

# Quantum Theory for Dielectric Properties of Conductors

## C. Effects of Magnetic Fields on Band-To-Band Transitions

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November, 2011, Viçosa, Brazil <sup>1</sup>

### Summary

The complex and frequency-dependent dielectric function  $\epsilon(\omega)$  describes how light interacts when propagating through matter. It determines the propagation speed, dispersion effects, absorption, and more esoteric phenomena such as Faraday rotation when a DC magnetic field is present. Of particular interest here is the description of  $\epsilon(\omega)$  in conductors using quantum mechanics, so that intrinsically quantum mechanical systems can be described. The goal is an appropriate understanding of the contributions from band-to-band transitions, such as in metals and semiconductors, with or without an applied DC magnetic field present.

Part A discusses the general theory of  $\epsilon(\omega)$  for a medium only in the presence of the optical electric field. The approach is to find how this electric field modifies the density matrix. It is applied to band-to-band transitions in the absence of an applied magnetic field.

In Part B, the effect of a DC magnetic field is discussed generally, with respect to how it causes Faraday rotation. For free electrons, it causes quantized Landau levels for the electrons; the dielectric function is found for that problem, and related problems are discussed.

In this part, the important problem is how to include the effect of a DC magnetic field on the band-to-band transitions, such as those in metals and semiconductors. Results are found for 1D and 3D band models, with and without a phenomenological damping.

Taken together, these theories should be complete enough to describe Faraday rotation effects in gold, whose dielectric function is strongly dependent on band-to-band transitions for wavelengths below 600 nm.

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<sup>1</sup>Last updated March, 2012, Florianópolis, Brazil

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## 6 Dielectrics in a DC Magnetic Field

The introduction to this topic appears in documents *Dielectrics: Part A* (general theory for dielectric functions) and *Dielectrics: Part B* (modifications due to magnetic field, especially, discussion of electronic Landau levels). Those may need to be reviewed in order to understand the discussion here. This part is concerned primarily with the contributions to the dielectric function due to the transitions between some bands (such as valence to conduction bands in a semiconductor).

## 7 Band to band transitions in a semiconductor/metal

So far the general theory for dielectric functions for right and left circular polarizations of the light,  $\epsilon_R$  and  $\epsilon_L$ , were derived. The result is seen to depend on the transitions that change angular momentum magnitude by  $\hbar$ , due to the magnitude of the photon angular momentum. After checking that all works out well for free electrons living in Landau levels, one can also look at some simple models where there are transitions only between a pair of bands.

Consider here electrons in a potential that produces bands, that have some quadratic kinetic energy dispersion combined with the magnetic dipole energy. The states could be similar to those considered earlier for almost-free electrons in a field, with the “unstable” states and energies:

$$\psi_{klm} = C j_l(kr) Y_{lm}(\theta, \phi), \quad E_{klm} = \frac{\hbar^2 k^2}{2m_e^*} - m\mu_B B. \quad (7.1)$$

For free electrons this was unstable because the angular momentum does not really have an upper limit, leading to unbounded negative energies. The correct theory for truly free electrons in a magnetic field is to consider their Landau levels, as is calculated in *Dielectrics: Part B*. This difficulty is not present in a band, because bands are usually of a selected angular momentum, and, the energies are not identical to this expression anyway.

Physically, electric dipole transitions nearly conserve electron momentum, so there is no change in the kinetic term. The band states are identified by a wavevector and by angular momentum quantum numbers  $l$  and  $m$ . Any transition that contributes to the susceptibility must change  $l$  by  $\pm 1$  and  $m$  by  $\pm 1$ . In terms of the spherical Bessel functions or indeed, any band states as the eigenstates, we can suppose that their wave vector  $k$  does not change, however, the nonzero terms do connect between different neighboring  $l$ 's. To decide the dependence on  $k$  it would be best to know the radial overlap integrals. We might get an estimate based on just looking at the transitions between some chosen  $l$  and  $l'$ , and ignore higher pairs, unless it is a simple extension to calculate them all. The wavevectors here are assumed to be three-dimensional, and a damping parameter  $\gamma$  is to be included for the dynamics.

So as a reasonable problem, I consider electrons living in two bands of angular momentum  $l_i$  and  $l_f$  separated by some gap,  $E_g$ , together with the splittings due to the magnetic field. One should assume the magnetic splitting is greater than thermal energy  $k_B T$ , otherwise, the magnetic splittings would be totally smeared out and they would not be observable. Let me assume that the band with  $l$  is lower in energy and is the valence band, while  $l_f = l_i \pm 1$  (to satisfy the selection rules) is the index for the conduction band. Between these two bands we can consider all transitions that additionally satisfy the azimuthal selection rule,  $\Delta m = \pm 1$ . We need to find the sums  $S_R$  and  $S_L$  appropriate for the two circular polarizations, that give  $\epsilon_R$  and  $\epsilon_L$ .

To be specific, the energies in each of the bands of interest are written as follows. There is the occupied hole quasi-particle band with effective mass  $m_h^*$  and the (mostly) unoccupied electron quasi-particle band with effective mass  $m_e^*$ . The zero of energy is placed at the center of the energy gap for the following formulas. Then these band energies are written (for positively charged “electrons”)

$$E_i = E_h = -\frac{1}{2}E_g - \frac{\hbar^2 k_i^2}{2m_h^*} - m_i \mu_B B, \quad E_f = E_e = +\frac{1}{2}E_g + \frac{\hbar^2 k_f^2}{2m_e^*} - m_f \mu_B B. \quad (7.2)$$

These are the eigenstates specified by band wavevector,  $k$ , and band index  $l$  and azimuthal quantum number  $m$ . The states might be written for a periodic lattice like  $u_{klm}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$ . Let me explain a few other things here, which are different than that in Boswarva, Howard and Lidiard (1962)<sup>2</sup>. As I have mentioned elsewhere, they made what I see as an error by including both a Landau-level energy together with the magnetic dipole interaction with the field; to me that is a double counting for the orbital angular momentum contribution. So I do not have a Landau-level energy. Besides, how can an electron be in a band, and yet have the motion/energy that it would have if in a free Landau-level? That does not make sense. The two bands have effective masses of opposite sign, as needed for electron and hole states. But the dipolar interaction is the same, because it refers to the states allowed for the electrons in the occupied levels. (The hole is not created until an upward transition takes place.) The  $m$  refers to the component of angular momentum along the applied magnetic field.

There is an important question about electron statistics, which are fermions and obey Fermi-Dirac statistics. The occupation factor  $w_i - w_f$  in most of these notes has been set to 1, which means

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<sup>2</sup>“Faraday effect in semiconductors,” I. M. Boswarva, R. E. Howard, A. B. Lidiard Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, Vol. 269, No. 1336 (Aug. 21, 1962), pp. 125-141. There seems to be various errors in that paper.

I am taking an extreme case that really may not apply to a metals like gold. This is equivalent to assuming that the Fermi energy is somewhere near the middle of the gap between the bands. That would be true in an intrinsic semiconductor, and may also apply to some doped semiconductors. So I should call it the “semiconductor approximation.” But in gold, as an example, according to Scaffardi and Tocho<sup>3</sup> the gap energy is 2.1 eV while the Fermi energy, apparently measured from the bottom of the gap, is 2.5 eV. If this is correct, it means the Fermi energy falls well within the conduction sp-band. Then, the factor of  $w_i - w_f$  cannot be set to unity. It must have some energy dependence. We can still take  $w_i = 1$ , as the valence d-band should be fully occupied, well below  $E_F$ , but the upper level needs to have its energy-dependent occupation number included correctly. So be aware that in much of these notes, I set the upper levels to be fully unoccupied, which helped with the integrations, but it is not always correct. More correctly, we should include the extra function as follows in the integrands,

$$g_{if} \equiv w_i - w_f \approx g(E_f) = 1 - F(E_f), \quad F(E_f) = \frac{1}{\exp\{\beta(E_f - E_F)\} + 1}, \quad (7.3)$$

where  $\beta$  is the inverse temperature and  $E_F$  is the Fermi energy. Both these energies obviously must be measured from the same reference level. This means that the energy difference that goes here is actually

$$E_f - E_F = (E_g - E_F) + \frac{\hbar^2 \mathbf{k}_f^2}{2m_e^*} - m_f \mu_B B. \quad (7.4)$$

Again, since a conducting metal could have  $E_g < E_F$  (need to verify this), then the energy difference  $E_f - E_F$  could be negative for a large part of the conduction band of interest, giving it a large occupation number. This would nearly zero out any contributions from the transitions in that wave vector range. Further, the size of that wave vectors range will change with the temperature.

The magnetic dipole term is taken with a **negative sign**, which would be the correct sign for **positively charged electrons**. In this way, the comparison with the theory in earlier sections and the different effects of right and left circular polarization will be clearer. In earlier sections, the sign of  $e$  was basically considered positive. But then, to compare these results with experiment, one needs to remember to change the sign of the charge carriers. It means reverse the sign of the Bohr magneton, or, of the magnetic frequency,  $\omega_B = eB/m_e c$ . To keep aware of the sign of the charges, the band energies could otherwise be written

$$E_i = E_h = -\frac{1}{2}E_g - \frac{\hbar^2 k_i^2}{2m_h^*} - m_i \frac{\hbar e B}{2m_e c}, \quad E_f = E_e = +\frac{1}{2}E_g + \frac{\hbar^2 k_f^2}{2m_e^*} - m_f \frac{\hbar e B}{2m_e c}, \quad (7.5)$$

or even with the last terms as proportional to  $\omega_B/2$ . In addition, the goal here is to consider nanoparticle samples, where the free Landau levels do not apply. Thus, I need to avoid that as an approximation, because those wave functions have de Broglie wave lengths much greater than the particle sizes.

The difference in the energies of two of these states gives the transition frequency, which is

$$\omega_{if} = \frac{E_i - E_f}{\hbar} = \frac{E_h - E_e}{\hbar} = -\frac{1}{\hbar} \left[ E_g + \frac{\hbar^2 k_i^2}{2m_h^*} + \frac{\hbar^2 k_f^2}{2m_e^*} - (m_f - m_i) \mu_B B \right]. \quad (7.6)$$

Since the wave vectors are taken as equal, this can be written with the effective mass  $\tilde{m}$ ,

$$\hbar \omega_{if} = - \left[ E_g + \frac{\hbar^2 k_i^2}{2\tilde{m}} - (m_f - m_i) \mu_B B \right], \quad \frac{1}{\tilde{m}} = \frac{1}{m_h^*} + \frac{1}{m_e^*}. \quad (7.7)$$

We will also refer to gap frequency  $\omega_g = E_g/\hbar$  for the first term.

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<sup>3</sup>“Size dependence of refractive index of gold nanoparticles,” Lucia B Scaffardi and Jorge O Tocho, Nanotechnology **17**, 1309–1315 (2006).

## 7.1 Expressions for permittivity for circular polarization, current averaging

The type of sum that is needed, say, for right circular polarization, comes from the symmetrization found earlier for transitions between states of defined  $l$  and  $m$ , using the expression based on **averaging of the current density**,

$$S_R = \frac{2m_e}{\hbar} \sum_i^o \sum_f^u (w_i - w_f) \omega_{if}^2 |\langle f|x|i \rangle|^2 \left\{ \frac{\delta_{m_f=m_i-1}}{\omega + i\gamma + \omega_{if}} - \frac{\delta_{m_f=m_i+1}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.8)$$

This could also be expressed more fundamentally with the matrix elements of  $\hat{\pi}$  operators,

$$S_R = \frac{2}{m_e \hbar} \sum_i^o \sum_f^u (w_i - w_f) |\langle f|\hat{\pi}_x|i \rangle|^2 \left\{ \frac{\delta_{m_f=m_i-1}}{\omega + i\gamma + \omega_{if}} - \frac{\delta_{m_f=m_i+1}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.9)$$

In the first expression from the “quasi-free” electron analysis I’ll assume that the bare electron mass  $m_e$  used to transform from  $\hat{\pi}$  to dipole matrix elements is OK, although I believe this is only going to be a good approximation when the electron and hole quasi-particle masses are not too different from  $m_e$ . The deltas come from a factor  $(1 - \Delta m)$  that forces only contributions from transitions with  $m_f = m_i - 1$  (before the  $o/u$  symmetrization). The expression for left polarization and  $S_L$  is similar, but with the two deltas swapped. For the  $\hat{\pi}$  form it will be

$$S_L = \frac{2}{m_e \hbar} \sum_i^o \sum_f^u (w_i - w_f) |\langle f|\hat{\pi}_x|i \rangle|^2 \left\{ \frac{\delta_{m_f=m_i+1}}{\omega + i\gamma + \omega_{if}} - \frac{\delta_{m_f=m_i-1}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.10)$$

Of course, we have seen much earlier that these two can be combined into a single formula, where helicity index  $\nu = +1$  for L-polarization and  $\nu = -1$  for R-polarization:

$$S_\nu = \frac{2}{m_e \hbar} \sum_i^o \sum_f^u (w_i - w_f) |\langle f|\hat{\pi}_x|i \rangle|^2 \left\{ \frac{\delta_{m_f=m_i+\nu}}{\omega + i\gamma + \omega_{if}} - \frac{\delta_{m_f=m_i-\nu}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.11)$$

This is somewhat similar to the form used in the absence of magnetic field—but that was based on averaging of the electric polarization, for the most part. I would like to be sure that this new theory reduces to that previous one in the limit of  $\mathbf{B} = 0$ . Although I cannot fully justify it, another approach would be to assume that the  $\hat{\pi}_x$  operator on which this is based is nearly the same as the standard momentum operator, which reduces to  $\hat{\pi}_x \rightarrow \hbar k_x$ . Then, the needed matrix element here might be written slightly differently, like

$$\langle i|\hat{\pi}_x|f \rangle \langle f|(\hat{\pi}_x - i\hat{\pi}_y)|i \rangle = |\langle f|\hat{\pi}_x|i \rangle|^2 (1 - \Delta m) \approx |\hbar k_x M(\mathbf{k}_i)|^2 \delta_{\mathbf{k}_i \mathbf{k}_f} 2\delta_{m_f=m_i-1} \quad (7.12)$$

This leads to an alternate expression for  $S_\nu$  that probably has a limit like the previous calculations,

$$S_\nu = \frac{2\hbar}{m_e} \sum_i^o \sum_f^u (w_i - w_f) k_{i,x}^2 |M(\mathbf{k}_i)|^2 \left\{ \frac{\delta_{m_f=m_i+\nu}}{\omega + i\gamma + \omega_{if}} - \frac{\delta_{m_f=m_i-\nu}}{\omega + i\gamma - \omega_{if}} \right\} \delta_{\mathbf{k}_i \mathbf{k}_f} \quad (7.13)$$

I think the main advantage of this form is that one can assume a nearly constant matrix element  $M(\mathbf{k}_i)$  between the bands, which is the same approximation that was made in the absence of the magnetic field. It may have some dependence on the band indexes  $l_i$  and  $l_f$ , which is suppressed. [Recall that this the similar matrix element squared for free electrons was proportional to  $\omega_B!$  That will not be the case here, due to the band separation.] The more important parts here are the dependencies on the azimuthal quantum numbers and their effects on the energies. Also note: that is the expression based on the **averaging of the current density**.

## 7.2 Expressions from averaging of electric polarization

In Part A of *Dielectrics* the results were worked out using the expression from averaging of the polarization, which I think is not as fundamental. However, I may need to evaluate on that basis simply to have the comparison of the results. The difference is that in place of a factor  $-\omega$  in the denominator for the susceptibility, there is a factor of  $+\omega_{kk'}$ . As mentioned earlier, these are almost the same, because the denominator of the original term is  $(\omega + i\gamma + \omega_{kk'})$ , which zeroes at  $\omega = -\omega_{kk'}$  (when damping is ignored). So, the theory expression for susceptibility, based on **averaging of the electric polarization**, comes from

$$\chi_{ij}(\omega) = \frac{-ne^2}{m_e\omega(\omega + i\gamma)} \left\{ \delta_{ij} - \frac{\omega}{m_e\hbar} \sum_{kk'} \frac{(w_k - w_{k'}) \langle k | \hat{\pi}_i | k' \rangle \langle k' | \hat{\pi}_j | k \rangle}{\omega_{kk'} [\omega + i\gamma + \omega_{kk'}]} \right\} \quad (7.14)$$

The second term leads to the sum  $S_R$  in the same way as described already from averaging of the current, and after symmetrizing for occupied and unoccupied levels, one gets

$$S_R = -\frac{2\omega}{m_e\hbar} \sum_i^o \sum_f^u (w_i - w_f) \frac{|\langle f | \hat{\pi}_x | i \rangle|^2}{\omega_{if}} \left\{ \frac{\delta_{m_f=m_i-1}}{\omega + i\gamma + \omega_{if}} + \frac{\delta_{m_f=m_i+1}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.15)$$

Swapping the deltas leads to the expression for left circular polarization,

$$S_L = -\frac{2\omega}{m_e\hbar} \sum_i^o \sum_f^u (w_i - w_f) \frac{|\langle f | \hat{\pi}_x | i \rangle|^2}{\omega_{if}} \left\{ \frac{\delta_{m_f=m_i+1}}{\omega + i\gamma + \omega_{if}} + \frac{\delta_{m_f=m_i-1}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.16)$$

In these expressions, there are two differences from the ones based on the current: (1) both terms now have the same sign, which causes some different cancellations, and (2) the extra factor of  $\omega_{if}$  in the denominator might make integrals that are easier to evaluate. This can be written for the general helicity index  $\nu = +1/-1$ , for *L/R* circular polarizations,

$$S_\nu = -\frac{2\omega}{m_e\hbar} \sum_i^o \sum_f^u (w_i - w_f) \frac{|\langle f | \hat{\pi}_x | i \rangle|^2}{\omega_{if}} \left\{ \frac{\delta_{m_f=m_i+\nu}}{\omega + i\gamma + \omega_{if}} + \frac{\delta_{m_f=m_i-\nu}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.17)$$

Then once the sums are known, the permittivity is obtained by the usual way, regardless of averaging of current or of polarization,

$$\epsilon_{R,L} = 1 + 4\pi\chi_{R,L} = 1 - \frac{4\pi ne^2}{m_e\omega(\omega + i\gamma)} (1 + S_{R,L}). \quad (7.18)$$

## 7.3 Evaluating $S_R$ , 3D bands with damping, current averaging

Now consider the summations over the initial and final states. The first sum over  $\mathbf{k}_f$  can be evaluated because of the Kronecker delta in wave vectors. For the sum over  $\mathbf{k}_i$ , I'll take the usual approximation of converting a sum over 3D wave vector into an integration,

$$\sum_{\mathbf{k}_i} \longrightarrow \frac{V}{(2\pi)^3} \int d^3k \quad (7.19)$$

(and now just write  $\mathbf{k}$  for  $\mathbf{k}_i$ ). There will also still be sums over the possible azimuthal numbers. To get further, it also has to be assumed that the matrix element  $M(\mathbf{k}_i)$  is a constant. Also, take  $w_i = 1$  and  $w_f = 0$  (Fermi level within the gap). With these approximations, one now has

$$S_R = \frac{2|M|^2\hbar}{m_e} \sum_{m_i} \sum_{m_f} \frac{V}{(2\pi)^3} \int d^3k k_x^2 \left\{ \frac{\delta_{m_f=m_i-1}}{\omega + i\gamma + \omega_{if}} - \frac{\delta_{m_f=m_i+1}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.20)$$

The angular parts of  $k$  can be integrated out, using  $k_x = k \sin \theta \cos \phi$  and  $d^3k = k^2 dk d(\cos \theta) d\phi$ , and one has as usual

$$\int d\Omega k_x^2 = \int_0^{2\pi} d\phi \int_{-1}^{+1} d(\cos \theta) (k \sin \theta \cos \phi)^2 = \frac{4\pi}{3} k^2 \quad (7.21)$$

Then there is still the integration over the magnitude of  $k$ ,

$$S_R = \frac{2|M|^2 \hbar}{m_e} \frac{V}{(2\pi)^3} \frac{4\pi}{3} \sum_{m_i} \sum_{m_f} \int_0^{k_F} dk k^4 \left\{ \frac{\delta_{m_f=m_i-1}}{\omega + i\gamma + \omega_{if}} - \frac{\delta_{m_f=m_i+1}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.22)$$

The upper limit must be the Fermi wave vector, defined in the usual way, which depends on the electron number density  $n$ .

Now the value of  $\omega_{if}$  is different in the two terms, due to the dependence on  $\Delta m$ . For the first term, with  $m_f = m_i - 1$ , there is

$$\omega_{if}^- = - \left[ \frac{E_g}{\hbar} + \frac{\hbar k^2}{2\tilde{m}} + \frac{\mu_B B}{\hbar} \right], \quad \Delta m = -1. \quad (7.23)$$

The first factor is the gap frequency  $\omega_g$ . With the Bohr magneton  $\mu_B = \frac{e\hbar}{2m_e c}$  and the magnetic frequency  $\omega_B = \frac{eB}{m_e c}$ , the last factor is  $\frac{\mu_B B}{\hbar} = \frac{1}{2}\omega_B$ . One can also make the definition of a scaled wavevector,

$$s \equiv \sqrt{\frac{\hbar}{2\tilde{m}}} k. \quad (7.24)$$

Then this transition frequency becomes

$$\omega_{if}^- = -\omega_g - s^2 - \frac{1}{2}\omega_B, \quad \Delta m = -1. \quad (7.25)$$

There is also the transition frequency for the  $\Delta m = +1$ , transition, which has the opposite sign on the magnetic part,

$$\omega_{if}^+ = -\omega_g - s^2 + \frac{1}{2}\omega_B, \quad \Delta m = +1. \quad (7.26)$$

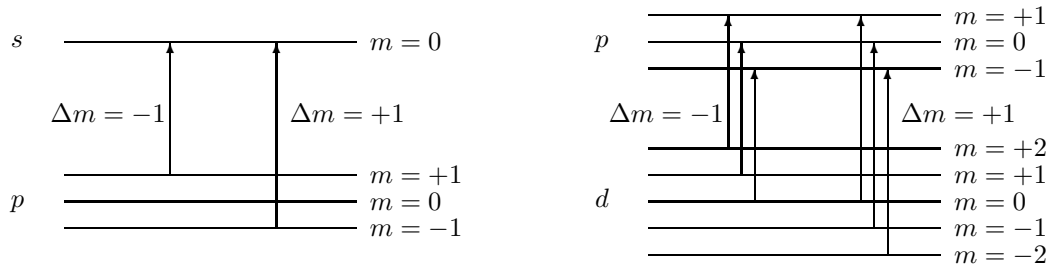
Including the frequency  $\omega + i\gamma$ , the integral becomes,

$$S_R = \frac{|M|^2 \hbar V}{3\pi^2 m_e} \sum_{m_i} \int_0^{k_F} dk k^4 \left\{ \frac{1}{\omega + i\gamma - \omega_g - s^2 - \frac{1}{2}\omega_B} - \frac{1}{\omega + i\gamma + \omega_g + s^2 - \frac{1}{2}\omega_B} \right\} \quad (7.27)$$

The wave vector also should be switched to  $s$ , so that the variable of integration is  $s$ ,

$$S_R = \frac{|M|^2 \hbar V}{3\pi^2 m_e} \left( \frac{2\tilde{m}}{\hbar} \right)^{5/2} \sum_{m_i} \int_0^{s_F} ds s^4 \left\{ \frac{1}{\omega + i\gamma - \omega_g - s^2 - \frac{1}{2}\omega_B} - \frac{1}{\omega + i\gamma + \omega_g + s^2 - \frac{1}{2}\omega_B} \right\} \quad (7.28)$$

The upper limit is the transformed Fermi wave vector,  $s_F = \sqrt{\frac{\hbar}{2\tilde{m}}} k_F$ . There is the sum over  $m_i$ . But that is related to how many transitions exist for each value of  $\Delta m$ . Let me consider some simple cases, like  $l_i = 1$  and  $l_f = 0$  (p-band to s-band transition). Refer to the following diagrams.



For the p to s-band transitions (or vice-versa) one sees there is only one term for each choice of  $\Delta m$ . For the d to p-band transitions, there are 3 terms. In fact, one can see the number is the minimum of  $2l + 1$  for the two bands, which turns out to be the same as  $l_i + l_f$  (because  $l_i = l_f \pm 1$ ). So the sum over  $m_i$  just gives a factor of  $l_i + l_f$ . Let me denote this azimuthal multiplicity as

$$g_m = \sum_{m_i} 1 = \min(2l_i + 1, 2l_f + 1) = 2\min(l_i, l_f) + 1 = l_i + l_f. \quad (7.29)$$

I'll have this factor if I do not account for the thermal population of the levels. In some cases below the Fermi distribution will be included. Then there is a separate sum over  $m_f$  and the Fermi function within the needed integrals. In that case, the  $g_m$  is replaced by that sum, i.e., set  $g_m = 1$  there when the integrals take care of that counting.

It will be convenient to have the eventual result for susceptibility,  $\chi_R$ , as physical factors times a dimensionless integral. The integral over  $s$  (a frequency<sup>1/2</sup>) in (7.28) has dimensions of frequency<sup>3/2</sup>. One can take that out,

$$S_R = \frac{|M|^2 \hbar V g_m}{3\pi^2 m_e} \left( \frac{2\tilde{m}}{\hbar} \right)^{5/2} \times I_R, \quad (7.30)$$

$$I_R = \int_0^{s_F} ds s^4 \left\{ \frac{1}{\omega + i\gamma - \omega_g - s^2 - \frac{1}{2}\omega_B} - \frac{1}{\omega + i\gamma + \omega_g + s^2 - \frac{1}{2}\omega_B} \right\} = I_2(a_1) - I_1(a_1). \quad (7.31)$$

The arguments in these integrals are the following frequency combinations,

$$a_2^2 = \omega - \frac{\omega_B}{2} - \omega_g + i\gamma, \quad a_1^2 = \omega - \frac{\omega_B}{2} + \omega_g + i\gamma, \quad (7.32)$$

Eventually, the sum  $S_R$  then gets converted to its contribution to the susceptibility by the following dimensionless factor,

$$\chi_R = \frac{-ne^2}{m_e \omega (\omega + i\gamma)} S_R. \quad (7.33)$$

From there, one can get it to my “standard” dimensionless factors like this:

$$\begin{aligned} \chi_R &= \frac{-ne^2}{m_e \omega (\omega + i\gamma)} \cdot \frac{|M|^2 \hbar V g_m}{3\pi^2 m_e} \left( \frac{2\tilde{m}}{\hbar} \right)^{5/2} \times I_R. \\ &= -(nV) \frac{2e^2 g_m \tilde{m}^2}{3\pi \hbar c m_e^2} |M|^2 \sqrt{\frac{2\tilde{m}c^2}{\hbar \omega_g}} \cdot \frac{\sqrt{\omega_g}}{\omega (\omega + i\gamma)} \frac{2}{\pi} \times I_R. \end{aligned} \quad (7.34)$$

The factor of  $(nV)$  is within parenthesis because I suspect it should be let to 1, due to the kind of normalization used for the density function. (The k-space sums already sum over all the electrons.) That needs checking later. The factors after the dot ( $\cdot$ ) are the factors convenient to make  $I_R$  in dimensionless form, and also, have all of the frequency dependence after the dot.

The integrals needed were evaluated in *Dielectrics: Part A*. There I had found the following basic indefinite integral:

$$I_1(a) = \int ds \frac{s^4}{a^2 + s^2} = \frac{1}{3}s^3 - a^2 s + a^3 \tan^{-1} \left( \frac{s}{a} \right). \quad (7.35)$$

The other one needed here can be expressed in some different ways, for  $a^2 > 0$ ,

$$I_2(a) = \int ds \frac{s^4}{a^2 - s^2} = \begin{cases} -\frac{1}{3}s^3 - a^2 s + a^3 \tanh^{-1} \left( \frac{s}{a} \right), & \text{for } s < a, \\ -\frac{1}{3}s^3 - a^2 s + a^3 \coth^{-1} \left( \frac{s}{a} \right), & \text{for } s > a. \end{cases} \quad (7.36)$$

$$I_2(a) = \int ds \frac{s^4}{a^2 - s^2} = -\frac{1}{3}s^3 - a^2 s + \frac{a^3}{2} \ln \left( \frac{|s+a|}{|s-a|} \right) \quad (7.37)$$

In a sense the log form is better because it contains the two cases together. These are expressed for real parameter  $a$  but actually with analytic continuation they indeed can apply even when  $a$  is



complex. However, that algebra to extract the real and imaginary parts of the results can be a mess. It also can be helpful to define a new function,

$$L(x) = \frac{1}{2} \ln \left( \frac{|1+x|}{|1-x|} \right) = \begin{cases} \tanh^{-1} x & \text{for } |x| < 1, \\ \coth^{-1} x & \text{for } |x| > 1. \end{cases} \quad (7.38)$$

Then the integral  $I_2$  can be expressed in a general way with this as

$$I_2(a) = \int ds \frac{s^4}{a^2 - s^2} = -\frac{1}{3}s^3 - a^2s + a^3L\left(\frac{s}{a}\right) \equiv F_2(s) \quad (7.39)$$

There is also one more way to do  $I_2$ , by using transformation  $s = iz$  and then it transforms into an analytically continued version of  $I_1$ ,

$$I_2(a) = i \int dz \frac{z^4}{a^2 + z^2} = i \left[ \frac{1}{3}z^3 - a^2z + a^3 \tan^{-1} \left( \frac{z}{a} \right) \right] = -\frac{1}{3}s^3 - a^2s + ia^3 \tan^{-1} \left( \frac{-is}{a} \right). \quad (7.40)$$

The first integral in  $S_R$  is of the form of  $I_2(a_2)$  with  $a_2^2 = \omega + i\gamma - \omega_g + \frac{1}{2}\omega_B$ . If one ignored the damping  $\gamma$ , this would be a positive  $a_2^2$  as long as the excitation frequency of the light satisfies  $\omega > \omega_g - \frac{1}{2}\omega_B$ . The second integral is of the form  $-I_1(a_1)$  with  $a_1^2 = \omega + i\gamma + \omega_g + \frac{1}{2}\omega_B$ . For zero damping, this is positive at any excitation frequency. So now the  $S_R$  sum has become

$$S_R = \frac{|M|^2 \hbar V}{3\pi^2 m_e} \left( \frac{2\tilde{m}}{\hbar} \right)^{5/2} (l_i + l_f) [I_2(a_2) - I_1(a_1)]_0^{s_F}. \quad (7.41)$$

### 7.3.1 Writing the integrals with Inouye *et al.* variable $x = \omega_g + s^2$

It is interesting to get the  $S_R$  and  $S_L$  integrals in terms of the Inouye *et al.* variable,  $x = \omega_g + s^2$ .<sup>4</sup> We should actually start from the general integral at either polarization, which is

$$I_\nu = \int_0^{s_F} ds s^4 \left\{ \frac{1}{\omega + i\gamma - \omega_g - s^2 + \frac{1}{2}\nu\omega_B} - \frac{1}{\omega + i\gamma + \omega_g + s^2 + \frac{1}{2}\nu\omega_B} \right\} \quad (7.42)$$

where the susceptibility sum that results is

$$S_\nu = \frac{|M|^2 \hbar V g m}{3\pi^2 m_e} \left( \frac{2\tilde{m}}{\hbar} \right)^{5/2} \times I_\nu. \quad (7.43)$$

Recall that  $\nu = +1/-1$  corresponds to  $L/R$  circular polarizations. We can simplify  $I_\nu$  somewhat, using the following definition of the Faraday-shifted complex optical frequency,  $\omega_\nu$ ,

$$\omega_\nu = \omega + i\gamma + \frac{1}{2}\nu\omega_B. \quad (7.44)$$

Then the integral becomes

$$I_\nu = \int_0^{s_F} ds s^4 \left\{ \frac{1}{\omega_\nu - \omega_g - s^2} - \frac{1}{\omega_\nu + \omega_g + s^2} \right\} \quad (7.45)$$

Then with  $dx = 2s ds$  or  $ds = \frac{1}{2}dx/\sqrt{x - \omega_g}$ , we get

$$I_\nu = \frac{1}{2} \int_{\omega_g}^{\omega_g + s_F^2} dx (x - \omega_g)^{3/2} \left\{ \frac{1}{\omega_\nu - x} - \frac{1}{\omega_\nu + x} \right\} = \int_{\omega_g}^{x_F} dx (x - \omega_g)^{3/2} \cdot \frac{x}{\omega_\nu^2 - x^2}. \quad (7.46)$$

The integral is not divergent due to the finite upper limit, which is  $x_F = \omega_g + s_F^2$ . It is simpler than the Inouye *et al.* expression found from polarization averaging. Note that the power  $3/2$  will change to  $1/2$  for a 1D band model. This is the result assuming  $w_i - w_f = 1$ .

<sup>4</sup>“Ultrafast dynamics of nonequilibrium electrons in a gold nanoparticle system,” Hideyuki Inouye, Koichiro Tanaka, Ichiro Tanahashi and Kazuyuki Hirao, Phys. Rev. B **57**, 11,334 (1998).

One could try to reinstall the thermal factor, if desired. But actually that is not so simple, because each term of the integrand gets a different Fermi function. The final state energy relative to the top of the valence band is

$$E_f = E_g + \frac{\hbar^2 k^2}{2m_e^*} - \frac{1}{2}m_f \hbar \omega_B. \quad (7.47)$$

This will depend on the variable  $x$  only if the hole and electron effective masses are the same. So I assume that,  $m_e^* = m_h^* = m^*$ . Then the energy here is now

$$E_f = \hbar \left( \omega_g + s^2 - \frac{1}{2}m_f \omega_B \right). \quad (7.48)$$

The first term in  $S_\nu$  comes from  $m_f = m_i + \nu$ , and the second term, from  $m_f = m_i - \nu$ . However, we can think now that the sums we had over  $m_i$  and  $m_f$  could be done in the opposite order: do the  $m_i$  sum first, leaving  $m_f$  for last. When the sum over  $m_i$  is done the first term in the integral uses only  $\Delta m = +\nu$ , and the second uses only  $\Delta m = -\nu$ . That is, the first term Kronecker delta selects only  $m_i = m_f - \nu$ , the second selects only  $m_i = m_f + \nu$ . These select the same values of  $\omega_{if}$ , etc., as before, to go in the denominator. The final state occupation is the same for all the transitions for a selected  $m_f$ , based on the final state energy:

$$E_f = \hbar \left( x - \frac{1}{2}m_f \omega_B \right). \quad (7.49)$$

The occupation function depends on this energy relative to the Fermi energy:

$$g_{m_f}(x) = w_i - w_f = 1 - F(E_f - E_F) = 1 - F(x, m_f). \quad (7.50)$$

Both terms have this same factor! That is good and convenient. Note that the energy difference is dominated by  $\hbar(\omega_g + s^2 - \omega_F)$ , where  $E_F = \hbar\omega_{FD}$  defines a Fermi frequency. Near the point where  $\omega_g + s^2 - \omega_F \approx 0$ , which is somewhere in the conduction band, the differences due to the magnetic frequency will be important. Away from that region, not so important. The best way to do the theory will be to keep these effects. In the end, small differences in this effect for the two polarizations could be important in the Faraday rotation.

With the total occupation effect included, now we write this with the sum over final azimuthal number  $m_f$  still to be done, (and remove or set to 1 the old  $g_m$  on its prefactor)

$$I_\nu = \frac{1}{2} \sum_{m_f} \int_{\omega_g}^{x_F} dx g_{m_f}(x) \cdot (x - \omega_g)^{3/2} \left\{ \frac{1}{\omega_\nu - x} - \frac{1}{\omega_\nu + x} \right\} \quad (7.51)$$

Because there is only one common factor of  $g_{m_f}$ , the same rearranging used earlier can bring it to the following form:

$$I_\nu = \sum_{m_f} \int_{\omega_g}^{x_F} dx g_{m_f}(x) \cdot (x - \omega_g)^{3/2} \cdot \frac{x}{\omega_\nu^2 - x^2}. \quad (7.52)$$

The sum is still present over  $m_f$ . Suppose that is a p-band with  $m_f = -1, 0, +1$ . Suppose the lower band is a d-band. It has five states,  $m_i = -2, -1, 0, +1, +2$ . But it doesn't matter what the initial states were, they have already been accounted for. For each final state  $m_f$ , only the states  $m_i = m_f \pm \nu$  have contributed to  $S_\nu$ . If the final state is a p-state, there will be three separate integrals like this, with slightly different results. Or, the sum over  $m_f$  could be placed inside the integral.

One more comment could be important. An interesting case is when the initial state is in an s-band ( $m_i = 0$  only) and then the final state must be in a p-band ( $m_f = -1, 0, +1$ ). [This may also apply to other cases where the final state has the higher angular momentum.] We do need to sum over all initial and final  $m$ . When  $m_f = 0$ , there is no  $m_i$  from which the transition takes place. When  $m_f = +1$ , then the only initial state is  $m_i = 0$ , which has  $\Delta m = +1$ . On the other

hand, when  $m_f = -1$ , of course the initial state is only  $m_i = 0$  and  $\Delta m = -1$ . So there are not two possibilities for each case, only one! The calculation really depends on the function inside the integrand,

$$f = \sum_{m_i, m_f} g_{m_f}(x) \cdot \left\{ \frac{\delta_{m_i=m_f-\nu}}{\omega_\nu - x} - \frac{\delta_{m_i=m_f+\nu}}{\omega_\nu + x} \right\} \quad (7.53)$$

Consider left polarization,  $\nu = +1$ . If we fix  $m_f = +1$ , then only the first term can be satisfied (with  $m_i = 0$ ), because the s-band does not have  $m_i = 2$  as required by the second delta. We get absolutely nothing when fixing  $m_f = 0$ . If we fix  $m_f = -1$ , then only the second term can be satisfied ( $m_i = 0$ ), and the first cannot be satisfied because the s-band does not have  $m_i = -2$ . So we get this result, doing the sum over  $m_f$  as well as  $m_i$ :

$$f_1 = \frac{g_1(x)}{\omega_1 - x} - \frac{g_{-1}(x)}{\omega_1 + x} \quad (7.54)$$

Consider instead right polarization,  $\nu = -1$ . Now the first term needs  $m_f = -1$  and the second needs  $m_f = +1$ . They are swapped. Now we get

$$f_{-1} = \frac{g_{-1}(x)}{\omega_{-1} - x} - \frac{g_1(x)}{\omega_{-1} + x} \quad (7.55)$$

Then we can see these combine into the one formula for both values of  $\nu$ ,

$$f_\nu = \frac{g_\nu(x)}{\omega_\nu - x} - \frac{g_{-\nu}(x)}{\omega_\nu + x} \quad (7.56)$$

Then the integral for  $I_\nu$  takes a slightly different form than before, for this special case of s  $\rightarrow$  p interband transitions only,

$$I_\nu = \frac{1}{2} \int_{\omega_g}^{x_F} dx (x - \omega_g)^{3/2} \left\{ \frac{g_\nu(x)}{\omega_\nu - x} - \frac{g_{-\nu}(x)}{\omega_\nu + x} \right\} \quad (7.57)$$

That's an interesting very simple result. In the constant that will multiply  $I_\nu$  one cant forget to remove the factor of  $g_m$  that was used earlier to do the transition counting, which is corrected by this new approach, that correctly include the Fermi-Dirac distribution of the final states.

### 7.3.2 Analytic continuation of the integrals

Technically, that last expression (7.41) is the closed form solution for  $S_R$  (without thermal effects). But from the numerical point of view, evaluation of its real and imaginary parts is slightly difficult and ugly. One can simplify the difference of integrals, using the values only at the upper limit (the lower limits give zero),

$$[I_2(a_2) - I_1(a_1)]_0^{s_F} = -\frac{2}{3} s_F^3 + 2\omega_g s_F - a_1^3 \tan^{-1} \left( \frac{s_F}{a_1} \right) + i a_2^3 \tan^{-1} \left( \frac{-i s_F}{a_2} \right). \quad (7.58)$$

One simplification used is that  $a_1^2 - a_2^2 = 2\omega_g$ . For the remaining parts the analytic continuation needs to be done. To do that, base it on the expression for inverse tangent with a complex argument, as

$$\tan^{-1} \left( \frac{s}{a} \right) = \frac{i}{2} \ln \left( \frac{a - is}{a + is} \right) \quad (7.59)$$

It will be convenient to denote the real combinations that appear in the integrals,

$$\omega_1 = \omega + \omega_g - \frac{1}{2}\omega_B, \quad \omega_2 = \omega - \omega_g - \frac{1}{2}\omega_B, \quad (7.60)$$

Then one needs the following square roots, which were worked out in *Dielectrics: Part A*,

$$a_1 = \sqrt{\omega_1 + i\gamma} = \sqrt{\frac{1}{2} \left( \sqrt{\omega_1^2 + \gamma^2} + \omega_1 \right)} + i \sqrt{\frac{1}{2} \left( \sqrt{\omega_1^2 + \gamma^2} - \omega_1 \right)} \equiv x_1 + iy_1. \quad (7.61)$$

$$a_2 = \sqrt{\omega_2 + i\gamma} = \sqrt{\frac{1}{2} \left( \sqrt{\omega_2^2 + \gamma^2} + \omega_2 \right)} + i\sqrt{\frac{1}{2} \left( \sqrt{\omega_2^2 + \gamma^2} - \omega_2 \right)} \equiv x_2 + iy_2. \quad (7.62)$$

For computations, one gets here the real and imaginary parts. Then for the inverse tangents, their real and imaginary parts can be worked out in terms of the  $x$  and  $y$ . For the term in  $I_1$  one needs

$$\begin{aligned} \tan^{-1} \left( \frac{s}{a_1} \right) &= \tan^{-1} \left[ \frac{s}{x_1 + iy_1} \right] = \frac{i}{2} \ln \left[ \frac{x_1 + iy_1 - is}{x_1 + iy_1 + is} \right] \\ &= \frac{1}{2} \tan^{-1} \left[ \frac{2x_1 s}{x_1^2 + y_1^2 - s^2} \right] + \frac{i}{4} \ln \left[ \frac{x_1^2 + (y_1 - s)^2}{x_1^2 + (y_1 + s)^2} \right] \end{aligned} \quad (7.63)$$

The term from  $I_3$  is a little bit different,

$$\begin{aligned} \tan^{-1} \left( \frac{-is}{a_2} \right) &= \tan^{-1} \left[ \frac{-is}{x_2 + iy_2} \right] = \frac{i}{2} \ln \left[ \frac{x_2 + iy_2 - s}{x_2 + iy_2 + s} \right] \\ &= -\frac{1}{2} \tan^{-1} \left[ \frac{2y_2 s}{x_2^2 + y_2^2 - s^2} \right] + \frac{i}{4} \ln \left[ \frac{(x_2 - s)^2 + y_2^2}{(x_2 + s)^2 + y_2^2} \right] \end{aligned} \quad (7.64)$$

All of this is to be evaluated at  $s = s_F$ . It's enough to calculate  $S_R$ , however, there is nothing pretty about the final formulas, which must be evaluated numerically from here.

### 7.3.3 Using the limit of $s_F \rightarrow \infty$

The limit of the letting the upper limit be very large is discussed in more detail in Section 7.9. With that limit, these inverse tangents give

$$\lim_{s \rightarrow \infty} \tan^{-1} \left( \frac{s}{a_1} \right) = \frac{\pi}{2} + i0, \quad (7.65)$$

$$\lim_{s \rightarrow \infty} \tan^{-1} \left( \frac{-is}{a_2} \right) = -\frac{\pi}{2} + i0. \quad (7.66)$$

These are reasonable, since these are the usual limits for real arguments. If one expects that it is OK to let the upper integration limit go to infinity, then the result for the  $I_R$  function can be simplified. First, the linear and cubic terms in  $s$  are roughly equal to an inverse tangent,

$$\begin{aligned} I_R = I_2(a_2) - I_1(a_1) &\approx 2\omega_g^{3/2} \tan^{-1} \left( \frac{s}{\sqrt{\omega_g}} \right) \\ &- \left[ \omega - \frac{\omega_B}{2} + \omega_g + i\gamma \right]^{3/2} \tan^{-1} \left( \frac{s}{\sqrt{\omega - \frac{\omega_B}{2} + \omega_g + i\gamma}} \right) \\ &+ i \left[ \omega - \frac{\omega_B}{2} - \omega_g + i\gamma \right]^{3/2} \tan^{-1} \left( \frac{s}{\sqrt{\omega - \frac{\omega_B}{2} - \omega_g + i\gamma}} \right) \end{aligned} \quad (7.67)$$

(See a later section for more explanation of the switch to all inverse tangents.) Then with letting  $s$  go to infinity, this will be further approximated, to a good precision, likely, as

$$I_R = \frac{\pi}{2} \left\{ 2\omega_g^{3/2} - \left[ \omega - \frac{\omega_B}{2} + \omega_g + i\gamma \right]^{3/2} + i \left[ \omega - \frac{\omega_B}{2} - \omega_g + i\gamma \right]^{3/2} \right\}. \quad (7.68)$$

Then this expression produces both the real and imaginary parts of the dielectric response under these approximations, in just this one expression. The next section shows how these could have been derived separately in the limit of very weak damping. For now, this will lead to the following result

for susceptibility,

$$\begin{aligned}
\chi_R &= -\frac{2e^2 g_m \tilde{m}^2}{3\pi\hbar c m_e^2} |M|^2 \sqrt{\frac{2\tilde{m}c^2}{\hbar\omega_g}} \cdot \frac{\sqrt{\omega_g}}{\omega(\omega+i\gamma)} \frac{2}{\pi} \times I_R. \\
&= -\frac{2e^2 g_m \tilde{m}^2}{3\pi\hbar c m_e^2} |M|^2 \sqrt{\frac{2\tilde{m}c^2}{\hbar\omega_g}} \\
&\times \frac{\sqrt{\omega_g}}{\omega(\omega+i\gamma)} \left\{ 2\omega_g^{3/2} - \left[ \omega - \frac{\omega_B}{2} + \omega_g + i\gamma \right]^{3/2} + i \left[ \omega - \frac{\omega_B}{2} - \omega_g + i\gamma \right]^{3/2} \right\}. \quad (7.69)
\end{aligned}$$

The last expression is split into dimensionless physical factors  $\times$  a dimensionless function of the frequencies. The last term is the imaginary part, in the limit of weak damping.

## 7.4 Finding $S_R$ for 3D bands, limit of zero damping, current averaging

To take the limit of very weak damping, we use the Sokchatsky-Weierstrass theorem for the denominators, in the form,

$$\lim_{\gamma \rightarrow 0^+} \frac{1}{x+i\gamma} = \text{p.v.} \left( \frac{1}{x} \right) - i\pi\delta(x) \quad (7.70)$$

Applied to the first term in expression (7.22) for  $S_R$  it gives

$$\frac{1}{\omega+i\gamma+\omega_{if}^-} \rightarrow \text{p.v.} \left( \frac{1}{\omega+\omega_{if}^-} \right) - i\pi\delta(\omega+\omega_{if}^-), \quad (7.71)$$

whereas, on the second term the effect is

$$\frac{1}{\omega+i\gamma-\omega_{if}^+} \rightarrow \text{p.v.} \left( \frac{1}{\omega-\omega_{if}^+} \right) - i\pi\delta(\omega-\omega_{if}^+), \quad (7.72)$$

### 7.4.1 The imaginary parts–delta functions

Now the transition frequency  $\omega_{if}$  is negative, as long as the magnetic frequency  $\omega_B$  is much less than the gap frequency. So only the  $\delta(\omega+\omega_{if}^-)$  will be satisfied at some particular wavevector magnitude  $k$ . The deltas produce the imaginary part of  $S_R$ – explained physically as resonant absorption. That imaginary part from (7.22) is

$$\text{Im}\{S_R\} = (-i\pi) \frac{|M|^2 \hbar V}{3\pi^2 m_e} \sum_{m_i} \int_0^{k_F} dk k^4 \delta(\omega+\omega_{if}^-) \quad (7.73)$$

The delta helps to do the integral, most easily if its argument is linear in the variable of integration. So it is helpful to switch to a new integration variable  $x = -\omega_{if}^-$ , and then solve for the corresponding value of  $k$ , through the transition frequency expression,

$$x = -\omega_{if}^- = \omega_g + \frac{\hbar k^2}{2\tilde{m}} + \frac{1}{2}\omega_B \implies k(x) = \sqrt{\frac{2\tilde{m}}{\hbar} \left( x - \omega_g - \frac{1}{2}\omega_B \right)}. \quad (7.74)$$

Also with

$$dx = \frac{\hbar}{m} k dk \quad (7.75)$$

this transforms the integral to

$$\text{Im}\{S_R\} = (-i) \frac{|M|^2 \hbar V}{3\pi m_e} \sum_{m_i} \int_0^{x_F} dx \frac{\tilde{m}}{\hbar} k^3(x) \delta(\omega-x) \quad (7.76)$$

The delta picks off only  $x = \omega$ , the excitation frequency. That chooses the particular wavevector  $k_0 = k(\omega)$  from the above expression that satisfies energy conservation. Including also the multiplicity of the azimuthal transitions,  $g_m \equiv (l_i + l_f)$ , one gets

$$\text{Im}\{S_R\} = (-i) \frac{|M|^2 \hbar V}{3\pi m_e} g_m \frac{\tilde{m}}{\hbar} k_0^3 = -i \frac{|M|^2 g_m \tilde{m}}{3\pi m_e} V k_0^3 \quad (7.77)$$

The result is dimensionless, as it should be, and negative, as expected for absorption (it will get multiplied by -1 to make a positive contribution to the imaginary part of  $\epsilon_R$ ). The only question not clear is the normalization, especially, what volume goes here, and perhaps it is the volume per electron?? If that were the case, it would explain how the density of electrons affects the result.

Also write its net contribution to the susceptibility, to compare with other results. That is

$$\text{Im}\{\chi_R\} = \frac{-ne^2}{m_e \omega^2} \text{Im}\{S_R\} = i \frac{ne^2}{m_e \omega^2} \frac{g_m}{3\pi} \frac{\tilde{m}}{m_e} |M|^2 V \left[ \frac{2\tilde{m}}{\hbar} \left( \omega - \omega_g - \frac{\omega_B}{2} \right) \right]^{3/2}. \quad (7.78)$$

I still have some confusion about the  $V$ , however, note that in CGS the susceptibility is dimensionless, and that is seen to work out correctly with this expression, even with the number density  $n$  present. However, this would still be correct if that number density were an inverse volume. But then, the result would not have a dependence on the number of electrons, which would not make sense. So the result is a little curious. On the other hand, the integrations over  $k$  are officially up to the Fermi wave vector, which is dependent on concentration of electrons. The point is that the sum is the sum over all electrons, even if an explicit dependence on  $n$  did not appear. My best guess right now is that I need  $nV \rightarrow 1$  here.

Let me take that guess and place this into a scaled form.

$$\text{Im}\{\chi_R\} = i g_m \frac{2e^2}{3\pi \hbar c} \frac{\tilde{m}^2}{m_e^2} |M|^2 \sqrt{\frac{2\tilde{m}c^2}{\hbar \omega_g}} \sqrt{\frac{\omega_g}{\omega}} \left[ \frac{\omega - \omega_g - \frac{1}{2}\omega_B}{\omega} \right]^{3/2}. \quad (7.79)$$

Surprisingly, this is almost the same as that obtained with the polarization averaging in the absence of the magnetic field, except primarily for the presence of the magnetic frequency  $\omega_B$  increasing the effective gap. There is also an extra factor of 2, and a factor of azimuthal multiplicity  $g_m$  that I did not have before. But these are both different from *Dielectrics: Part A* because there I did not worry about summing over  $m_l$  for any states, although I should have included that. In fact, if done correctly, the sum for  $S_R$  should be about half of that for  $S_{xx}$ , since  $S_R$  includes only the  $\Delta m = -1$  transitions, which are half of the total possible transitions.

If the calculation is repeated for  $S_L$ , the only change will be that the Kronecker deltas switch places, and that means we use instead use  $\delta(\omega + \omega_{if}^+)$ . The net result is that this changes the sign of  $\omega_B$  in the final answer, but nothing else is modified:

$$\text{Im}\{\chi_L\} = i g_m \frac{2e^2}{3\pi \hbar c} \frac{\tilde{m}^2}{m_e^2} |M|^2 \sqrt{\frac{2\tilde{m}c^2}{\hbar \omega_g}} \sqrt{\frac{\omega_g}{\omega}} \left[ \frac{\omega - \omega_g + \frac{1}{2}\omega_B}{\omega} \right]^{3/2}. \quad (7.80)$$

It seems like an insignificant difference, however, when these are subtracted to give  $\chi_{xy} = (\chi_R - \chi_L)/2i$  or better, to give  $\epsilon_{xy}$ , which determines the Faraday rotation, one will see that the Faraday effects will depend on the scale of  $\omega_B$  relative to  $\omega - \omega_g$ . It is fairly clear that at least this imaginary part of  $\epsilon_{xy}$  should be proportional to  $\omega_B$  at small magnetic field, as one expects! [If  $\omega_B = 0$ , then the imaginary parts of  $\chi_R$  and  $\chi_L$  will become the same, leading to  $\chi_{xy} = 0$ . One could expand the radicals for small  $\omega_B$ .]

One more thing to note is that finding these by the formulas from averaging of the electric polarization will lead to the identical results, because the presence of the delta functions pick off exactly the one frequency  $\omega = -\omega_{fi}^\pm$  where the appropriate denominator goes to zero. So there is no need to do that comparison for these imaginary parts.

### 7.4.2 The real parts—principal value

Next is to do the real part of  $S_R$ , that comes from the principal valued integral. From (7.22) that is

$$\operatorname{Re}\{S_R\} = \frac{|M|^2 \hbar V}{3\pi^2 m_e} \sum_{m_i} \text{p.v.} \left\{ \int_0^{k_F} dk k^4 \left[ \frac{1}{\omega + \omega_{if}^-} - \frac{1}{\omega - \omega_{if}^+} \right] \right\} \quad (7.81)$$

Now since both transition frequencies are negative, only the first term has a pole; the second denominator never goes to zero. So the principal part is not really needed on the second term; it is a normal integral. These integrals are aided by transforming to the variable  $s$  introduced earlier for integral (7.28). Here, the integral is like (7.28), but pure real with  $\gamma = 0$ , so the algebra is simpler.

$$\operatorname{Re}\{S_R\} = \frac{|M|^2 \hbar V}{3\pi^2 m_e} \left[ \frac{2\tilde{m}}{\hbar} \right]^{\frac{5}{2}} g_m \text{p.v.} \left\{ \int_0^{s_F} ds s^4 \left[ \frac{1}{\omega - \omega_g - \frac{\omega_B}{2} - s^2} - \frac{1}{\omega + \omega_g - \frac{\omega_B}{2} + s^2} \right] \right\} \quad (7.82)$$

The second term was already found, and since no p.v. is needed, it is the function  $I_1(a_1)$ , where  $a_1^2 = \omega + \omega_g - \frac{\omega_B}{2}$ , i.e.,

$$I_1(a) = \int_0^{s_F} ds \frac{s^4}{a^2 + s^2} = \frac{1}{3} s_F^3 - a^2 s_F + a^3 \tan^{-1} \left( \frac{s_F}{a} \right). \quad (7.83)$$

The first term also was found in *Dielectrics: Part A*, but let me repeat part of that here. The basic indefinite integral is the function  $I_2(a_2)$  introduced earlier here, where  $a_2^2 = \omega - \omega_g + \frac{\omega_B}{2}$ , and

$$I_2(a) = \int ds \frac{s^4}{a^2 - s^2} = -\frac{1}{3} s^3 - a^2 s + a^3 L \left( \frac{s}{a} \right) = F_2(s), \quad L(x) = \frac{1}{2} \ln \left( \frac{|1+x|}{|1-x|} \right). \quad (7.84)$$

For the p.v. integral, jump over the point  $s = a = a_2$  which is singular. Do this by combining the two integrals,

$$\text{p.v.} \int_0^{s_F} ds = \lim_{\gamma \rightarrow 0} \left\{ \int_0^{a-\gamma} ds + \int_{a+\gamma}^{s_F} ds \right\} \quad (7.85)$$

This means the following evaluations,

$$\text{p.v.} \int_0^{s_F} ds = \lim_{\gamma \rightarrow 0} \{ F_2(a-\gamma) - F_2(0) + F_2(s_F) - F_2(a+\gamma) \} \quad (7.86)$$

The only part that is singular is the function  $L(s)$ . Also,  $F_2(0) = 0$ . So this is the same as

$$\begin{aligned} \text{p.v.} \int_0^{s_F} ds &= \lim_{\gamma \rightarrow 0} a^3 \left\{ L \left( \frac{a-\gamma}{a} \right) - L \left( \frac{a+\gamma}{a} \right) \right\} + F_2(s_F) \\ &= \lim_{\gamma \rightarrow 0} \frac{a^3}{2} \left\{ \ln \left| \frac{1 + (1 - \frac{\gamma}{a})}{1 - (1 - \frac{\gamma}{a})} \right| - \ln \left| \frac{1 + (1 + \frac{\gamma}{a})}{1 - (1 + \frac{\gamma}{a})} \right| \right\} + F_2(s_F) \\ &= \lim_{\gamma \rightarrow 0} \frac{a^3}{2} \ln \left\{ \left| \frac{2 - \frac{\gamma}{a}}{\frac{\gamma}{a}} \right| \cdot \left| \frac{\frac{\gamma}{a}}{2 + \frac{\gamma}{a}} \right| \right\} + F_2(s_F) \longrightarrow F_2(s_F). \end{aligned} \quad (7.87)$$

The principal value just removes the singularity, and all that is left is the function at the ends of the interval. So then the combination of the two integrals over  $s$  is

$$\begin{aligned} \text{p.v.} \int_0^{s_F} ds = I_2(a_2) - I_1(a_1) &= -\frac{1}{3} s_F^3 - a_2^2 s_F + a_2^3 L \left( \frac{s_F}{a_2} \right) \\ &\quad - \left[ \frac{1}{3} s_F^3 - a_1^2 s_F + a_1^3 \tan^{-1} \left( \frac{s_F}{a_1} \right) \right] \end{aligned} \quad (7.88)$$

We have that  $a_1^2 - a_2^2 = 2\omega_g$ , and  $L(x)$  is the hyperbolic inverse cotangent,  $\coth^{-1}(x)$  when  $x > 1$  or inverse hyperbolic tangent,  $\tanh^{-1}(x)$  for  $x < 1$ , so

$$\begin{aligned} \text{p.v.} \int_0^{s_F} ds = & -\frac{2}{3}s_F^3 + 2\omega_g s_F + \left[\omega - \omega_g - \frac{\omega_B}{2}\right]^{\frac{3}{2}} L\left(\frac{s_F}{\sqrt{\omega - \omega_g - \frac{\omega_B}{2}}}\right) \\ & - \left[\omega + \omega_g - \frac{\omega_B}{2}\right]^{\frac{3}{2}} \tan^{-1}\left(\frac{s_F}{\sqrt{\omega + \omega_g - \frac{\omega_B}{2}}}\right) \end{aligned} \quad (7.89)$$

Interestingly, this is very close to a result found from polarization averaging in the absence of the magnetic field. An inverse tangent term there is approximately equal to the cubic and linear terms in  $s$  here. So one can see that current averaging and polarization averaging give almost the same result. The connection would be that, approximately, the first two terms are related to inverse tangent, whose expansion begins

$$2\omega_g^{3/2} \tan^{-1}\left(\frac{s_F}{\sqrt{\omega_g}}\right) = 2\omega_g s_F - \frac{2}{3}s_F^3 + \frac{2}{5}\frac{s_F^5}{\omega_g} - \dots \quad (7.90)$$

Therefore, the two approaches are closer to each other, provided the ratio  $\frac{s_F^2}{\omega_g}$  is small enough. But  $\hbar s_F^2$  is an effective Fermi energy for the bands (but not the true Fermi energy in the middle of the gap), so for a given material situation, this ratio can be calculated and checked whether it is much less than 1.

One can note a way to make this result just like the result for zero magnetic field. That is to define an effective Faraday frequency for the optical field, that depends on the circular polarization. For right polarization, let me define that frequency as

$$\omega_R \equiv \omega - \frac{\omega_B}{2}. \quad (7.91)$$

Then the p.v. integral above (and also the delta integral result) involves this combination, and it becomes

$$\begin{aligned} \text{p.v.} \int_0^{s_F} ds = & -\frac{2}{3}s_F^3 + 2\omega_g s_F + [\omega_R - \omega_g]^{3/2} L\left(\frac{s_F}{\sqrt{\omega_R - \omega_g}}\right) \\ & - [\omega_R + \omega_g]^{3/2} \tan^{-1}\left(\frac{s_F}{\sqrt{\omega_R + \omega_g}}\right) \end{aligned} \quad (7.92)$$

These are *the same form* as without the magnetic field, except for this shifted optical frequency. It is as if the right circular polarization photons have a lower effective energy for causing transitions and other physical effects. The first term, that depends only on the gap, however, has no dependence on the magnetic field. For left circular polarization, the effective Faraday frequency is instead increased compared to the optical frequency,

$$\omega_L \equiv \omega + \frac{\omega_B}{2}. \quad (7.93)$$

These photons have a shorter way to get across the gap, hence their effect is greater, in some sense. In many subsequent formulas I could use these effective Faraday frequencies, however, for the most part I left them with the magnetic frequency explicitly displayed.

**Excitation above the gap,**  $\omega > \omega_g$ : The calculation so far assumed this condition. Then including the other physical factors, the right polarization sum is

$$\begin{aligned} \text{Re}\{S_R\} = & \frac{|M|^2 \hbar V}{3\pi^2 m_e} \left[\frac{2\tilde{m}}{\hbar}\right]^{\frac{5}{2}} g_m \left\{ -\frac{2}{3}s_F^3 + 2\omega_g s_F \right. \\ & + \left[\omega - \omega_g - \frac{\omega_B}{2}\right]^{\frac{3}{2}} L\left(\frac{s_F}{\sqrt{\omega - \omega_g - \frac{\omega_B}{2}}}\right) \\ & \left. - \left[\omega + \omega_g - \frac{\omega_B}{2}\right]^{\frac{3}{2}} \tan^{-1}\left(\frac{s_F}{\sqrt{\omega + \omega_g - \frac{\omega_B}{2}}}\right) \right\} \end{aligned} \quad (7.94)$$



There are extra factors needed to convert to its contribution to the susceptibility, and that result is

$$\begin{aligned} \text{Re}\{\chi_R\} = \frac{-ne^2}{m_e\omega^2}\text{Re}\{S_R\} &= \frac{-ne^2}{m_e\omega^2} \frac{|M|^2\hbar V}{3\pi^2 m_e} \left[ \frac{2\tilde{m}}{\hbar} \right]^{\frac{5}{2}} g_m \left\{ -\frac{2}{3}s_F^3 + 2\omega_g s_F \right. \\ &+ \left[ \omega - \omega_g - \frac{\omega_B}{2} \right]^{\frac{3}{2}} L \left( \frac{s_F}{\sqrt{\omega - \omega_g - \frac{\omega_B}{2}}} \right) \\ &\left. - \left[ \omega + \omega_g - \frac{\omega_B}{2} \right]^{\frac{3}{2}} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega + \omega_g - \frac{\omega_B}{2}}} \right) \right\} \end{aligned} \quad (7.95)$$

Again I'll take the guess that the normalization needs to be with  $nV \rightarrow 1$ . Then we should try to scale it to dimensionless form the same as for the imaginary part. That becomes

$$\begin{aligned} \text{Re}\{\chi_R\} = & -g_m \frac{2e^2}{3\pi\hbar c} \frac{\tilde{m}^2}{m_e^2} |M|^2 \sqrt{\frac{2\tilde{m}c^2}{\hbar\omega_g}} \\ & \times \frac{2}{\pi} \frac{\sqrt{\omega_g}}{\omega^2} \left\{ -\frac{2}{3}s_F^3 + 2\omega_g s_F + \left[ \omega - \omega_g - \frac{\omega_B}{2} \right]^{\frac{3}{2}} L \left( \frac{s_F}{\sqrt{\omega - \omega_g - \frac{\omega_B}{2}}} \right) \right. \\ & \left. - \left[ \omega + \omega_g - \frac{\omega_B}{2} \right]^{\frac{3}{2}} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega + \omega_g - \frac{\omega_B}{2}}} \right) \right\} \end{aligned} \quad (7.96)$$

Here the factors in the first line are the same as the corresponding imaginary part. All the frequency dependent parts are in the second and third lines.

There is one more approximation that probably makes a lot of sense, to take the limit of large  $s_F$ . But that can be done only if the cubic and linear terms are replaced by the inverse tangent. If one does this, the inverse tangent terms give  $\pi/2$ , while the  $L(x)$  function becomes  $\coth^{-1}(x)$  which goes to zero. So supposing this limit is good, it gives

$$\text{Re}\{\chi_R\} \approx -g_m \frac{2e^2}{3\pi\hbar c} \frac{\tilde{m}^2}{m_e^2} |M|^2 \sqrt{\frac{2\tilde{m}c^2}{\hbar\omega_g}} \times \frac{\sqrt{\omega_g}}{\omega^2} \left\{ 2\omega_g^{3/2} - \left[ \omega + \omega_g - \frac{\omega_B}{2} \right]^{3/2} \right\} \quad (7.97)$$

To get the result for  $\chi_L$  for left circular polarization, reverse the sign on  $\omega_B$ .

**Excitation below the effective gap,  $\omega < \omega_g(B)$ :** Look at the  $I_2$  integral when the excitation energy is below the band gap more carefully. The relevant integral is

$$I_2(a_2) = \text{p.v.} \int ds \frac{s^4}{a_2^2 - s^2} = \text{p.v.} \int ds \frac{s^4}{\omega - (\omega_g + \frac{\omega_B}{2}) - s^2}. \quad (7.98)$$

In one sense, the effective gap (for right circular photons) is the enhanced gap,

$$\omega_g(B) \equiv \omega_g + \frac{\omega_B}{2}. \quad (7.99)$$

However, that is just an alternative way of thinking, rather than using the effective Faraday frequency,

$$\omega_R = \omega - \frac{\omega_B}{2} < \omega_g. \quad (7.100)$$

These are two different ways to state that the photons do not cause real transitions (i.e., absorbed). More generally, I could say there is a Faraday frequency  $\omega_F$  that is either  $\omega_R$  or  $\omega_L$ , depending on the choice of polarization, and “below the gap” excitation means,

$$\omega_F < \omega_g. \quad (7.101)$$

I may use this way or the effective band gap concept alternatively.

When  $\omega < \omega_g(B)$  (or equivalently,  $\omega_F < \omega_g$ ), all factors in the denominator of the  $I_2$  integrand are negative, and the integral is not singular any more, so the p.v. is not needed. Indeed, now the integral just becomes the negative of the  $I_1$  integral (but at a different argument  $b = ia_2$ ). So now it is

$$I_2(b) = - \int_0^{s_F} ds \frac{s^4}{b^2 + s^2}, \quad \text{where } b = \sqrt{\omega_g(B) - \omega} = \sqrt{\omega_g - \omega_R} = ia_2. \quad (7.102)$$

But that really is the same as

$$\begin{aligned} I_2(b) = -I_1(b) &= - \left[ \frac{1}{3} s_F^3 - b^2 s_F + b^3 \tan^{-1} \left( \frac{s_F}{b} \right) \right] \\ &= - \frac{1}{3} s_F^3 + [\omega_g(B) - \omega] s_F - [\omega_g(B) - \omega]^{3/2} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g(B) - \omega}} \right) \end{aligned} \quad (7.103)$$

There is no change in the integral  $I_1(a_1)$ . Now the combined integrals are

$$\begin{aligned} \int_0^{s_F} ds &= I_2(a_2) - I_1(a_1) = -I_1(b) - I_1(a_1) \\ &= - \frac{1}{3} s_F^3 + b^2 s_F - b^3 \tan^{-1} \left( \frac{s_F}{b} \right) - \left[ \frac{1}{3} s_F^3 - a_1^2 s_F + a_1^3 \tan^{-1} \left( \frac{s_F}{a_1} \right) \right] \end{aligned} \quad (7.104)$$

Inserting the physical arguments, the result from current averaging is

$$\begin{aligned} \left[ \int_0^{s_F} ds \right]_{\langle J \rangle} &= - \frac{2}{3} s_F^3 + 2\omega_g s_F - \left[ \omega_g + \frac{\omega_B}{2} - \omega \right]^{\frac{3}{2}} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g + \frac{\omega_B}{2} - \omega}} \right) \\ &\quad - \left[ \omega_g - \frac{\omega_B}{2} + \omega \right]^{\frac{3}{2}} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g - \frac{\omega_B}{2} + \omega}} \right) \end{aligned} \quad (7.105)$$

Also there is the approximate variation for averaging of the electric polarization, which changes the first terms into an arctangent,

$$\begin{aligned} \left[ \int_0^{s_F} ds \right]_{\langle P \rangle} &= 2\omega_g^{\frac{3}{2}} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g}} \right) - \left[ \omega_g + \frac{\omega_B}{2} - \omega \right]^{\frac{3}{2}} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g + \frac{\omega_B}{2} - \omega}} \right) \\ &\quad - \left[ \omega_g - \frac{\omega_B}{2} + \omega \right]^{\frac{3}{2}} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g - \frac{\omega_B}{2} + \omega}} \right) \end{aligned} \quad (7.106)$$

Now the susceptibility sum  $S_R$  becomes

$$\begin{aligned} \text{Re}\{S_R\} &= \frac{|M|^2 \hbar V}{3\pi^2 m_e} \left[ \frac{2\tilde{m}}{\hbar} \right]^{\frac{5}{2}} g_m \left\{ - \frac{2}{3} s_F^3 + 2\omega_g s_F \right. \\ &\quad - \left[ \omega_g + \frac{\omega_B}{2} - \omega \right]^{\frac{3}{2}} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g + \frac{\omega_B}{2} - \omega}} \right) \\ &\quad \left. - \left[ \omega_g - \frac{\omega_B}{2} + \omega \right]^{\frac{3}{2}} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g - \frac{\omega_B}{2} + \omega}} \right) \right\} \end{aligned} \quad (7.107)$$

With the factors needed to convert it to susceptibility, and  $nV$  set to 1, and scaling with dimensionless factors, there is

$$\begin{aligned} \text{Re}\{\chi_R\} &= -g_m \frac{2e^2}{3\pi \hbar c} \frac{\tilde{m}^2}{m_e^2} |M|^2 \sqrt{\frac{2\tilde{m}c^2}{\hbar\omega_g}} \\ &\quad \times \frac{2}{\pi} \frac{\sqrt{\omega_g}}{\omega^2} \left\{ - \frac{2}{3} s_F^3 + 2\omega_g s_F - \left[ \omega_g + \frac{\omega_B}{2} - \omega \right]^{\frac{3}{2}} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g + \frac{\omega_B}{2} - \omega}} \right) \right. \\ &\quad \left. - \left[ \omega_g - \frac{\omega_B}{2} + \omega \right]^{\frac{3}{2}} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g - \frac{\omega_B}{2} + \omega}} \right) \right\} \end{aligned} \quad (7.108)$$

Now finally for completeness, the value of  $s_F$  really isn't well defined. So one supposes it can be let to go to infinity, but again with the assumption that the cubic and linear terms in  $s_F$  become the mentioned inverse tangent. These inverse tangents will tend towards the value of  $\pi/2$ , and we will get the approximate but simplified result,

$$\begin{aligned} \text{Re}\{\chi_R\} &\approx -g_m \frac{2e^2}{3\pi\hbar c} \frac{\tilde{m}^2}{m_e^2} |M|^2 \sqrt{\frac{2\tilde{m}c^2}{\hbar\omega_g}} \\ &\times \frac{\sqrt{\omega_g}}{\omega^2} \left\{ 2\omega_g^{3/2} - \left[\omega_g + \frac{\omega_B}{2} - \omega\right]^{3/2} - \left[\omega_g - \frac{\omega_B}{2} + \omega\right]^{3/2} \right\} \end{aligned} \quad (7.109)$$

To reiterate, this applies only when the excitation photon has insufficient energy to be absorbed;  $\omega_R = \omega - \frac{\omega_B}{2} < \omega_g$ . One can see we could have substituted the Faraday frequency  $\omega_R$  in here, and the formula has *the same form* as in the absence of the magnetic field. To get the related results for left circular polarization, reverse the sign on  $\omega_B$ , i.e., change  $\omega_R$  into  $\omega_L$ .

Even though there is no real absorption of photons, the electron gas is polarized by them and there is a dielectric response. One can see that this agrees with the result for above-gap excitation, at the crossover point,  $\omega = \omega_g + \frac{\omega_B}{2}$ , as it should! Also, this is only the interband contribution; there is also a separate plasmon term, as usual.

## 7.5 Evaluating $S_\nu$ , 3D bands with damping, polarization averaging

Now instead as a check, let's do the same calculation but using the expression (7.17) from averaging of the electric polarization, repeated here:

$$S_\nu = -\frac{2\omega}{m_e\hbar} \sum_i^o \sum_f^u (w_i - w_f) \frac{|\langle f|\hat{\pi}_x|i\rangle|^2}{\omega_{if}} \left\{ \frac{\delta_{m_f=m_i+\nu}}{\omega + i\gamma + \omega_{if}} + \frac{\delta_{m_f=m_i-\nu}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.110)$$

If we install the matrix element as  $\langle f|\hat{\pi}_x|i\rangle = \hbar k_{i,x} M$  and convert to the 3D integration over wave vector, after summing over  $\mathbf{k}_f = \mathbf{k}_i$ , and using the approximation  $w_i - w_f = 1$ , we have

$$S_\nu = -\frac{2\hbar\omega|M|^2}{m_e} \sum_{m_i}^o \sum_{m_f}^u \frac{V}{(2\pi)^3} \int d\mathbf{k}_i k_{i,x}^2 \frac{1}{\omega_{if}} \left\{ \frac{\delta_{m_f=m_i+\nu}}{\omega + i\gamma + \omega_{if}} + \frac{\delta_{m_f=m_i-\nu}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.111)$$

Doing the angular integration with  $d\mathbf{k} = k^2 d\Omega dk$  and  $k_i \rightarrow k$  gives a factor of  $4\pi k^2/3$  and leads to

$$S_\nu = -\frac{2\hbar\omega|M|^2}{m_e} \frac{V}{(2\pi)^3} \frac{4\pi}{3} \sum_{m_i}^o \sum_{m_f}^u \int_0^{k_F} dk k^4 \frac{1}{\omega_{if}} \left\{ \frac{\delta_{m_f=m_i+\nu}}{\omega + i\gamma + \omega_{if}} + \frac{\delta_{m_f=m_i-\nu}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.112)$$

To proceed further requires the transition frequencies, which are recalled to be

$$\omega_{if} = -\omega_g - \frac{\hbar k_i^2}{2\tilde{m}} + \Delta m \frac{eB}{2m_e c} = -\omega_g - s^2 + \frac{1}{2}\Delta m \omega_B. \quad (7.113)$$

It is important to keep in mind, for real negatively charged electrons,  $\omega_B < 0$ , which determines the direction of the Zeeman energy shifts. The sum over  $m_f$  is restricted according to the Kronecker deltas, differently for the two terms. The first contains  $\Delta m = +\nu$  and the second has  $\Delta m = -\nu$ . So in terms of the variable  $s$ , the integral needed is really a sum of two integrals, and letting the overall constant be positive, and keeping the frequency in the needed integrals,

$$S_\nu = +\frac{g_m\hbar|M|^2V}{3\pi^2m_e} \left(\frac{2\tilde{m}}{\hbar}\right)^{5/2} \times [K_1 + K_2], \quad (7.114)$$

where the parts needed are

$$K_1 = \omega \int_0^{s_F} \frac{-ds s^4}{(-\omega_g - s^2 + \frac{1}{2}\nu\omega_B)(\omega + i\gamma - \omega_g - s^2 + \frac{1}{2}\nu\omega_B)} \quad (7.115)$$

$$K_2 = \omega \int_0^{s_F} \frac{-ds s^4}{(-\omega_g - s^2 - \frac{1}{2}\nu\omega_B)(\omega + i\gamma + \omega_g + s^2 + \frac{1}{2}\nu\omega_B)} \quad (7.116)$$

I like to beautify these somewhat, using the following definition of the Faraday-shifted complex optical frequency,  $\omega_\nu$  and the polarization-effected Zeeman shift frequency  $\zeta$ ,

$$\omega_\nu = \omega + i\gamma + \frac{1}{2}\nu\omega_B, \quad \zeta = \frac{1}{2}\nu\omega_B. \quad (7.117)$$

Then some simple manipulations rewrite these as

$$K_1 = \omega \int_0^{s_F} \frac{-ds s^4}{(\omega_g + s^2 - \zeta)(\omega_g + s^2 - \omega_\nu)} \quad (7.118)$$

$$K_2 = \omega \int_0^{s_F} \frac{+ds s^4}{(\omega_g + s^2 + \zeta)(\omega_g + s^2 + \omega_\nu)} \quad (7.119)$$

These have a nice symmetry. Note that the thermal occupation is in the semiconductor approximation, where  $g_m = l_i + l_f$ .

### 7.5.1 3D polarization integrals in the Inouye *et al.* variable $x = \omega_g + s^2$

Before evaluating them, it is interesting to get  $K_1$  and  $K_2$  in terms of the Inouye *et al.* variable,  $x = \omega_g + s^2$ . Then with  $dx = 2s ds$  or  $ds = \frac{1}{2}dx/\sqrt{x - \omega_g}$ , we get

$$K_1 = \int_{\omega_g}^{\omega_g + s_F^2} dx \frac{\omega}{2\sqrt{x - \omega_g}} \frac{-(x - \omega_g)^2}{[x - \zeta][x - \omega_\nu]} = \frac{1}{2} \int_{\omega_g}^{x_F} dx \frac{-\omega (x - \omega_g)^{3/2}}{(x - \zeta)(x - \omega_\nu)} \quad (7.120)$$

$$K_2 = \int_{\omega_g}^{\omega_g + s_F^2} dx \frac{\omega}{2\sqrt{x - \omega_g}} \frac{+(x - \omega_g)^2}{[x + \zeta][x + \omega_\nu]} = \frac{1}{2} \int_{\omega_g}^{x_F} dx \frac{+\omega (x - \omega_g)^{3/2}}{(x + \zeta)(x + \omega_\nu)} \quad (7.121)$$

Best to combine into one integral,  $I_\nu = K_1 + K_2$ . Find the integrand as proportional to

$$\begin{aligned} f &= \frac{1}{2} \left\{ \frac{-1}{(x - \zeta)(x - \omega_\nu)} + \frac{1}{(x + \zeta)(x + \omega_\nu)} \right\} \\ &= \frac{1}{2} \left\{ \frac{-(x + \zeta)(x + \omega_\nu)}{(x^2 - \zeta^2)(x^2 - \omega_\nu^2)} + \frac{(x - \zeta)(x - \omega_\nu)}{(x^2 - \zeta^2)(x^2 - \omega_\nu^2)} \right\} = \frac{-x(\omega_\nu + \zeta)}{(x^2 - \zeta^2)(x^2 - \omega_\nu^2)}. \end{aligned} \quad (7.122)$$

But curiously the combination  $\omega_\nu + \zeta$  has an interesting value,

$$\omega_\nu + \zeta = \omega + i\gamma + \frac{1}{2}\nu\omega_B + \frac{1}{2}\nu\omega_B = \omega + i\gamma + \nu\omega_B = \omega_{2\nu}. \quad (7.123)$$

It has double the Zeeman shift. Now the combined integral is

$$I_\nu = \int_{\omega_g}^{x_F} dx (x - \omega_g)^{3/2} \cdot \frac{x\omega}{x^2 - \frac{1}{4}\omega_B^2} \cdot \frac{\omega_{2\nu}}{\omega_\nu^2 - x^2}. \quad (7.124)$$

Since  $\nu = \pm 1$  its square is always 1 so  $\zeta^2 = \frac{1}{4}\omega_B^2$ . Only the last factor contains polarization information. That last factor is positive for excitation above the gap. The factor between the dots is close to  $1/x$ , as in the Inouye *et al.* expression for no magnetic field. The 3/2 power on the other factor will change to 1/2 when this is done for 1D, as in the Inouye problem. So this looks pretty good, and equivalent to their result, when  $B \rightarrow 0$ . The result is similar to the result found for current averaging, but clearly not identical.

That does not have the thermal occupation number included. To put that back in, works the same as we did earlier for the current density calculation. It will replace the factor  $g_m = \sum_{m_i, m_f}$  in  $I_\nu$  by doing the sum including the temperature effects. The sum is done first over  $m_i$ , using the Kronecker deltas, at fixed  $m_f$ , which select only the values  $m_i = m_f - \nu$ , for  $K_1$  and  $m_i = m_f + \nu$  for  $K_2$ . We assume both those transitions exist (they don't if the initial band is an s-band, for example). Then each integral is weighted by the occupation factor depending on the final state energy,

$$E_f = \hbar \left( x - \frac{1}{2}m_f \omega_B \right). \quad (7.125)$$

The occupation function depends on this energy relative to the Fermi energy:

$$g_{m_f}(x) = w_i - w_f = 1 - F(E_f - E_F) = 1 - F(x, m_f). \quad (7.126)$$

Since we take this as fixed in each integral, it simply goes into each integrand, and hence into their combined integrand, together with the sum over the possible final values:

$$I_\nu = \sum_{m_f} \int_{\omega_g}^{x_F} dx g_{m_f}(x) \cdot (x - \omega_g)^{3/2} \cdot \frac{x\omega}{x^2 - \frac{1}{4}\omega_B^2} \cdot \frac{\omega_{2\nu}}{\omega_\nu^2 - x^2}. \quad (7.127)$$

To be clear, this  $I_\nu$  is used in the usual expression, with these factors,

$$S_\nu = + \frac{\hbar|M|^2V}{3\pi^2m_e} \left( \frac{2\tilde{m}}{\hbar} \right)^{5/2} \times I_\nu. \quad (7.128)$$

If a material has the Fermi energy high into the upper band, the thermal effect must be taken into account like this. Also keep in mind, if the upper band has the higher angular momentum, then this is not quite right, see an earlier discussion about this where the current averaging calculation was written in the Inouye *et al.* variable,  $x$ .

### 7.5.2 Evaluating the integrals, 3D+damping, when $w_i - w_f$ (no thermal factors)

Now go back to the evaluation of the  $K_1$  and  $K_2$  integrals in terms of the variable  $s$ , ignoring the thermal occupation effects, then the constant  $g_m$  represents the multiplicity of allowed transitions. Assume here the Fermi level is well within the gap, as in semiconductors. Consider using for  $K_1$  a partial fraction expansion,

$$\frac{1}{(\omega_g + s^2 - \zeta)(\omega_g + s^2 - \omega_\nu)} = \frac{1}{\omega_\nu - \zeta} \left[ \frac{-1}{\omega_g + s^2 - \zeta} + \frac{1}{\omega_g + s^2 - \omega_\nu} \right] \quad (7.129)$$

But  $\omega_\nu - \zeta = \omega + i\gamma$ , it has no Zeeman shift. For the  $K_2$  integral we need instead (switching the signs on  $\omega_\nu$  and  $\zeta$ )

$$\frac{1}{(\omega_g + s^2 + \zeta)(\omega_g + s^2 + \omega_\nu)} = \frac{1}{-\omega_\nu + \zeta} \left[ \frac{-1}{\omega_g + s^2 + \zeta} + \frac{1}{\omega_g + s^2 + \omega_\nu} \right] \quad (7.130)$$

Then the integrals are now expressed as

$$K_1 = \frac{\omega}{\omega + i\gamma} \int_0^{s_F} ds s^4 \left[ \frac{1}{s^2 + \omega_g - \zeta} - \frac{1}{s^2 + \omega_g - \omega_\nu} \right] \quad (7.131)$$

$$K_2 = \frac{\omega}{\omega + i\gamma} \int_0^{s_F} ds s^4 \left[ \frac{1}{s^2 + \omega_g + \zeta} - \frac{1}{s^2 + \omega_g + \omega_\nu} \right] \quad (7.132)$$

They have a nice symmetry. One is obtained from the other by reversing the signs of  $\omega_\nu$  and  $\zeta$ .

We know how to do all of these integrals. Let me just write them as general complex integrals, with the understanding that their analytic continuation can be done to extract the real and imaginary parts. The basic needed integral is mentioned earlier in Part B,

$$I_1(a) = \int ds \frac{s^4}{a^2 + s^2} = \frac{1}{3}s^3 - a^2s + a^3 \tan^{-1} \left( \frac{s}{a} \right). \quad (7.133)$$

Really, only the second term in  $K_1$  has the likelihood of the parameter  $a$  being pure imaginary, however, the damping in the frequency makes these all complex, in general. We can apply this integral with that understanding that it defines some complex function. For  $K_1$  this apparently gives

$$\begin{aligned} K_1 &= \frac{\omega}{\omega + i\gamma} \left\{ \frac{1}{3}s^3 - (\omega_g - \zeta)s + (\omega_g - \zeta)^{3/2} \tan^{-1} \left( \frac{s}{\sqrt{\omega_g - \zeta}} \right) \right\} \\ &- \frac{\omega}{\omega + i\gamma} \left\{ \frac{1}{3}s^3 - (\omega_g - \omega_\nu)s + (\omega_g - \omega_\nu)^{3/2} \tan^{-1} \left( \frac{s}{\sqrt{\omega_g - \omega_\nu}} \right) \right\} \end{aligned} \quad (7.134)$$

These are evaluated at the upper limit,  $s_F$ . It is wonderful that the cubic term cancel. It is curious that the optical frequency does not enter in the first line (except in denominator). Combining the two lines gives

$$\frac{K_1}{\omega} = -s + \frac{1}{\omega + i\gamma} \left\{ (\omega_g - \zeta)^{3/2} \tan^{-1} \left( \frac{s}{\sqrt{\omega_g - \zeta}} \right) - (\omega_g - \omega_\nu)^{3/2} \tan^{-1} \left( \frac{s}{\sqrt{\omega_g - \omega_\nu}} \right) \right\} \quad (7.135)$$

The  $K_2$  integral is similar, as obtained changing the signs of  $\omega_\nu$  and  $\zeta$ ,

$$\frac{K_2}{\omega} = +s + \frac{1}{\omega + i\gamma} \left\{ (\omega_g + \zeta)^{3/2} \tan^{-1} \left( \frac{s}{\sqrt{\omega_g + \zeta}} \right) - (\omega_g + \omega_\nu)^{3/2} \tan^{-1} \left( \frac{s}{\sqrt{\omega_g + \omega_\nu}} \right) \right\} \quad (7.136)$$

We actually want the sum of these,  $I_\nu = K_1 + K_2$ , which is rather interesting. There are no cubic nor linear terms in  $s$ . Only the inverse tangents survive.

$$I_\nu = \frac{\omega}{\omega + i\gamma} \times \left[ (\omega_g - \zeta)^{3/2} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g - \zeta}} \right) + (\omega_g + \zeta)^{3/2} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g + \zeta}} \right) \right. \\ \left. - (\omega_g - \omega_\nu)^{3/2} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g - \omega_\nu}} \right) - (\omega_g + \omega_\nu)^{3/2} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g + \omega_\nu}} \right) \right] \quad (7.137)$$

That is not a bad result. However, it has an interesting feature that I was not sure would happen. Indeed, it seems that instead of the Zeeman shifting the optical frequency, it makes more sense to think of it as changing the effective gap. Suppose we group the  $\zeta$  not with  $\omega$  but instead with  $\omega_g$ . Specifically, the ones involving the photon frequency are

$$\omega_g - \omega_\nu = (\omega_g - \zeta) - (\omega + i\gamma), \quad \omega_g + \omega_\nu = (\omega_g + \zeta) + (\omega + i\gamma). \quad (7.138)$$

However, the first line in  $I_\nu$ , that does not have the photon frequency, really shows how the magnetic field affects the gap, regardless of the photon frequency. This type of term was present in the original results with  $B = 0$ , that is, a term depending only on the gap frequency, not the photon.

Consider letting the upper limit of integration go to infinity. The limit of  $s_F \rightarrow \infty$  is discussed in Sec. 7.9. It may help first to reverse the order in one of the terms, i.e.,

$$\frac{\omega + i\gamma}{\omega} I_\nu = (\omega_g - \zeta)^{3/2} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g - \zeta}} \right) + (\omega_g + \zeta)^{3/2} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g + \zeta}} \right) \\ - i(\omega_\nu - \omega_g)^{3/2} \tan^{-1} \left( \frac{is_F}{\sqrt{\omega_\nu - \omega_g}} \right) - (\omega_g + \omega_\nu)^{3/2} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g + \omega_\nu}} \right) \quad (7.139)$$

This makes more sense, thinking that the photon energy is above the gap, although this isn't actually necessary. In Sec. 7.9 it is shown that the limits are

$$\lim_{s \rightarrow \infty} \tan^{-1} \frac{s}{a} \rightarrow \text{sgn}(\text{Re}\{a\}) \frac{\pi}{2}, \quad \lim_{s \rightarrow \infty} \tan^{-1} \frac{is}{a} \rightarrow \text{sgn}(\text{Im}\{a\}) \frac{\pi}{2}, \quad (7.140)$$

The optical frequency include  $+\gamma$  with positive  $\gamma$ . So for the imaginary term we have  $\text{sgn}(\text{Im}\{a\}) = +1$ . Then we can see the limit with  $s_F \rightarrow \infty$  becomes a simple expression:

$$I_\nu = \frac{\pi\omega}{2(\omega + i\gamma)} \left\{ (\omega_g - \zeta)^{3/2} + (\omega_g + \zeta)^{3/2} - i(\omega_\nu - \omega_g)^{3/2} - (\omega_\nu + \omega_g)^{3/2} \right\}. \quad (7.141)$$

We can note that really it could have been left without the switching in the one term,

$$I_\nu = \frac{\pi\omega}{2(\omega + i\gamma)} \left\{ (\omega_g - \zeta)^{3/2} + (\omega_g + \zeta)^{3/2} - (\omega_g - \omega_\nu)^{3/2} - (\omega_\nu + \omega_g)^{3/2} \right\}. \quad (7.142)$$

That's an incredibly simple result, compared to what we started with. Note that it is used in (7.114) with  $K_1 + K_2 \equiv I_\nu$ . The main question about it will be, how much does the thermal

population factor (that was set to a constant) affect this calculation? Are we really only doing states that are far from the Fermi level and therefore not much affected by the Fermi-distribution? Further, we split into occupied and unoccupied states. The distinction between them should be at the Fermi level. Yet, we let the integration go to infinity, it is an inconsistency. The plan was to integrate only over roughly the half of states  $|i\rangle$  that are occupied. If we then integrate over all states, it is a double counting.

Recall, however, that if the Fermi energy falls inside the upper band, this approach is wrong, and the Fermi occupation must be taken into account, as mentioned slightly above in this section. Thus, the more correct approach takes care of most of these difficult questions.

Let me also write this result one more time, showing how really the gap gets shifts, rather than the photon:

$$I_\nu = \frac{\pi\omega}{2(\omega + i\gamma)} \left\{ (\omega_g - \zeta_\nu)^{3/2} + (\omega_g + \zeta_\nu)^{3/2} - [(\omega_g - \zeta_\nu) - (\omega + i\gamma)]^{3/2} - [(\omega_g + \zeta_\nu) + (\omega + i\gamma)]^{3/2} \right\}. \quad (7.143)$$

I added the  $\nu$  subscript to  $\zeta_\nu = \frac{1}{2}\nu\omega_B$  to show it depends on the polarization. Curiously, there are terms where the gap is modified in both directions, for a chosen polarization. These come from the symmetrization in terms of occupied/unoccupied states. One can imagine that some are absorptions and some are emissions, because of the way the second terms were obtained by swapping  $i$  and  $f$  indices. But one cannot just say that the gap gets shifted in a certain direction for each polarization. There are terms in both directions! Thus it makes more sense to say that the primary effect is the shift the photon frequency in opposite directions for the two polarization, although it is not the only thing that happens.

## 7.6 Expression for $S_R$ for 1D bands with damping, current averaging

The application to 1D bands is an approximation to a full 3D band structure, along some direction where there is a gap. For gold it was already discussed that there is a gap of about 2 eV in the 111 direction near the Fermi surface. Although the actual physical problem is 3D, one needs to reduce to the important 1D direction and integration only of that degree of freedom. I have worked this out in *Dielectrics: Part A*, as far as how to get down to a 1D integral. It is based on assuming  $N$  electrons, but living in a cubical box rather than the usual spherical symmetry for wavevectors. One can find the effective Fermi wavevector, along a Cartesian coordinate, needed to fill up  $N$  states in a volume  $V = L^3$ . If the wavevectors range from  $-k_F$  to  $+k_F$  along each Cartesian axis, then the needed Fermi wave vector is

$$k_F = \left( \frac{\pi^3 n}{2} \right)^{1/3}. \quad (7.144)$$

This was derived by setting

$$N = 2 \left( \frac{L}{2\pi} \right)^3 (2k_F)^3. \quad (7.145)$$

With that, any summation over allowed states first has its transverse integrations carried out, leaving only the final longitudinal one ( $k_x$ ) along the band direction. It means a sum transforms as follows:

$$\sum_k \rightarrow \frac{2V}{(2\pi)^3} (2k_F)^2 \int_{-k_F}^{+k_F} dk_x = \frac{V k_F^2}{\pi^3} \int_{-k_F}^{+k_F} dk_x. \quad (7.146)$$

The first “2” counts spin states, and the squared factors of  $2k_F$  are due to the transverse integrations, already carried out. By this type of transformation, the correct units will be preserved on all quantities.

With that, consider the sum  $S_R$  for a 1D band with the damping  $\gamma$  included. After using momentum conservation to sum out the final wave vector, the sum with this transformation is

$$S_R = \frac{2|M|^2\hbar}{m_e} \sum_{m_i} \sum_{m_f} \frac{V k_F^2}{(\pi)^3} \int_{-k_F}^{+k_F} dk_x k_x^2 (w_i - w_f) \left\{ \frac{\delta_{m_f=m_i-1}}{\omega + i\gamma + \omega_{if}} - \frac{\delta_{m_f=m_i+1}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.147)$$

There seems to be a lot of questionable approximation to get to this. Really, it is hard to understand what is meant by  $k_x$  here, that is, how does that direction relate to the direction in which the light is propagating? Even when this calculation is carried out in the absence of magnetic field, there is this unsettling question about the direction of  $k_x$  relative to the direction of the light waves. There is also of course lack of knowledge about the matrix element, which is probably connected to these questions. I will ignore these difficulties here, for the time being.

The integral can be transformed to one over  $s = \sqrt{\hbar/2\tilde{m}} k_x$ , which is my preferred variable, and including the transition frequencies and sums over  $m_i, m_f$ , we have

$$S_R = \frac{4|M|^2\hbar V k_F^2}{m_e (\pi)^3} \left(\frac{2\tilde{m}}{\hbar}\right)^{3/2} \times I_R,$$

$$I_R = \sum_{m_f} \int_0^{+s_F} ds g_{m_f}(s^2) s^2 \left\{ \frac{1}{\omega + i\gamma - \frac{\omega_B}{2} - \omega_g - s^2} - \frac{1}{\omega + i\gamma - \frac{\omega_B}{2} + \omega_g + s^2} \right\} \quad (7.148)$$

The range of integration was modified because the integrand is an even function of  $s$ . I will evaluate using this form, however, first it will be interesting to see how this looks in the  $x$  variable used by Inouye *et al.*, where  $x = \omega_g + s^2$  was its original definition. It looks as if one can try that same definition here, since that same factor appears in both denominators. Also with  $\omega_\nu \equiv \omega + i\gamma - \frac{\omega_B}{2}$  (this is right polarization or  $\nu = -1$ ), the factor in the braces here becomes

$$\frac{1}{\omega_\nu - x} - \frac{1}{\omega_\nu + x} = \frac{2x}{\omega_\nu^2 - x^2} = \frac{2x}{(\omega + i\gamma - \frac{\omega_B}{2})^2 - x^2} = \frac{2x}{(\omega - \frac{\omega_B}{2})^2 - x^2 - \gamma^2 + 2i\gamma(\omega - \frac{\omega_B}{2})} \quad (7.149)$$

This is similar to the results at zero field, however, with the magnetic frequency subtracted from the optical frequency, which is rather interesting. To compare with Inouye *et al.* it is best to bring the  $i$  to the numerator so real and imaginary parts are separated, although it makes for an ugly formula,

$$\frac{1}{\omega_\nu - x} - \frac{1}{\omega_\nu + x} = 2x \frac{\left[ (\omega - \frac{\omega_B}{2})^2 - x^2 - \gamma^2 \right] - 2i\gamma(\omega - \frac{\omega_B}{2})}{\left[ (\omega - \frac{\omega_B}{2})^2 - x^2 - \gamma^2 \right]^2 + 4\gamma^2(\omega - \frac{\omega_B}{2})^2} \quad (7.150)$$

Of course, this is the result of current averaging and Inouye *et al.* used polarization averaging, but what can be seen as the main consequence of the magnetic field is the shift it gives to the optical frequency. This is similar to what was seen earlier, that it effectively increases the band gap (or reduces the effective photon energy).

The change from integration over  $s$  to integration over  $x = \omega_g + s^2$ , with  $dx = 2s ds$ , is effected by

$$\int_0^{s_F} ds s^2 f(s^2) = \frac{1}{2} \int_{\omega_g}^{x_F} dx \sqrt{x - \omega_g} f(x - \omega_g) \quad (7.151)$$

The upper limit is  $x_F = \omega_g + s_F^2$ . So the integral  $I_R$  in terms of  $x$ -integration is

$$I_R = \sum_{m_f} \int_{\omega_g}^{x_F} dx g_{m_f}(x) \sqrt{x - \omega_g} x \frac{\left[ (\omega - \frac{\omega_B}{2})^2 - x^2 - \gamma^2 \right] - 2i\gamma(\omega - \frac{\omega_B}{2})}{\left[ (\omega - \frac{\omega_B}{2})^2 - x^2 - \gamma^2 \right]^2 + 4\gamma^2(\omega - \frac{\omega_B}{2})^2} \quad (7.152)$$

Keep in mind, with the factors to produce the susceptibility contribution, this is applied as

$$\chi_R = \frac{-ne^2 S_R}{m_e \omega(\omega + i\gamma)} = \frac{-ne^2(\omega - i\gamma)}{m_e \omega(\omega^2 + \gamma^2)} \times \frac{4|M|^2\hbar V k_F^2}{m_e (\pi)^3} \left(\frac{2\tilde{m}}{\hbar}\right)^{3/2} \times I_R. \quad (7.153)$$

The definition of a real Faraday effective optical frequency, for right/left circular polarizations,

$$\omega_R \equiv \omega - \frac{\omega_B}{2}, \quad \omega_L \equiv \omega + \frac{\omega_B}{2}. \quad (7.154)$$



can be written generally with the effective real “Faraday frequency” (does not include the damping)

$$\omega_F = \omega + \nu \frac{\omega_B}{2} \quad (7.155)$$

Then this integral is expressed more simply,

$$I_R = \sum_{m_f} \int_{\omega_g}^{x_F} dx g_{m_f}(x) \sqrt{x - \omega_g} x \frac{[\omega_R^2 - x^2 - \gamma^2] - 2i\gamma\omega_R}{[\omega_R^2 - x^2 - \gamma^2]^2 + 4\gamma^2\omega_R^2} \quad (7.156)$$

The result for left polarization is contained in the same formula, with  $\omega_L$  in the place of  $\omega_R$ . (Or just put  $\omega_F$  in the place of  $\omega_R$  for general case.) These expressions are OK for numerical integration, and should be very good because the temperature effects are included. If one wants the result ignoring those factors (limit of  $w_i - w_f = 1$ ), then use  $\sum_{m_f} g_{m_f}(x) \rightarrow g_m = l_i + l_f$ , as worked out earlier.

The  $I_R$  integral here has dimensions of frequency<sup>1/2</sup>. I will assume the normalization gives  $nV \rightarrow 1$ . Knowing these, it may help also to express the sum and the susceptibility in terms of dimensionless factors, which are expressions for either  $R$  or  $L$  polarization

$$S_{R|L} = \frac{4|M|^2}{\pi^2} \left( \frac{m_e V \omega_g^2}{\hbar c} \right) \left( \frac{\hbar k_F}{m_e c} \right)^2 \left( \frac{2\tilde{m}c^2}{\hbar \omega_g} \right)^{3/2} \cdot \frac{1}{\sqrt{\omega_g}} \frac{2}{\pi} I_{R|L} \quad (7.157)$$

$$\chi_{R|L} = -\frac{4|M|^2}{\pi^2} \left( \frac{e^2}{\hbar c} \right) \left( \frac{\hbar k_F}{m_e c} \right)^2 \left( \frac{2\tilde{m}c^2}{\hbar \omega_g} \right)^{3/2} \cdot \frac{\omega_g^{3/2}}{\omega(\omega + i\gamma)} \frac{2}{\pi} I_{R|L} \quad (7.158)$$

The last factors after the dot are the dimensionless form of  $I_{R|L}$  that will have a convenient limit, and all the frequency dependence is in that part.

## 7.7 Expressions for 1D bands with damping, electric polarization averaging. I.

Here I discuss a calculation of the susceptibility, using the general complex optical frequency variable,  $\omega_\nu$ , that was introduced earlier. The section that follows discusses the same problem, but getting an expression in terms of real variables.

I can start from the expression (7.147) from current averaging, but make the appropriate modifications for polarization averaging: add factor of  $-\omega/\omega_{if}$ , and terms come with the same signs. I am also going to include the thermal occupation terms here, which I have found to be more important than I imagined earlier when writing these notes.

So for electric polarization averaging we have the sum for the  $\nu$  polarization,

$$S_\nu = -\frac{2|M|^2 \hbar}{m_e} \sum_{m_i} \sum_{m_f} \frac{V k_F^2}{(\pi)^3} \int_{-k_F}^{+k_F} dk_x k_x^2 \frac{\omega(w_i - w_f)}{\omega_{if}} \left\{ \frac{\delta_{m_f=m_i+\nu}}{\omega + i\gamma + \omega_{if}} + \frac{\delta_{m_f=m_i-\nu}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.159)$$

This can be transformed to the variable  $s = \sqrt{\hbar/2\tilde{m}} k_x$ , and I will also keep track of the initial and final angular momentum states:

$$S_\nu = -\frac{2|M|^2 \hbar V k_F^2}{m_e (\pi)^3} \left( \frac{2\tilde{m}}{\hbar} \right)^{3/2} \sum_{m_i} \sum_{m_f} 2\omega \int_0^{+s_F} ds s^2 \frac{w_i - w_f}{\omega_{if}} \left\{ \frac{\delta_{m_f=m_i+\nu}}{\omega + i\gamma + \omega_{if}} + \frac{\delta_{m_f=m_i-\nu}}{\omega + i\gamma - \omega_{if}} \right\} \quad (7.160)$$

But the transition frequency is

$$\omega_{if} = -\omega_g - s^2 + \frac{1}{2} \Delta m \omega_B. \quad (7.161)$$

So there results a constant times the sum of two separate integrals  $K_1 + K_2 = I_\nu$ :

$$S_\nu = \frac{2|M|^2 \hbar V k_F^2}{m_e (\pi)^3} \left( \frac{2\tilde{m}}{\hbar} \right)^{3/2} \times 2 \times (K_1 + K_2). \quad (7.162)$$

where the integrals include the minus sign and the  $\omega$  and are

$$K_1 = \omega \sum_{m_i, m_f} \int_0^{s_F} \frac{-ds (w_i - w_f) s^2 \delta_{m_f = m_i + \nu}}{(-\omega_g - s^2 + \frac{1}{2}\nu\omega_B) (\omega + i\gamma - \omega_g - s^2 + \frac{1}{2}\nu\omega_B)} \quad (7.163)$$

$$K_2 = \omega \sum_{m_i, m_f} \int_0^{s_F} \frac{-ds (w_i - w_f) s^2 \delta_{m_f = m_i - \nu}}{(-\omega_g - s^2 - \frac{1}{2}\nu\omega_B) (\omega + i\gamma + \omega_g + s^2 + \frac{1}{2}\nu\omega_B)} \quad (7.164)$$

These are very similar to the expressions I had for  $K_1$  and  $K_2$  for 3D, and really the only main change is the factor of  $s^2$  instead of  $s^4$ . They can be written with

$$\omega_\nu = \omega + i\gamma + \frac{1}{2}\nu\omega_B, \quad \zeta = \frac{1}{2}\nu\omega_B. \quad (7.165)$$

Then they are

$$K_1 = \omega \sum_{m_i, m_f} \int_0^{s_F} \frac{-ds g_{m_f}(s) s^2 \delta_{m_f = m_i + \nu}}{(\omega_g + s^2 - \zeta) (\omega_g + s^2 - \omega_\nu)} \quad (7.166)$$

$$K_2 = \omega \sum_{m_i, m_f} \int_0^{s_F} \frac{+ds g_{m_f}(s) s^2 \delta_{m_f = m_i - \nu}}{(\omega_g + s^2 + \zeta) (\omega_g + s^2 + \omega_\nu)} \quad (7.167)$$

Including the thermal population effects, the best way to write them for real calculations will probably be in terms of the Inouye *et al.* variable  $x = \omega_g + s^2$ . That becomes

$$K_1 = -\frac{\omega}{2} \sum_{m_i, m_f} \int_{\omega_g}^{\omega_g + s_F^2} dx \frac{g_{m_f}(x) \sqrt{x - \omega_g}}{(x - \zeta)(x - \omega_\nu)} \delta_{m_i = m_f - \nu} \quad (7.168)$$

$$K_2 = +\frac{\omega}{2} \sum_{m_i, m_f} \int_{\omega_g}^{\omega_g + s_F^2} dx \frac{g_{m_f}(x) \sqrt{x - \omega_g}}{(x + \zeta)(x + \omega_\nu)} \delta_{m_i = m_f + \nu} \quad (7.169)$$

I changed the deltas here to show how they select certain  $m_i$  for fixed  $m_f$ . When the  $m_i$  sum is done first (it already selected the transitions in the denominators), it chose particular transitions. We do this at fixed final  $m_f$ . For a chosen  $m_f$ , there are (usually) two  $m_i$ , one corresponding to each integral. Then both integrals have the same population factors then.<sup>5</sup> When the population factors are the same, the two integrals can be combined into one. The integrand depends on

$$\begin{aligned} f &= \frac{1}{2} \left\{ \frac{-1}{(x - \zeta)(x - \omega_\nu)} + \frac{1}{(x + \zeta)(x + \omega_\nu)} \right\} \\ &= \frac{1}{2} \left\{ \frac{-(x + \zeta)(x + \omega_\nu) + (x - \zeta)(x - \omega_\nu)}{(x^2 - \zeta^2)(x^2 - \omega_\nu^2)} \right\} = \frac{-x(\omega_\nu + \zeta)}{(x^2 - \zeta^2)(x^2 - \omega_\nu^2)}. \end{aligned} \quad (7.170)$$

This same factor was encountered in the 3D problem. So the rest of the calculation is very similar. With  $\omega_\nu + \zeta = \omega_{2\nu}$ , we have for the combined integral  $I_\nu = K_1 + K_2$ ,

$$I_\nu = \sum_{m_f} \int_{\omega_g}^{x_F} dx g_{m_f}(x) \cdot \sqrt{x - \omega_g} \cdot \frac{x\omega}{x^2 - \frac{1}{4}\omega_B^2} \cdot \frac{\omega_{2\nu}}{\omega_\nu^2 - x^2}. \quad (7.171)$$

This result for  $I_\nu$  should not be too bad to calculate, and usually it is customary to let the upper limit go to infinity. At large  $x$  the integrand varies as  $x^{-5/2}$  so the integration should be convergent. There still remains the sum over the final state, which modifies the population factor.

<sup>5</sup>Recall, however, if the higher band has the larger angular momentum, this counting needs to be done differently. We did the case of s to p transitions earlier. Even for, say, p to d transitions, if you have  $m_f = +2$ , for example, there is only one available  $m_i = 1$ , because there will not be  $m_i = +3$  in a p-band.

We note that the population factor is taken as

$$g_{m_f}(x) = 1 - F_{m_f}(x), \quad F(E_f) = \frac{1}{\exp\{\beta(E_f - E_F)\} + 1}. \quad (7.172)$$

where we need to insert the final state energy as

$$E_f = \hbar \left( \omega_g + s^2 - \frac{1}{2} m_f \omega_B \right) = \hbar \left( x - \frac{1}{2} m_f \omega_B \right). \quad (7.173)$$

The final state energy depends on the Zeeman state, hence I keep the index  $m_f$  on the occupation factor.

Summarizing, this will give the sum for polarization averaging, in the 1D damped model,

$$S_\nu = \frac{4|M|^2 \hbar V k_F^2}{m_e (\pi)^3} \left( \frac{2\tilde{m}}{\hbar} \right)^{3/2} \times I_\nu. \quad (7.174)$$

All these constants will be typically renamed as some constant, say,  $Q$  as in the Scaffardi and Tocho paper. It would be a fitting constant, made to match experiment.

## 7.8 Expressions for 1D bands with damping, electric polarization averaging. II.

This part discusses an expression for  $I_{R|L}$  in terms of real variables. In the previous section the calculation was done in the complex more general notation using  $\omega_\nu$ .

Let me note how  $\chi_R$  works out instead if the expression from polarization averaging were used, because that will be better for comparison with the theory in the absence of the magnetic field! This requires the two terms for  $\Delta m = \pm 1$  to come in with the same sign, and the whole integrand gets multiplied by a factor of  $-\omega/\omega_{if}$ . Going back to the integrand for  $S_R$ , Eq. (7.147), the part in braces {...} now becomes

$$\begin{aligned} \{...\} &\rightarrow -\frac{\omega}{\omega_{if}} \left\{ \frac{\delta_{m_f=m_i-1}}{\omega + i\gamma + \omega_{if}} + \frac{\delta_{m_f=m_i+1}}{\omega + i\gamma - \omega_{if}} \right\} = \left\{ \frac{-\omega}{\omega_{if}^-(\omega + i\gamma + \omega_{if}^-)} + \frac{-\omega}{\omega_{if}^+(\omega + i\gamma - \omega_{if}^+)} \right\} \\ &= \frac{-\omega}{(-\frac{\omega_B}{2} - \omega_g - s^2)(\omega + i\gamma - \frac{\omega_B}{2} - \omega_g - s^2)} + \frac{-\omega}{(\frac{\omega_B}{2} - \omega_g - s^2)(\omega + i\gamma - \frac{\omega_B}{2} + \omega_g + s^2)} \\ &= \frac{\omega}{(x + \frac{\omega_B}{2})(\omega + i\gamma - \frac{\omega_B}{2} - x)} + \frac{\omega}{(x - \frac{\omega_B}{2})(\omega + i\gamma - \frac{\omega_B}{2} + x)} \end{aligned} \quad (7.175)$$

Here I am using the same definition,  $x = \omega_g + s^2$ . The presence of different factors with the magnetic frequency and  $x$  is interesting. It is probably simplest to keep the  $\Delta m = \pm 1$  terms separated, they do not combine into anything too beautiful! But I like the result. If we rationalize each one separately, there results

$$\{...\} = \frac{\omega}{(x + \frac{\omega_B}{2})} \cdot \frac{(\omega - \frac{\omega_B}{2} - x - i\gamma)}{(\omega - \frac{\omega_B}{2} - x)^2 + \gamma^2} + \frac{\omega}{(x - \frac{\omega_B}{2})} \cdot \frac{(\omega - \frac{\omega_B}{2} + x - i\gamma)}{(\omega - \frac{\omega_B}{2} + x)^2 + \gamma^2} \quad (7.176)$$

Just for the record, if instead we did put them together and rationalize, see what comes out:

$$\begin{aligned} \{...\} &= \frac{\omega}{x^2 - (\frac{\omega_B}{2})^2} \cdot \left\{ \frac{x - \frac{\omega_B}{2}}{\omega_\nu - x} + \frac{x + \frac{\omega_B}{2}}{\omega_\nu + x} \right\} \\ &= \frac{\omega}{x^2 - (\frac{\omega_B}{2})^2} \cdot \left\{ \frac{(x - \frac{\omega_B}{2})(\omega_\nu + x) + (x + \frac{\omega_B}{2})(\omega_\nu - x)}{\omega_\nu^2 - x^2} \right\} \\ &= \frac{\omega}{x^2 - (\frac{\omega_B}{2})^2} \cdot \left\{ \frac{(2\omega_\nu - \omega_B)x}{\omega_\nu^2 - x^2} \right\} = \frac{2\omega x(\omega + i\gamma - \omega_B)}{\left[ x^2 - (\frac{\omega_B}{2})^2 \right] \left[ (\omega + i\gamma - \frac{\omega_B}{2})^2 - x^2 \right]} \end{aligned} \quad (7.177)$$

Again I used  $\omega_\nu = \omega + i\gamma - \frac{\omega_B}{2}$ , where this example has  $\nu = -1$  for R polarization. Now finally get it rationalized, ugh, with all the  $i$ 's in the top,

$$\{\dots\} = \frac{2\omega x(\omega + i\gamma - \omega_B)}{\left[x^2 - \left(\frac{\omega_B}{2}\right)^2\right]} \cdot \frac{\left[\left(\omega - \frac{\omega_B}{2}\right)^2 - x^2 - \gamma^2\right] - 2i\gamma\left(\omega - \frac{\omega_B}{2}\right)}{\left[\left(\omega - \frac{\omega_B}{2}\right)^2 - x^2 - \gamma^2\right]^2 + 4\gamma^2\left(\omega - \frac{\omega_B}{2}\right)^2} \quad (7.178)$$

The factor of “2” is taken out as a prefactor, then with real Faraday frequency  $\omega_R = \omega - \frac{\omega_B}{2}$ , the integral that will be needed is now

$$I_R = \sum_{m_f} \int_{\omega_g}^{x_F} dx g_{m_f}(x) \sqrt{x - \omega_g} x \cdot \frac{\omega(\omega + i\gamma - \omega_B)}{x^2 - \left(\frac{\omega_B}{2}\right)^2} \cdot \frac{[\omega_R^2 - x^2 - \gamma^2] - 2i\gamma\omega_R}{[\omega_R^2 - x^2 - \gamma^2]^2 + 4\gamma^2\omega_R^2} \quad (7.179)$$

Obviously there is a similar expression for  $I_L$ , changing  $\omega_R$  to  $\omega_L = \omega + \frac{\omega_B}{2}$ . This is the same as the complex expression in the previous section, which is a good check of all this algebra. The part between the dots is what is different from current averaging. However, one expects that the main contribution to the integral comes from the region,  $x \approx \omega_R$ . Then the factor between the dots is close to “1” if the damping and magnetic field are small, as should be assumed. So this should not be significantly different from the corresponding integral that came from current averaging. It may be slightly preferred because it looks more convergent at large  $x$ , however, that is probably of little importance, and, the current averaging expression is generally simpler.

## 7.9 Finding $S_R$ , 1D bands, with damping, current averaging

The last sections gave the expression for  $S_R$ , but concentrated mostly on the integrals in terms of the variable  $x = \omega_g + s^2$ . For analytic evaluations, however, it is better to set up the integrals in terms of  $s$ . Here I try to get their exact analytic results, where the main approximation not used by Inouye *et al.* is that I have already set the occupation probabilities to 1 and zero for occupied and unoccupied states.

So here I want to evaluate the integral needed for  $S_R$  in expression (7.148), taking out a factor of “2” to stay with the prefactor, which comes from converting to an integral only over positive  $s$ , one needs

$$\begin{aligned} I_R &= \int_0^{s_F} ds s^2 \left\{ \frac{1}{\omega + i\gamma - \frac{\omega_B}{2} - \omega_g - s^2} - \frac{1}{\omega + i\gamma - \frac{\omega_B}{2} + \omega_g + s^2} \right\} \\ &= \int_0^{s_F} ds s^2 \left\{ \frac{1}{\omega_R + i\gamma - \omega_g - s^2} - \frac{1}{\omega_R + i\gamma + \omega_g + s^2} \right\} \end{aligned} \quad (7.180)$$

As complex functions, these two integrals are of similar forms, whose integrations are quite simple. The second term is simplest,

$$I_1(a_1) = \int ds \frac{s^2}{a_1^2 + s^2} = s - a_1 \tan^{-1} \left( \frac{s}{a_1} \right) = s - \frac{ia_1}{2} \ln \left( \frac{a_1 - is}{a_1 + is} \right). \quad (7.181)$$

The last form is a general analytic function for the inverse tangent, used earlier. The squared parameter we have already met,

$$a_1^2 = \omega_R + \omega_g + i\gamma \equiv \omega_1 + i\gamma, \quad a_1 = \sqrt{\omega_1 + i\gamma} \quad (7.182)$$

and the square root of this is also known,

$$a_1 = x_1 + iy_1 = \sqrt{\frac{1}{2} \left( \sqrt{\omega_1^2 + \gamma^2} + \omega_1 \right)} + i\sqrt{\frac{1}{2} \left( \sqrt{\omega_1^2 + \gamma^2} - \omega_1 \right)} \quad (7.183)$$

These can be used to find the arctangent, there is no difference from the analysis already done for 3D damped bands, and one will get the same result,

$$\begin{aligned}\tan^{-1}\left(\frac{s}{a_1}\right) &= \tan^{-1}\left[\frac{s}{x_1 + iy_1}\right] = \frac{i}{2} \ln \left[\frac{x_1 + iy_1 - is}{x_1 + iy_1 + is}\right] \\ &= \frac{1}{2} \tan^{-1}\left[\frac{2x_1s}{x_1^2 + y_1^2 - s^2}\right] + \frac{i}{4} \ln \left[\frac{x_1^2 + (y_1 - s)^2}{x_1^2 + (y_1 + s)^2}\right]\end{aligned}\quad (7.184)$$

For the other integral with  $-s^2$ , let its parameter be  $a_2$ , defined as

$$a_2^2 = \omega_R - \omega_g + i\gamma \equiv \omega_2, \quad a_2 = \sqrt{\omega_2 + i\gamma} \quad (7.185)$$

and the square root is given by the same algorithm as for  $a_1$ . The integral itself is aided by the transformation  $s = iz$ , which converts it to

$$\begin{aligned}I_2(a_2) &= \int ds \frac{s^2}{a_2^2 - s^2} = -i \int dz \frac{z^2}{a_1^2 + z^2} = -i \left[ z - a_2 \tan^{-1}\left(\frac{z}{a_2}\right) \right] \\ &= -s + ia_2 \tan^{-1}\left(\frac{-is}{a_2}\right) = -s - \frac{a_2}{2} \ln \left(\frac{a_2 - s}{a_2 + s}\right)\end{aligned}\quad (7.186)$$

Again the inverse tangent can be evaluated using the real and imaginary parts, which was

$$\begin{aligned}\tan^{-1}\left(\frac{-is}{a_2}\right) &= \tan^{-1}\left[\frac{-is}{x_2 + iy_2}\right] = \frac{i}{2} \ln \left[\frac{x_2 + iy_2 - s}{x_2 + iy_2 + s}\right] \\ &= -\frac{1}{2} \tan^{-1}\left[\frac{2y_2s}{x_2^2 + y_2^2 - s^2}\right] + \frac{i}{4} \ln \left[\frac{(x_2 - s)^2 + y_2^2}{(x_2 + s)^2 + y_2^2}\right]\end{aligned}\quad (7.187)$$

Then the combination to get the needed integral  $I_R$  is

$$\begin{aligned}I_R = I_2(a_2) - I_1(a_1) &= \left[ -s_F + ia_2 \tan^{-1}\left(\frac{-is_F}{a_2}\right) \right] - \left[ s_F - a_1 \tan^{-1}\left(\frac{s_F}{a_1}\right) \right] \\ &= i\sqrt{\omega_R - \omega_g + i\gamma} \tan^{-1}\left(\frac{-is_F}{\sqrt{\omega_R - \omega_g + i\gamma}}\right) \\ &\quad + \sqrt{\omega_R + \omega_g + i\gamma} \tan^{-1}\left(\frac{s_F}{\sqrt{\omega_R + \omega_g + i\gamma}}\right) - 2s_F\end{aligned}\quad (7.188)$$

Of course, the inverse tangents are defined above for these complex arguments. These results apply no matter whether the excitation frequency is above or below the gap, due to the way this way derived, with generalized complex square roots. The only possible difficulty, is the choice of the upper limit,  $s_F$ , especially, what to do about the linear term.

Based on results in *Dielectrics: Part A*, the main change for polarization averaging will be that instead of the term  $-2s_F$ , there is

$$-2s_F \longrightarrow -2\sqrt{\omega_g} \tan^{-1}\left(\frac{s_F}{\sqrt{\omega_g}}\right). \quad (7.189)$$

For taking the limit  $s_F \rightarrow \infty$ , this would go over to  $-\pi\sqrt{\omega_g}$ , rather than diverging, which could be a useful approximation. What about the other inverse tangents as  $s_F \rightarrow \infty$ ? This must be done carefully, else they seem to give zero. But those tangents do go to zero, however, while their denominators are negative. So  $\tan^{-1}(y/x)$  gives an angle in the second quadrant if  $y$  is positive while  $x$  is negative, and in the third quadrant if  $y$  is negative while  $x$  is also negative. That is, the form  $\tan^{-1}(y/x) \rightarrow \pi \operatorname{sgn}(y)$  for  $x \rightarrow -\infty$ . For the square roots used here, all the factors  $x_1, y_1, x_2, y_2$  are taken as positive numbers. Then there are the following simple limits:

$$\lim_{s \rightarrow \infty} \frac{1}{2} \tan^{-1}\left[\frac{2x_1s}{x_1^2 + y_1^2 - s^2}\right] = \frac{1}{2} \pi \operatorname{sgn}(x_1) = \frac{\pi}{2}, \quad (7.190)$$

$$\lim_{s \rightarrow \infty} -\frac{1}{2} \tan^{-1} \left[ \frac{2y_2 s}{x_2^2 + y_2^2 - s^2} \right] = -\frac{1}{2} \pi \operatorname{sgn}(y_2) = -\frac{\pi}{2}, \quad (7.191)$$

The logarithmic parts of the complex inverse tangents vanish in the same limits, so we have

$$\lim_{s \rightarrow \infty} \tan^{-1} \left( \frac{s}{a_1} \right) = \frac{\pi}{2} + i0, \quad (7.192)$$

$$\lim_{s \rightarrow \infty} \tan^{-1} \left( \frac{-is}{a_2} \right) = -\frac{\pi}{2} + i0, \quad (7.193)$$

So if one takes the upper limit  $s_F$  to infinity, the  $I_R$  integral becomes approximately,

$$\begin{aligned} I_R &= [I_2(a_2) - I_1(a_1)]_{s_F \rightarrow \infty} = -\pi \sqrt{\omega_g} + ia_2 \cdot \frac{-\pi}{2} + a_1 \cdot \frac{\pi}{2} \\ I_R &= \frac{\pi}{2} [a_1 - ia_2 - 2\sqrt{\omega_g}] = \frac{\pi}{2} \left[ \sqrt{\omega_R + \omega_g + i\gamma} - i\sqrt{\omega_R - \omega_g + i\gamma} - 2\sqrt{\omega_g} \right] \end{aligned} \quad (7.194)$$

That clearly shows how one integral is the complex rotation of the other, due to the  $i$  on  $a_2$ . To get the similar result for left polarization, it is necessary to switch  $\omega_R = \omega - \frac{\omega_B}{2}$  to  $\omega_L = \omega + \frac{\omega_B}{2}$ .

### 7.9.1 Getting the effective sums

Going back to (7.148) and equations following it, the sum that goes to the susceptibility is written, with the dimensionless factors as

$$\begin{aligned} S_R &= g_m \frac{2|M|^2}{\pi^2} \left( \frac{m_e V \omega_g^2}{\hbar c} \right) \left( \frac{\hbar k_F}{m_e c} \right)^2 \left( \frac{2\tilde{m}c^2}{\hbar \omega_g} \right)^{3/2} \cdot \frac{1}{\sqrt{\omega_g}} \frac{2}{\pi} I_R \\ &= g_m \frac{2|M|^2}{\pi^2} \left( \frac{m_e V \omega_g^2}{\hbar c} \right) \left( \frac{\hbar k_F}{m_e c} \right)^2 \left( \frac{2\tilde{m}c^2}{\hbar \omega_g} \right)^{3/2} \left[ \frac{\sqrt{\omega_R + \omega_g + i\gamma}}{\sqrt{\omega_g}} - i \frac{\sqrt{\omega_R - \omega_g + i\gamma}}{\sqrt{\omega_g}} - 2 \right] \end{aligned} \quad (7.195)$$

The associated susceptibility contribution is

$$\chi_R = -g_m \frac{2|M|^2}{\pi^2} \left( \frac{e^2}{\hbar c} \right) \left( \frac{\hbar k_F}{m_e c} \right)^2 \left( \frac{2\tilde{m}c^2}{\hbar \omega_g} \right)^{3/2} \frac{\omega_g^{3/2}}{\omega(\omega + i\gamma)} \left[ \sqrt{\omega_R + \omega_g + i\gamma} - i\sqrt{\omega_R - \omega_g + i\gamma} - 2\sqrt{\omega_g} \right] \quad (7.196)$$

One can check this in the limit of small damping, letting  $\gamma \rightarrow 0$ , it goes over to

$$\chi_R \approx -g_m \frac{2|M|^2}{\pi^2} \left( \frac{e^2}{\hbar c} \right) \left( \frac{\hbar k_F}{m_e c} \right)^2 \left( \frac{2\tilde{m}c^2}{\hbar \omega_g} \right)^{3/2} \frac{\omega_g^{3/2}}{\omega^2} \left[ \sqrt{\omega_R + \omega_g} - 2\sqrt{\omega_g} - i\sqrt{\omega_R - \omega_g} \right] \quad (7.197)$$

I changed the order to keep the real and imaginary parts separated. But one must keep in mind that the last term is imaginary (as written) if the excitation is above the gap, but it becomes real if the excitation is below the gap. This is to be expected, as below-the-gap excitation does not have any physical absorption. As a check of this, we can do the integrals, taking the limit of  $\gamma \rightarrow 0$  first, as shown in the next section.

### 7.10 Finding $S_R$ , 1D bands, limit of zero damping, current averaging

Again we want to apply the zero damping limit, using the SW theorem before integration,

$$\lim_{\gamma \rightarrow 0^+} \frac{1}{x + i\gamma} = \text{p.v.} \left( \frac{1}{x} \right) - i\pi\delta(x) \quad (7.198)$$

Applied to the first term in the integrand for  $I_R$ , (7.180), for the 1D bands model, it gives

$$\frac{1}{\omega_R + i\gamma - \omega_g - s^2} \longrightarrow \text{p.v.} \left( \frac{1}{\omega_R - \omega_g - s^2} \right) - i\pi\delta(\omega_R - \omega_g - s^2), \quad (7.199)$$

whereas, on the second term the effect is

$$\frac{1}{\omega_R + i\gamma + \omega_g + s^2} \longrightarrow \text{p.v.} \left( \frac{1}{\omega_R + \omega_g + s^2} \right) - i\pi\delta(\omega_R + \omega_g + s^2), \quad (7.200)$$

There is also an additional factor of  $s^2$  in the integrand.

### 7.10.1 The imaginary part – integration of the delta functions

I am doing this slightly differently than what was done for the zero damping limit in 3D bands. This time, switch to the variable  $x = \omega_g + s^2$ , which is present in both integrands. Now one has  $dx = 2sds$  and there results some trivial integration steps,

$$\begin{aligned} \text{Im}\{I_R\} &= -i\pi \int_0^{s_F} ds s^2 [\delta(\omega_R - \omega_g - s^2) - \delta(\omega_R + \omega_g + s^2)] \\ &= -i\pi \int_{\omega_g}^{x_F} dx \frac{1}{2} \sqrt{x - \omega_g} [\delta(\omega_R - x) - \delta(\omega_R + x)] \\ &= -i\frac{\pi}{2} \sqrt{\omega_R - \omega_g}. \end{aligned} \quad (7.201)$$

Because  $x > \omega_g$ , the second delta is never satisfied, so only the first one gives any contribution. It is a fantastically simple result. Recall,  $\omega_R = \omega - \frac{1}{2}\omega_B$ . There is the opposite sign on  $\omega_B$  to get  $\omega_L$  and hence the integral  $I_L$ . This is clearly consistent with the results from the previous section in the limit  $\gamma \rightarrow 0$ .

### 7.10.2 The real part – principal valued integration

Now one wants the real part,

$$\text{Re}\{I_R\} = \text{p.v.} \int_0^{s_F} ds s^2 \left[ \frac{1}{\omega_R - \omega_g - s^2} - \frac{1}{\omega_R + \omega_g + s^2} \right] \quad (7.202)$$

It is best to leave these in terms of  $s$ , which we know how to integrate. The second integral is not singular and p.v. is not necessary there. With my usual definitions,

$$a_1^2 = \omega_R + \omega_g, \quad a_2^2 = \omega_R - \omega_g, \quad (7.203)$$

These are easily integrated with some simple rearranging,

$$\begin{aligned} \text{Re}\{I_R\} &= \text{p.v.} \int_0^{s_F} ds \left[ \frac{-a_2^2 + s^2 + a_2^2}{a_2^2 - s^2} - \frac{a_1^2 + s^2 - a_1^2}{a_1^2 + s^2} \right] \\ &= \text{p.v.} \int_0^{s_F} ds \left[ -2 + \frac{a_2^2}{a_2^2 - s^2} + \frac{a_1^2}{a_1^2 + s^2} \right] \\ &= -2s_F + a_1 \tan^{-1} \left( \frac{s_F}{a_1} \right) + a_2 \text{p.v.} \int_0^{s_F/a_2} dx \frac{1}{1 - x^2} \end{aligned} \quad (7.204)$$

The latter integral gives an inverse hyperbolic tangent where  $x < 1$ , but it gives an inverse hyperbolic cotangent where  $x > 1$ . It is possible to express this as a single function introduced earlier, most usefully written using a logarithm,

$$\int \frac{dx}{1 - x^2} = L(x) = \frac{1}{2} \ln \left( \frac{|1 + x|}{|1 - x|} \right). \quad (7.205)$$

When the p.v. is taken, it simply ignores anything singular happening at  $x = 1$ . Only the upper limit ends up contributing, so we get very simply (assuming  $s_F > a_2$ ),

$$\begin{aligned} \text{Re}\{I_R\} &= -2s_F + a_1 \tan^{-1} \left( \frac{s_F}{a_1} \right) + a_2 \coth^{-1} \left( \frac{s_F}{a_2} \right) \\ &= -2s_F + \sqrt{\omega_R + \omega_g} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_R + \omega_g}} \right) + \sqrt{\omega_R - \omega_g} \coth^{-1} \left( \frac{s_F}{\sqrt{\omega_R - \omega_g}} \right). \end{aligned} \quad (7.206)$$

If a good estimate of  $s_F$  is known, this is then easy to evaluate. On the other hand, if one wants to let  $s_F \rightarrow \infty$ , that does not work unless the first term is replaced by the approximation appropriate for electric polarization averaging, as seen earlier,

$$2s_F \approx 2\sqrt{\omega_g} \tan^{-1} \left( \frac{s_F}{\sqrt{\omega_g}} \right). \quad (7.207)$$

Then this expression does have a finite limit for large  $s_F$ , of  $2\sqrt{\omega_g} \times \pi/2$ . If one didn't think this is a reasonable approximation, another possibility for choosing the upper limit of integration is to use the value from the following equality,

$$s_F \approx \sqrt{\omega_g} \frac{\pi}{2}, \quad (7.208)$$

although this is of some questionable justification. Nevertheless, if the polarization averaging approximation is used, one gets while letting the upper limit go to to infinity,

$$\text{Re}\{I_R\} \approx \frac{\pi}{2} [\sqrt{\omega_R + \omega_g} - 2\sqrt{\omega_g}] \quad (7.209)$$

because the limit of the inverse hyperbolic cotangent vanishes. That is also in complete agreement with the real part of  $I_R$  as obtained in the earlier section where  $\gamma$  was let to vanish at the end of the calculation.

### 7.10.3 The net integral for 1D bands, zero damping limit, discussion

Combining the real and imaginary parts for the integral from current density averaging, one gets

$$\begin{aligned} I_R &\approx \frac{\pi}{2} [\sqrt{\omega_R + \omega_g} - 2\sqrt{\omega_g} - i\sqrt{\omega_R - \omega_g}] \\ I_R &\approx \frac{\pi}{2} \left[ \sqrt{\omega - \frac{\omega_B}{2} + \omega_g} - 2\sqrt{\omega_g} - i\sqrt{\omega - \frac{\omega_B}{2} - \omega_g} \right] \end{aligned} \quad (7.210)$$

As always, switch the sign of  $\omega_B$  to get the corresponding result for left circular polarization. This last formula summarizes very succinctly what I wanted to find when I started this quest! After scaling with the physical factors, it will determine the main features of a DC magnetic field acting on the interband transitions in a metal, such as gold, that I was interested in. It is even simpler than I could have imagined, considering the amount of theory that was needed to arrive here. Note that it gets multiplied by a negative constant to produce  $\chi$ . Also, the second term would typically be the largest. As the frequency increases, the first two (real) terms tend to cancel more so, up to the point  $\omega \approx 3\omega_g$ , where they just about cancel. Both the real and imaginary contributions to  $\chi$  appear to be positive. When the excitation is below gap, the last term also becomes a real contribution; there is no true absorption when  $\omega - \frac{1}{2}\omega_B < \omega_g$ .

Need to keep in mind, however, that this above result applies only under the approximation,  $w_i - w_f = 1$ . It does not have the important thermal effects that would be present in the Fermi level falls in the upper band, as should be the case for metals, like gold, silver, copper.

The dependence on the circular polarization is very interesting. It seems to show that the right circular photons have a lower effective energy, because the magnetic frequency *subtracts* from the photon frequency in that case. Conversely, the left circular photons have to cross a smaller effective gap, or, they have an enhanced ability to cross the band gap. Of course, these effects are very small, but they have implications for the Faraday rotation. Perhaps experimentalists have thought of ways to excite with one polarization or the other, and measure different responses, to exploit the differences of the two polarizations, besides looking at the Faraday rotation.

So this calculation seems to be pretty complete, in that we know how the band-to-band transitions influence the susceptibility and dielectric functions in the presence of a DC magnetic field. All that is left to do is check how it works with some real physical constants included, for a real application. Further, there might be some other additional analysis of the effects these results predict for the Faraday rotation.



#### 7.10.4 More about the Faraday effect contributions–1D, current averaging

One knows that the bulk Faraday rotation angle depends on the following combination, ignoring some numerical factors,

$$\theta_F \propto \frac{\mathcal{E}_{xy}}{\sqrt{\epsilon_{xx}}} \quad (7.211)$$

But these Cartesian components are related to the circular permittivity components by

$$\epsilon_R = \epsilon_{xx} + \mathcal{E}_{xy}, \quad \epsilon_L = \epsilon_{xx} - \mathcal{E}_{xy}, \quad (7.212)$$

or solved the other way,

$$\epsilon_{xx} = \frac{1}{2}(\epsilon_R + \epsilon_L), \quad \mathcal{E}_{xy} = \frac{1}{2}(\epsilon_R - \epsilon_L). \quad (7.213)$$

So without keeping track of all physical factors, one can extract the dependence on magnetic field by just using the results for the  $I_R$  and  $I_L$  integrals, because  $\epsilon_R$  and  $\epsilon_L$  are proportional to those (for only the band-to-band parts here). The main thing to look at is the off diagonal permittivity. Assuming weak enough magnetic field, do expansions,

$$\begin{aligned} I_R &= \frac{\pi}{2} \left\{ \sqrt{\omega + \omega_g} \left[ 1 - \frac{1}{2} \frac{\omega_B}{\omega + \omega_g} \right]^{1/2} - 2\sqrt{\omega_g} - i\sqrt{\omega - \omega_g} \left[ 1 - \frac{1}{2} \frac{\omega_B}{\omega - \omega_g} \right]^{1/2} \right\} \\ &\approx \frac{\pi}{2} \left\{ \sqrt{\omega + \omega_g} - 2\sqrt{\omega_g} - i\sqrt{\omega - \omega_g} - \frac{\omega_B}{4} \left[ \frac{1}{\sqrt{\omega + \omega_g}} - \frac{i}{\sqrt{\omega - \omega_g}} \right] \right\} \end{aligned} \quad (7.214)$$

The same approximations for  $I_L$  lead to

$$I_L \approx \frac{\pi}{2} \left\{ \sqrt{\omega + \omega_g} - 2\sqrt{\omega_g} - i\sqrt{\omega - \omega_g} + \frac{\omega_B}{4} \left[ \frac{1}{\sqrt{\omega + \omega_g}} - \frac{i}{\sqrt{\omega - \omega_g}} \right] \right\} \quad (7.215)$$

Therefore the contribution to the diagonal part of permittivity has little dependence on magnetic field,

$$I_{xx} = \frac{1}{2}(I_R + I_L) \approx \frac{\pi}{2} \left\{ \sqrt{\omega + \omega_g} - 2\sqrt{\omega_g} - i\sqrt{\omega - \omega_g} \right\} \quad (7.216)$$

The contribution to the off-diagonal part is approximately linear in the magnetic field,

$$I_{xy} = \frac{1}{2}(I_R - I_L) \approx -\frac{\pi\omega_B}{8} \left\{ \frac{1}{\sqrt{\omega + \omega_g}} - \frac{i}{\sqrt{\omega - \omega_g}} \right\} \quad (7.217)$$

This last combination is most important for the Faraday rotation, as

$$\mathcal{E}_{xy} = \frac{1}{2}(\epsilon_R - \epsilon_L) \propto \frac{1}{2}(I_R - I_L) \quad (7.218)$$

If the excitation is above the gap, then the formula shows both a real and imaginary part, however, the imaginary part will contribute to the ellipticity effect. On the other hand, if the excitation is below the gap, then both terms here become real and both give contributions to the Faraday rotation. This suggests that there could be a very interesting crossover effect from the one regime to the other. Possibly the F.R. rapidly reduces (with the square root dependence on excitation frequency) as the gap energy is crossed. However, these must be well-known effects, and my interest is otherwise, in the eventual implications for affecting the dielectric properties of magnetic particles covered with a gold shell (also a system where the band theory is questionable, oh well..).

#### 7.11 Finding $S_\nu$ , 1D bands, with damping, polarization averaging

This part looks at evaluating the integral (7.162) for  $S_\nu$  for the 1D band model from polarization averaging, in the limit where the thermal population factor is  $w_i - w_f = 1$ . To do this, look at the

$K_1$  and  $K_2$  integrals, which combine into  $I_\nu = K_1 + K_2$ , supposing that the sums over  $m_i, m_f$  are already done, and give a factor of  $g_m = l_i + l_f$  included in the constants,

$$K_1 = \omega \int_0^{s_F} \frac{-ds s^2}{(\omega_g + s^2 - \zeta)(\omega_g + s^2 - \omega_\nu)} \quad (7.219)$$

$$K_2 = \omega \int_0^{s_F} \frac{+ds s^2}{(\omega_g + s^2 + \zeta)(\omega_g + s^2 + \omega_\nu)} \quad (7.220)$$

The usual definitions  $\omega_\nu = \omega + i\gamma + \zeta$  and  $\zeta = \nu \frac{\omega_B}{2}$  are used here. Recall the partial fraction expansion for  $K_1$ 's integrand,

$$\frac{1}{(\omega_g + s^2 - \zeta)(\omega_g + s^2 - \omega_\nu)} = \frac{1}{\omega_\nu - \zeta} \left[ \frac{-1}{\omega_g + s^2 - \zeta} + \frac{1}{\omega_g + s^2 - \omega_\nu} \right] \quad (7.221)$$

Then this has  $\omega_\nu - \zeta = \omega + i\gamma$ , no Zeeman term in the first factor. For the other integral we need to switch the signs on  $\omega_\nu$  and  $\zeta$ , so

$$\frac{1}{(\omega_g + s^2 + \zeta)(\omega_g + s^2 + \omega_\nu)} = \frac{1}{-\omega_\nu + \zeta} \left[ \frac{-1}{\omega_g + s^2 + \zeta} + \frac{1}{\omega_g + s^2 + \omega_\nu} \right] \quad (7.222)$$

Then we get nearly the same as in 3D expressions earlier,

$$K_1 = \frac{\omega}{\omega + i\gamma} \int_0^{s_F} ds s^2 \left[ \frac{1}{s^2 + \omega_g - \zeta} + \frac{1}{\omega_\nu - \omega_g - s^2} \right] \quad (7.223)$$

$$K_2 = \frac{\omega}{\omega + i\gamma} \int_0^{s_F} ds s^2 \left[ \frac{1}{s^2 + \omega_g + \zeta} - \frac{1}{s^2 + \omega_g + \omega_\nu} \right] \quad (7.224)$$

I wrote the second term in  $K_1$  in such a way that is convenient, thinking that  $\omega_\nu > \omega_g$ . These are all integrals found earlier, for example,

$$I_1(a_1) = \int ds \frac{s^2}{a_1^2 + s^2} = s - a_1 \tan^{-1} \left( \frac{s}{a_1} \right) = s - \frac{ia_1}{2} \ln \left( \frac{a_1 - is}{a_1 + is} \right). \quad (7.225)$$

For the one with the reversed sign on  $s^2$  we showed in *Part A*

$$I_3(a_1) = \int ds \frac{s^2}{a_1^2 - s^2} = -s + a_1 \tanh^{-1} \left( \frac{s}{a_1} \right), \quad (7.226)$$

where this requires the complex continuation of the inverse function. Thus we can write out each one and sum the two integrals. We have (with  $s \rightarrow s_F$  later)

$$K_1 = \frac{\omega}{\omega + i\gamma} \left[ s - \sqrt{\omega_g - \zeta} \tan^{-1} \frac{s}{\sqrt{\omega_g - \zeta}} - s + \sqrt{\omega_\nu - \omega_g} \tanh^{-1} \frac{s}{\sqrt{\omega_\nu - \omega_g}} \right] \quad (7.227)$$

$$K_2 = \frac{\omega}{\omega + i\gamma} \left[ s - \sqrt{\omega_g + \zeta} \tan^{-1} \frac{s}{\sqrt{\omega_g + \zeta}} - s + \sqrt{\omega_g + \omega_\nu} \tan^{-1} \frac{s}{\sqrt{\omega_g + \omega_\nu}} \right] \quad (7.228)$$

The linear term in  $s$  drops out; only the arctangents survive. Then the total integral  $I_\nu$  is their sum,

$$I_\nu = \frac{\omega}{\omega + i\gamma} \times \left[ -\sqrt{\omega_g - \zeta_\nu} \tan^{-1} \frac{s_F}{\sqrt{\omega_g - \zeta_\nu}} - \sqrt{\omega_g + \zeta_\nu} \tan^{-1} \frac{s_F}{\sqrt{\omega_g + \zeta_\nu}} \right. \\ \left. + \sqrt{\omega_\nu - \omega_g} \tanh^{-1} \frac{s_F}{\sqrt{\omega_\nu - \omega_g}} + \sqrt{\omega_g + \omega_\nu} \tan^{-1} \frac{s_F}{\sqrt{\omega_g + \omega_\nu}} \right] \quad (7.229)$$

I added the  $\nu$  on  $\zeta_\nu = \nu \frac{\omega_B}{2}$  to show that it depends on the polarization.

We can suppose as earlier that the upper integration limit can be let to go to infinity. Only the term with  $\omega_\nu \omega_g$  gives any difficulty here. I think the case of most interest is when  $\omega_\nu$  is above the gap (ignoring the damping). That is why I reversed the order in the term. But we know from *Part A* that the limit is

$$\lim_{s_F \rightarrow \infty} \sqrt{\omega_\nu - \omega_g} \tanh^{-1} \frac{s_F}{\sqrt{\omega_\nu - \omega_g}} = -i \sqrt{\omega_\nu - \omega_g} \frac{\pi}{2}. \quad (7.230)$$

On the other hand, if we didn't do this switch, the expression would come out  $\frac{\pi}{2} \sqrt{\omega_g - \omega_\nu}$ , but that is equivalent, regardless of the relative sizes of  $\omega_g$  and  $\omega_\nu$  (one needs some consistent way to choose which square root is being used, however). So there is no absolute need to do this, really. Then I can take the limit  $s_F \rightarrow \infty$  and get the approximate but simple result,

$$I_\nu = \frac{\pi\omega}{2(\omega + i\gamma)} \left[ -\sqrt{\omega_g - \zeta_\nu} - \sqrt{\omega_g + \zeta_\nu} - i\sqrt{\omega_\nu - \omega_g} + \sqrt{\omega_\nu + \omega_g} \right] \quad (7.231)$$

This is very similar to the formula in 3D, however, the powers are 1/2 instead of 3/2. One can write it to highlight the shifts in the gap, in some sense, but these go both directions:

$$I_\nu = \frac{\pi\omega}{2(\omega + i\gamma)} \left[ -\sqrt{\omega_g - \zeta_\nu} - \sqrt{\omega_g + \zeta_\nu} - i\sqrt{(\omega + i\gamma) - (\omega_g - \zeta_\nu)} + \sqrt{(\omega + i\gamma) + (\omega_g + \zeta_\nu)} \right] \quad (7.232)$$

So it is not really possible to say that the Faraday effect simply raises or lowers the gap for each polarization. It does affect the photon frequency oppositely for the two polarizations, but in addition, there are the first two terms that do not involve the photon frequency. This result is different than the result from current averaging!

We can also easily take the limit, additionally, of zero damping, and compare later with a more direct approach to that. As  $\gamma \rightarrow 0$ , we have  $\omega_\nu \rightarrow \omega + \zeta_\nu$ . This gives

$$I_\nu \rightarrow \frac{\pi}{2} \left[ -\sqrt{\omega_g - \zeta_\nu} - \sqrt{\omega_g + \zeta_\nu} - i\sqrt{(\omega + \zeta_\nu) - \omega_g} + \sqrt{(\omega + \zeta_\nu) + \omega_g} \right] \quad (7.233)$$

The third term is the only imaginary part, assuming the excitation is above the gap. It is correct as far as having a negative sign: it gives a positive contribution to  $\chi$  after multiplying by a negative constant. The combination  $\omega + \zeta_\nu$  is just the real Faraday frequency  $\omega_\nu$ . Furthermore, in the limit that  $\omega \rightarrow 0$  now, the whole expression vanishes. So the terms that do not explicitly have the photon present, can be thought of as giving this zero normalization at zero frequency (together with  $\gamma = 0$ ).

### 7.11.1 About $\tan^{-1}$ and $\tanh^{-1}$ at complex arguments.

I saw above some confusion when the argument inside these functions changes from real to imaginary. This is a short section to clarify some math. Note the factor we had above that started out with  $\sqrt{\omega_g - \omega_\nu}$ . It is perfectly fine, however, the more physical limit will be when  $\omega_\nu > \omega_g$ , so it does make sense to reverse inside the square root. This produces:

$$\tan^{-1} \frac{s}{\sqrt{\omega_g - \omega_\nu}} = \tan^{-1} \frac{s}{i\sqrt{\omega_\nu - \omega_g}} = \tan^{-1} \frac{-is}{\sqrt{\omega_\nu - \omega_g}}. \quad (7.234)$$

Now look at the function  $\tanh ix$ . We have

$$\tanh ix = \frac{\sinh ix}{\cosh ix} = \frac{e^{ix} - e^{-ix}}{e^{ix} + e^{-ix}} = \frac{i \sin x}{\cos x} = i \tan x. \quad (7.235)$$

Now consider the inverse tangent:

$$y = \tan x \Rightarrow x = \tan^{-1} y. \quad (7.236)$$

Alternatively,

$$y = \tan x = -i \tanh ix \Rightarrow iy = \tanh ix \Rightarrow ix = \tanh^{-1} iy = i \tan^{-1} y. \quad (7.237)$$

So both  $\tanh$  and  $\tanh^{-1}$  of an imaginary argument give  $i$  times the circular function.

$$\tanh ix = i \tan x, \quad \tanh^{-1} ix = i \tan^{-1} x. \quad (7.238)$$

Instead, change  $x \rightarrow ix$  to go the other direction, using the oddness of these functions:

$$\tan ix = i \tanh x, \quad \tan^{-1} ix = i \tanh^{-1} x. \quad (7.239)$$

Applying this to the term in  $I_\nu$ , this gives

$$\sqrt{\omega_g - \omega_\nu} \tan^{-1} \frac{s}{\sqrt{\omega_g - \omega_\nu}} = i \sqrt{\omega_\nu - \omega_g} \tan^{-1} \frac{-is}{\sqrt{\omega_\nu - \omega_g}} = \sqrt{\omega_\nu - \omega_g} \tanh^{-1} \frac{s}{\sqrt{\omega_\nu - \omega_g}}. \quad (7.240)$$

Unfortunately, this seems to hide that the limit at large argument is imaginary. Indeed, the difficulty is that  $\tanh x \leq 1$ . So this is undefined at large argument, while the  $\tan^{-1}$  does not have this difficulty at large argument. Instead, need to transform to an expression with  $\coth^{-1} x$ .

Actually, most of what I needed now appears at the end of *Part A*, concerning the real and imaginary parts of the complex functions  $\tan^{-1}$  and  $\tanh^{-1}$ .

## 7.12 Finding $S_\nu$ , 1D bands, limit of zero damping, polarization averaging

Again we want to apply the zero damping limit for the case of polarization averaged expressions. This can be applied only under the approximation of no thermal factor,  $w_i - w_f = 1$ , in the expression for the  $S_\nu$  integral, (7.162). We use again the SW theorem before integration,

$$\lim_{\gamma \rightarrow 0^+} \frac{1}{x + i\gamma} = \text{p.v.} \left( \frac{1}{x} \right) - i\pi\delta(x) \quad (7.241)$$

Applied to the second term in the integrand for  $K_1$ , (7.163), for the 1D bands model, it gives

$$\frac{1}{\omega + i\gamma - \omega_g - s^2 + \zeta_\nu} \rightarrow \text{p.v.} \left( \frac{1}{\omega - \omega_g - s^2 + \zeta_\nu} \right) - i\pi\delta(\omega - \omega_g - s^2 + \zeta_\nu), \quad (7.242)$$

whereas, on the second term in the integrand for  $K_2$ , the effect is

$$\frac{1}{\omega + i\gamma + \omega_g + s^2 + \zeta_\nu} \rightarrow \text{p.v.} \left( \frac{1}{\omega + \omega_g + s^2 + \zeta_\nu} \right) - i\pi\delta(\omega + \omega_g + s^2 + \zeta_\nu), \quad (7.243)$$

There is also an additional factor of  $s^2$  in the integrand, and the sum over  $m_i, m_f$  produces the multiplicity factor  $g_m$  that goes to the constants. As mentioned,  $w_i - w_f$  is set to 1. There is also the factor of  $-\omega s^2$  and the reciprocals of  $(-\omega_g - s^2 \pm \zeta_\nu)$ .

### 7.12.1 The imaginary parts – delta functions.

The imaginary part of  $K_1$  and  $K_2$  comes from using the delta functions. These can be combined into the imaginary part of  $I_\nu = K_1 + K_2$ . For  $K_1$  this is

$$\text{Im} \{K_1\} = (-i\pi)(\omega) \int_0^{s_F} ds \frac{-s^2}{-\omega_g - s^2 + \zeta_\nu} \delta(\omega - \omega_g - s^2 + \zeta_\nu) \quad (7.244)$$

Using the variable  $x = \omega_g + s^2$ , and  $dx = 2s ds$ , this is converted to an integral that selects only the Faraday point,  $x = \omega + \zeta_\nu = \omega_\nu$ . Note that this requires the assumption that  $\omega_\nu > \omega_g$ , otherwise, this integral will be zero:

$$\text{Im} \{K_1\} = i\pi\omega \int_{\omega_g}^{x_F} \frac{1}{2} dx \frac{\sqrt{x - \omega_g}}{-x + \zeta_\nu} \delta(\omega - x + \zeta_\nu) = -i\frac{\pi}{2} g_m \sqrt{\omega_\nu - \omega_g} \quad (7.245)$$

For the  $K_2$  integral we have something similar,

$$\text{Im} \{K_2\} = (-i\pi)(\omega) \int_0^{s_F} ds \frac{-s^2}{-\omega_g - s^2 - \zeta_\nu} \delta(\omega + \omega_g + s^2 + \zeta_\nu) \quad (7.246)$$

Then converted to integration over  $x$ , the delta selects the negative Faraday frequency,  $x = -\omega - \zeta = -\omega_\nu$ . But that point is outside the range of integration, so the integral is zero:

$$\text{Im} \{K_2\} = -i\pi\omega \int_{\omega_g}^{x_F} \frac{1}{2} dx \frac{\sqrt{x - \omega_g}}{x + \zeta_\nu} \delta(\omega + x + \zeta_\nu) = 0. \quad (7.247)$$

Therefore the combination gives for R or L polarizations, a very simple result,

$$\text{Im} \{I_{R|L}\} = -i\frac{\pi}{2} \sqrt{\omega_{R|L} - \omega_g}. \quad (7.248)$$

Note, the sign is correct. This is multiplied by a negative constant to get the contribution to susceptibility. This applies only when  $\omega_{R|L} > \omega_g$ , above the gap excitation. If the excitation is below the gap,  $\omega_{R|L} < \omega_g$ , there is no imaginary part to  $I_{R|L}$ . This is equal to the result in the previous section, in the limit of zero damping, good!

### 7.12.2 The real parts – principal valued integral.

Now do the calculation of the principal valued integral from  $K_1$ . We need

$$\text{Re} \{K_1\} = \omega \text{ p.v.} \int_0^{s_F} ds \frac{-s^2}{(-\omega_g - s^2 + \zeta_\nu)(\omega - \omega_g - s^2 + \zeta_\nu)} \quad (7.249)$$

This involves the combination  $\omega_G \equiv \omega_g - \zeta_\nu$ , so it can be slightly changed to

$$\text{Re} \{K_1\} = \omega \text{ p.v.} \int_0^{s_F} ds \frac{s^2}{(\omega_G + s^2)(\omega - \omega_G - s^2)} \quad (7.250)$$

The usual partial fraction expansion will help,

$$\frac{1}{(\omega_G + s^2)(\omega - \omega_G - s^2)} = \frac{1}{\omega} \left[ \frac{1}{\omega_G + s^2} + \frac{1}{\omega - \omega_G - s^2} \right] \quad (7.251)$$

Further, this gets multiplied by  $s^2$  so just do the following as well before integrating:

$$\frac{s^2}{\omega_G + s^2} = \frac{\omega_G + s^2 - \omega_G}{\omega_G + s^2} = 1 - \frac{\omega_G}{\omega_G + s^2}. \quad (7.252)$$

$$\frac{s^2}{\omega - \omega_G - s^2} = \frac{-\omega + \omega_G + s^2 + \omega - \omega_G}{\omega - \omega_G - s^2} = -1 + \frac{\omega - \omega_G}{\omega - \omega_G - s^2}. \quad (7.253)$$

This gives the partial fraction expansion of the whole integrand as

$$\frac{s^2}{(\omega_G + s^2)(\omega - \omega_G - s^2)} = \frac{1}{\omega} \left[ \frac{-\omega_G}{\omega_G + s^2} + \frac{\omega - \omega_G}{\omega - \omega_G - s^2} \right]. \quad (7.254)$$

We are assuming above gap excitation,  $\omega - \omega_G > 0$ . Now the integral is

$$\text{Re} \{K_1\} = \text{p.v.} \int_0^{s_F} ds \left[ \frac{-\omega_G}{\omega_G + s^2} + \frac{\omega - \omega_G}{\omega - \omega_G - s^2} \right] \quad (7.255)$$

The first part has no singularity and p.v. is not needed there—it gives an inverse tangent.

$$\int_0^{s_F} ds \frac{-\omega_G}{\omega_G + s^2} = -\sqrt{\omega_G} \tan^{-1} \frac{s_F}{\sqrt{\omega_G}}. \quad (7.256)$$

The second term has a singularity at  $s_1 = \sqrt{\omega - \omega_G}$ , assumed to be on the real axis with  $\omega > \omega_G$ . Recall how this was done in *Dielectrics, Part A*. Setting  $a^2 = \omega - \omega_G$ , we can use the indefinite integral

$$\int ds \frac{a^2}{a^2 - s^2} = \frac{a}{2} \int ds \left( \frac{1}{s+a} - \frac{1}{s-a} \right) = \frac{a}{2} \ln \left[ \frac{s+a}{s-a} \right] = \begin{cases} a \tanh^{-1} \frac{s}{a} & \text{for } s < a, \\ a \coth^{-1} \frac{s}{a} & \text{for } s > a. \end{cases} \quad (7.257)$$

I have it in terms of inverse hyperbolic functions, but the log is easier to think about. But we saw in *Part A* that the singular point is just passed right through, and we need only the result at the upper limit. Check how that worked. Note that if the upper limit  $s_F < a$ , then no p.v. is needed, and the integral is

$$\int_0^{s_F} ds \frac{a^2}{a^2 - s^2} = \frac{a}{2} \left\{ \ln \left[ \frac{s_F + a}{s_F - a} \right] - \ln \left[ \frac{0 + a}{0 - a} \right] \right\} = \frac{a}{2} \ln \left[ \frac{a + s_F}{a - s_F} \right]. \quad (7.258)$$

On the other hand, when  $s_F > a$  we pass through the singular point and the p.v. is done as follows:

$$\text{p.v.} \int_0^{s_F} ds \frac{a^2}{a^2 - s^2} = \lim_{\varepsilon \rightarrow 0} \left\{ \int_0^{a-\varepsilon} + \int_{a+\varepsilon}^{s_F} \right\} \quad (7.259)$$

Then inserting the limits, we get for  $s_F > a$ ,

$$\begin{aligned} \text{p.v.} &= \frac{a}{2} \left\{ -\ln \left[ \frac{0+a}{0-a} \right] + \ln \left[ \frac{a-\varepsilon+a}{a-\varepsilon-a} \right] - \ln \left[ \frac{a+\varepsilon+a}{a+\varepsilon-a} \right] + \ln \left[ \frac{s_F+a}{s_F-a} \right] \right\} \\ &= \frac{a}{2} \left\{ +\ln \left[ -1 \times \frac{2a-\varepsilon}{-\varepsilon} \frac{\varepsilon}{2a+\varepsilon} \right] + \ln \left[ \frac{s_F+a}{s_F-a} \right] \right\} \rightarrow \frac{a}{2} \ln \left[ \frac{s_F+a}{s_F-a} \right]. \end{aligned} \quad (7.260)$$

One sees that the two cases are equivalent if always the absolute value is used within the log. Inserting the value  $a = \sqrt{\omega - \omega_G}$  with  $\omega > \omega_G$  assumed, this gives for either  $s_F < a$  or  $s_F > a$ ,

$$\text{p.v.} \int_0^{s_F} ds \frac{a^2}{a^2 - s^2} = \frac{1}{2} \sqrt{\omega - \omega_G} \ln \left| \frac{s_F + \sqrt{\omega - \omega_G}}{s_F - \sqrt{\omega - \omega_G}} \right|. \quad (7.261)$$

Then combining the results, we have for the total principal valued integral,

$$\text{Re} \{K_1\} = \left[ -\sqrt{\omega_G} \tan^{-1} \frac{s_F}{\sqrt{\omega_G}} + \frac{1}{2} \sqrt{\omega - \omega_G} \ln \left| \frac{s_F + \sqrt{\omega - \omega_G}}{s_F - \sqrt{\omega - \omega_G}} \right| \right]. \quad (7.262)$$

Inserting the value  $\omega_G = \omega_g - \zeta_\nu$ , this is

$$\text{Re} \{K_1\} = \left[ -\sqrt{\omega_g - \zeta_\nu} \tan^{-1} \frac{s_F}{\sqrt{\omega_g - \zeta_\nu}} + \sqrt{\omega_\nu - \omega_g} \ln \left| \frac{s_F + \sqrt{\omega_\nu - \omega_g}}{s_F - \sqrt{\omega_\nu - \omega_g}} \right| \right], \quad (7.263)$$

where  $\omega_\nu = \omega + \zeta_\nu$  was used.

Next for the  $K_2$  principal valued integral, there is

$$\text{Re} \{K_2\} = \omega \text{ p.v.} \int_0^{s_F} ds \frac{-s^2}{(-\omega_g - s^2 - \zeta_\nu)(\omega + \omega_g + s^2 + \zeta_\nu)}. \quad (7.264)$$

In this case, the gap shifted frequency is  $\omega_G = \omega_g + \zeta_\nu$ . The integral looks like

$$\text{Re} \{K_2\} = \omega \text{ p.v.} \int_0^{s_F} ds \frac{s^2}{(\omega_G + s^2)(\omega + \omega_G + s^2)}. \quad (7.265)$$

This is nearly the same as the  $K_1$  integral, but in the second term instead of  $\omega - \omega_G$  there is  $\omega + \omega_G$ . But there is nothing singular here and no p.v. is needed! The partial fractions gives:

$$\frac{s^2}{(\omega_G + s^2)(\omega + \omega_G + s^2)} = \frac{1}{\omega} \left[ \frac{-\omega_G}{\omega_G + s^2} + \frac{\omega + \omega_G}{\omega + \omega_G + s^2} \right]. \quad (7.266)$$

Then here both integrations just give inverse tangents directly, and the non-p.v. integral is

$$\text{Re}\{K_2\} = \left[ -\sqrt{\omega_G} \tan^{-1} \frac{s_F}{\sqrt{\omega_G}} + \sqrt{\omega + \omega_G} \tan^{-1} \frac{s_F}{\sqrt{\omega + \omega_G}} \right]. \quad (7.267)$$

Then inserting the new value of  $\omega_G = \omega_g + \zeta_\nu$  gives

$$\text{Re}\{K_2\} = \left[ -\sqrt{\omega_g + \zeta_\nu} \tan^{-1} \frac{s_F}{\sqrt{\omega_g + \zeta_\nu}} + \sqrt{\omega_\nu + \omega_g} \tan^{-1} \frac{s_F}{\sqrt{\omega_\nu + \omega_g}} \right]. \quad (7.268)$$

Then finally the results get combined to get the real part of  $I_\nu$ :

$$\text{Re}\{I_\nu\} = \left\{ -\sqrt{\omega_g - \zeta_\nu} \tan^{-1} \frac{s_F}{\sqrt{\omega_g - \zeta_\nu}} - \sqrt{\omega_g + \zeta_\nu} \tan^{-1} \frac{s_F}{\sqrt{\omega_g + \zeta_\nu}} \right. \quad (7.269)$$

$$\left. + \sqrt{\omega_\nu - \omega_g} \ln \left| \frac{s_F + \sqrt{\omega_\nu - \omega_g}}{s_F - \sqrt{\omega_\nu - \omega_g}} \right| + \sqrt{\omega_\nu + \omega_g} \tan^{-1} \frac{s_F}{\sqrt{\omega_\nu + \omega_g}} \right\} \quad (7.270)$$

Also there is the presence of the Faraday shifted frequency here. This is nearly the same as the  $\gamma \rightarrow 0$  limit of an expression found earlier for this problem. The only difference is in the log term. However, those two terms are probably the same, when calculated more carefully, taking into account all the possibilities of the real and imaginary parts for the previous result.

### 7.12.3 Total $I_\nu$ at zero damping and $s_F \rightarrow \infty$ limit.

So we have obtained the following for the 1D bands model from polarization averaging, in the limit of zero damping:

$$\begin{aligned} I_\nu = & -\sqrt{\omega_g - \zeta_\nu} \tan^{-1} \frac{s_F}{\sqrt{\omega_g - \zeta_\nu}} - \sqrt{\omega_g + \zeta_\nu} \tan^{-1} \frac{s_F}{\sqrt{\omega_g + \zeta_\nu}} \quad (7.271) \\ & + \sqrt{\omega_\nu - \omega_g} \ln \left| \frac{s_F + \sqrt{\omega_\nu - \omega_g}}{s_F - \sqrt{\omega_\nu - \omega_g}} \right| + \sqrt{\omega_\nu + \omega_g} \tan^{-1} \frac{s_F}{\sqrt{\omega_\nu + \omega_g}} - i \frac{\pi}{2} \sqrt{\omega_\nu - \omega_g}. \end{aligned}$$

Then when the limit  $s_F \rightarrow \infty$  is done, the result simplifies, as all the  $\tan^{-1} \rightarrow \pi/2$ , the  $\ln \rightarrow 0$ ,

$$I_\nu = \frac{\pi}{2} \left[ \sqrt{\omega_\nu + \omega_g} - \sqrt{\omega_g - \zeta_\nu} - \sqrt{\omega_g + \zeta_\nu} - i \sqrt{\omega_\nu - \omega_g} \right]. \quad (7.272)$$

That is identical to what was derived from the more general calculation in a previous section, which is very good. The last part could become real, however, for below the gap excitation. In that case, it would imply no absorption, as there would be no imaginary part in the permittivity.

In comparing to the expression (7.210) from current averaging, the only difference is the presence of the magnetic frequency and polarization factor ( $\zeta_\nu$ ) in the constant terms involving the gap, but not the photon. These are somewhat strange terms. This will not make much difference between current averaging and polarization averaging at usual optical frequencies. Significant differences are present only as the frequency goes towards zero.

Summarized, the contribution to the susceptibility comes from dimensionless  $S_\nu$  as normalized in (7.159) and (7.162),

$$S_\nu = \frac{4|M|^2 \hbar V k_F^2}{m_e (\pi)^3} \left( \frac{2\tilde{m}}{\hbar} \right)^{3/2} \times I_\nu. \quad (7.273)$$

Then this gives the actual interband transitions contribution to  $\chi$  according to

$$\chi_\nu = \frac{-ne^2}{m_e \omega (\omega + i\gamma)} S_\nu. \quad (7.274)$$

Also can point out that it is easy to put the damping back into the expression for  $I_\nu$ . The factor  $i\gamma$  adds linearly into  $\omega_{nu}$ , without really affecting  $\omega_g$ . Also, one can re-install the prefactor  $\omega/(\omega + i\gamma)$  on the whole expression, which became 1 in the zero damping limit.

#### 7.12.4 Faraday effect from 1D band model – polarization averaging

We know the small changes in electric susceptibility with magnetic field lead to the Faraday rotation. Let me expand the integral  $I_\nu$  (or equivalently,  $I_R$  and  $I_L$ ) in the limit of a weak applied magnetic field. Do this using the electric polarization averaging expressions without damping. This has some extra terms due to the gap plus/minus zeta parts:

$$\begin{aligned}
 I_\nu &= \frac{\pi}{2} \left\{ \sqrt{\omega + \omega_g} \left[ 1 + \frac{\nu}{2} \frac{\omega_B}{\omega + \omega_g} \right]^{1/2} - i \sqrt{\omega - \omega_g} \left[ 1 + \frac{\nu}{2} \frac{\omega_B}{\omega - \omega_g} \right]^{1/2} \right. \\
 &\quad \left. - \sqrt{\omega_g} \left( 1 - \frac{\nu}{2\omega_g} \omega_B \right)^{1/2} - \sqrt{\omega_g} \left( 1 + \frac{\nu}{2\omega_g} \omega_B \right)^{1/2} \right\} \\
 &\approx \frac{\pi}{2} \left\{ \sqrt{\omega + \omega_g} - 2\sqrt{\omega_g} - i \sqrt{\omega - \omega_g} + \frac{\nu\omega_B}{4} \left[ \frac{1}{\sqrt{\omega + \omega_g}} - \frac{i}{\sqrt{\omega - \omega_g}} \right] \right\} \quad (7.275)
 \end{aligned}$$

However, those extra terms cancel out in linear order in  $B$ , which is all we usually need. So the Faraday rotation results will be the same as in the calculation from averaging of the current density, as found earlier. Of course, keep in mind that these are only very approximate results. It will be best to keep the damping parameter  $\gamma > 0$  and especially important to include the thermal population factor, which requires the full integrals be done with  $\sum_{m_f} g_{m_f}(x)$  present.