nm} = -\frac{1}{\hbar\omega_{m0}} \frac{1}{\hbar\omega_{n0}} \left(-\frac{\hbar^2}{2m_1} \right)^2 \int_0^{\infty} \left(\frac{d\xi_m}{dz} \xi_0 - \xi_m \frac{d\xi_0}{dz} \right) \left(\frac{d\xi_n}{dz} \xi_0 - \xi_n \frac{d\xi_0}{dz} \right) dz \quad (146)$$

Note that Ando defines $\hbar\omega_m = E_m - E_0$ whereas I use ω_{m0} and $\hbar\omega_m = E_m$.

If the effective mass is z dependent then, we have to keep it inside of the integral giving

$$S_{nm} = -\frac{1}{\hbar\omega_{m0}} \frac{1}{\hbar\omega_{n0}} \left(-\frac{\hbar^2}{2} \right)^2 \int_0^{\infty} \left(\frac{1}{m^*(z)} \right)^2 \left(\frac{d\xi_m}{dz} \xi_0 - \xi_m \frac{d\xi_0}{dz} \right) \left(\frac{d\xi_n}{dz} \xi_0 - \xi_n \frac{d\xi_0}{dz} \right) dz \quad (147)$$

This can be proved using the correct form of Schrodinger's equation

$$\xi_m(z) \equiv \frac{1}{\hbar\omega_m} \left[-\frac{\hbar^2}{2m_1} \frac{d}{dz} \left(\frac{1}{m^*(z)} \frac{d}{dz} \right) + V_{eff}(z) \right] \xi_m(z) \quad (148)$$

Note that if the effective masses are different for each level then I do not think that this proof can work.

G Derivation of the Conductivity Tensor

Ando defines the conductivity perpendicular to the 2D plane as

$$\sigma_{zz} = \frac{1}{D} \int_0^{\infty} j(z) dz \quad (149)$$

then the equation of continuity is used to derive j

$$\nabla j + \frac{\partial \tilde{n}}{\partial t} = 0 \quad (150)$$

$$\Rightarrow \frac{\partial j_x}{\partial x} + \frac{\partial j_y}{\partial y} + \frac{\partial j_z}{\partial z} + \frac{\partial \tilde{n}(z)}{\partial t} = 0 \quad (151)$$

as given the long-wavelength limit that we are always assuming, \tilde{n} (the charge density) is a function only of z

so the equations becomes

$$\frac{\partial j_z}{\partial z} + \frac{\partial \tilde{n}}{\partial t} = 0 \quad (152)$$

where we have already found

$$\tilde{n}(z, t) = -e(n(z) + \Delta n(z) \cos \omega t + \dots) \quad (153)$$

where \tilde{n} is the charge density and n is the carrier density. So

$$j_z = e \int_0^z \Delta n(z) dz (-\omega) \sin \omega t \quad (154)$$

Using

$$\Delta n(z) = -\sum_i n_i \sum_m \frac{2}{\hbar} \xi_i(z') \xi_m(z') M_{mi} \left(\frac{\omega_{mi}}{\omega_{mi}^2 - \omega^2} \right) \quad (155)$$

we have

$$j_z = -e(-\omega) \sin \omega t 2 \sum_i \left[n_i \sum_m \left\{ M_{mi} \left(\frac{\hbar \omega_{mi}}{\hbar^2 \omega_{mi}^2 - \hbar^2 \omega^2} \right) \int_0^z \xi_i(z') \xi_m(z') dz' \right\} \right] \quad (156)$$

and so

$$\sigma_{zz} = \frac{1}{D} - e(-\omega) \sin \omega t 2 \sum_i \left[n_i \sum_m \left\{ M_{mi} \left(\frac{\hbar \omega_{mi}}{\hbar^2 \omega_{mi}^2 - \hbar^2 \omega^2} \right) \int_0^\infty \int_0^z \xi_i(z') \xi_m(z') dz' dz \right\} \right] \quad (157)$$

Now

$$\begin{aligned} & \int_0^\infty \int_0^z \xi_i(z') \xi_m(z') dz' dz \Rightarrow \int_0^\infty \int_0^\infty H(z - z') \xi_i(z') \xi_m(z') dz' dz \\ \Rightarrow & \int_0^\infty \int_0^\infty H(z - z') \xi_i(z') \xi_m(z') dz' dz \Rightarrow \lim_{z \rightarrow \infty} \int_0^\infty (z - z') H(z - z') \xi_i(z') \xi_m(z') dz' \\ & \Rightarrow \lim_{z \rightarrow \infty} \int_0^z (z - z') \xi_i(z') \xi_m(z') dz' \Rightarrow \lim_{z \rightarrow \infty} \int_0^z (z - z') \xi_i(z') \xi_m(z') dz' \\ z \rightarrow \infty & \left[z \int_0^z \xi_i(z') \xi_m(z') dz' - \int_0^z z' \xi_i(z') \xi_m(z') dz' \right] \Rightarrow - \int_0^\infty z' \xi_i(z') \xi_m(z') dz' \\ & = -d_{mi} \end{aligned} \quad (158)$$

and if we switch to complex notation then $\sigma_{zz} \rightarrow \sigma_{zz}(\omega)$, $\sin \omega t \rightarrow i$, giving

$$\sigma_{zz}(\omega) = (-i\omega) \frac{2e}{D} \sum_i \left[n_i \sum_m \left\{ M_{mi} \left(\frac{\hbar \omega_{mi}}{\hbar^2 \omega_{mi}^2 - \hbar^2 \omega^2} \right) d_{mi} \right\} \right] \quad (159)$$