Quantum Theory for Dielectric Properties of Conductors
B. Magnetic Fields and Landau Levels

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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 this Part, 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 Part C, 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 phenomenolgical 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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Contents

3 Dielectrics in a DC Magnetic Field

Here is the main topic why I am interested in dielectric response: I want to understand what happens in the presence of a constant magnetic field, in addition to the optical field, because many interesting and curious effects then take place. Classically, the electrons tend to move in circular cyclotron orbits. But in the combination of the DC magnetic field and the AC fields of light, there is a competition, especially if the light is circularly polarized. So I want to get an accurate QM theory of the dielectric function, $\epsilon(\omega)$ for this situation. It will be important for describing mainly, the Faraday rotation. It should provide input into describing FR in small metallic and magnetic particles in composites.

3.1 Classical electron motion in a DC magnetic field

For simplicity consider the case where an EM wave is incident on electrons in a metal. The electrons are assumed to be damped (parameter γ) and bound by some local harmonic potential (spring constant $m_e\omega_0^2$). The DC magnetic field, denoted by $\bar{\mathbf{B}}$ to distinguish it from the field in the EM waves, points in the same direction (along $\hat{z}$) as the waves are propagating. This is the situation that leads to Faraday rotation. Assume the usual $e^{-i\omega t}$ time dependencies for the optical field. The transverse EM waves have x and y components. We concentrate primarily on the motion of an electron in the xy plane. The electron position is $\mathbf{r} = (x(t), y(t))$. Its equation of motion is

$$m_e\ddot{\mathbf{r}} = e\mathbf{E} + \frac{e}{c}\dot{\mathbf{r}}\times\bar{\mathbf{B}} - m_e\omega_0^2\mathbf{r} - m_e\gamma\dot{\mathbf{r}}, \quad \text{or} \quad -m_e\omega^2\mathbf{r} = e\mathbf{E} + \frac{-i\omega e}{c}\mathbf{r}\times\bar{\mathbf{B}} - m_e\omega_0^2\mathbf{r} + m_e\gamma i\omega\mathbf{r}. \tag{3.1}$$

The force of the optical magnetic field on the electron can be ignored in a first approximation. It is convenient to re-arrange so that the applied $\mathbf{E}$ is the source on the RHS,

$$\left[m_e(\omega_0^2 - \omega^2 - i\omega\gamma) - \frac{i\omega e}{c}\bar{\mathbf{B}}\times\right]\mathbf{r} = e\mathbf{E} \tag{3.2}$$

In terms of components, this simple situation gives a matrix eigenvalue problem. That a matrix is helpful can be seen because of the presence of the cross product operator with $\bar{\mathbf{B}}$. Note that the magnetic field has only a z-component, $\mathbf{B} = B\hat{z}$. Then by components, there is

$$\begin{array}{ll} \text{along } \hat{x}: & m_e(\omega_0^2 - \omega^2 - i\omega\gamma)x + i\omega\frac{eB}{c}y = eE_x \\ \text{along } \hat{y}: & m_e(\omega_0^2 - \omega^2 - i\omega\gamma)y - i\omega\frac{eB}{c}x = eE_x \end{array} \tag{3.3}$$

Put this into a more usual matrix form:

$$\begin{bmatrix} m_e(\omega_0^2 - \omega^2 - i\omega\gamma) & i\omega\frac{eB}{c} \\ -i\omega\frac{eB}{c} & m_e(\omega_0^2 - \omega^2 - i\omega\gamma) \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} eE_x \\ eE_y \end{bmatrix} \tag{3.4}$$

Now, so far it is just mathematics. We could grind along and solve for the position by inverting the square matrix on the LHS. While that would work for any source field (E_x, E_y), it is not very enlightening. It is more interesting to suppose that the applied field is arranged in such a way that it is an eigenvector of that square matrix. If that were the case, the solution for the position is trivial. Eventually, knowledge of $\mathbf{r}(t)$ will give the electric polarization and hence the dielectric function.

Before doing that, do note one thing, the appearance of the classical cyclotron frequency,

$$\omega_B = \frac{eB}{m_e c} \tag{3.5}$$

With that, it is convenient to rewrite the matrix relationship as

$$\begin{bmatrix} (\omega_0^2 - \omega^2 - i\omega\gamma) & i\omega\omega_B \\ -i\omega\omega_B & (\omega_0^2 - \omega^2 - i\omega\gamma) \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} \frac{e}{m_e}E_x \\ \frac{e}{m_e}E_y \end{bmatrix} \tag{3.6}$$

The matrix M on the LHS contains only different frequencies; the source on the RHS is scaled with the charge to mass ratio of the electron.

Look for the eigenspectrum of the matrix on the LHS, call it M. Denote the factors on the diagonal as $D = \omega_0^2 - \omega^2 - i\omega\gamma$. Look for eigenvectors $\mathbf{u}$ of

$$M\cdot\mathbf{u} = \lambda\mathbf{u}, \qquad M = \begin{bmatrix} D & i\omega\omega_B \\ -i\omega\omega_B & D \end{bmatrix}. \tag{3.7}$$

The determinant needed is

$$\det(M - \lambda\mathbf{I}) = (D-\lambda)^2 - (-i\omega\omega_B)(i\omega\omega_B) = (D-\lambda)^2 - \omega^2\omega_B^2 = 0. \tag{3.8}$$

The eigenvalues come out trivially,

$$\lambda_1 = D + \omega\omega_B, \qquad \lambda_2 = D - \omega\omega_B. \tag{3.9}$$

For the first eigenvalue, the components of its eigenvector are found from,

$$(D-\lambda_1)u_x + i\omega\omega_B u_y = 0, \quad \text{or } -u_x + iu_y = 0, \Longrightarrow u_y = -iu_x \tag{3.10}$$

For the second eigenvalue, the components of its eigenvector are found from,

$$(D-\lambda_2)u_x + i\omega\omega_B u_y = 0, \quad \text{or } u_x + iu_y = 0, \Longrightarrow u_y = iu_x \tag{3.11}$$

Therefore the normalized eigenspectrum is summarized:

$$\begin{array}{llll} \hat{u}_1 = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{y}), & \lambda_1 = D + \omega\omega_B, & \hat{u}_1^* \cdot \hat{u}_1 = 1, & \hat{u}_2^* \cdot \hat{u}_1 = 0, \\ \hat{u}_2 = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{y}), & \lambda_1 = D - \omega\omega_B, & \hat{u}_2^* \cdot \hat{u}_2 = 1, & \hat{u}_1^* \cdot \hat{u}_2 = 0. \end{array} \tag{3.12}$$

We are solving the matrix equation,

$$M \cdot \mathbf{r} = \frac{e}{m_e}\mathbf{E}. \tag{3.13}$$

But what is the source field $\mathbf{E}$ is already known in terms of its eigenvector components, that is, we have the expansion,

$$\mathbf{E} = E_1\hat{u}_1 + E_2\hat{u}_2, \qquad \text{where } \; E_1 = \hat{u}_1^* \cdot \mathbf{E}, \;\; E_2 = \hat{u}_2^* \cdot \mathbf{E}. \tag{3.14}$$

Then the solution $\mathbf{r}$ also could be expanded in the eigenvectors the same way, like $\mathbf{r} = r_1\hat{u}_1 + r_2\hat{u}_2$. The orthogonality of the two eigenvectors leads to some trivial dynamics solution:

$$\begin{array}{l} M \cdot (r_1\hat{u}_1 + r_2\hat{u}_2) = (\lambda_1 r_1\hat{u}_1 + \lambda_2 r_2\hat{u}_2) = \frac{e}{m}(E_1\hat{u}_1 + E_2\hat{u}_2) \\ r_1 = eE_1/m_e\lambda_1, \qquad r_2 = eE_2/m_e\lambda_2. \end{array} \tag{3.15}$$

The solution is essentially separated. Let write it out as if the original EM waves were specified by their x and y components. Then we have

$$E_1 = \hat{u}_1^* \cdot \mathbf{E} = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{y})^* \cdot (E_x\hat{x} + E_y\hat{y}) = \frac{1}{\sqrt{2}}(E_x + iE_y) \tag{3.16}$$

$$E_2 = \hat{u}_2^* \cdot \mathbf{E} = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{y})^* \cdot (E_x\hat{x} + E_y\hat{y}) = \frac{1}{\sqrt{2}}(E_x - iE_y) \tag{3.17}$$

It means we are expressing the field as this combination, which obviously works out:

$$\mathbf{E} = E_1\hat{u}_1 + E_2\hat{u}_2 = \frac{1}{\sqrt{2}}(E_x + iE_y) \cdot \frac{1}{\sqrt{2}}(\hat{x} - i\hat{y}) + \frac{1}{\sqrt{2}}(E_x - iE_y) \cdot \frac{1}{\sqrt{2}}(\hat{x} + i\hat{y}) \tag{3.18}$$

Then the corresponding position of the electron is doing the following:

$$\begin{aligned} \mathbf{r} &= \frac{eE_1}{m_e\lambda_1}\hat{u}_1 + \frac{eE_2}{m_e\lambda_2}\hat{u}_2 \\ &= \frac{e/m_e}{D + \omega\omega_B}\frac{1}{\sqrt{2}}(E_x + iE_y)\frac{1}{\sqrt{2}}(\hat{x} - i\hat{y}) + \frac{e/m_e}{D - \omega\omega_B}\frac{1}{\sqrt{2}}(E_x - iE_y)\frac{1}{\sqrt{2}}(\hat{x} + i\hat{y}) \end{aligned} \tag{3.19}$$

It's a mess because going back to the Cartesian coordinates isn't really natural for the problem, the eigen vectors make more sense and simplicity, that's what they are there for. Nevertheless, look at its Cartesian components, if you like:

$$x(t) = \frac{e}{2m_e}\left[\frac{E_x + iE_y}{D + \omega\omega_B} + \frac{E_x - iE_y}{D - \omega\omega_B}\right] = \frac{e}{2m_e}\left[\frac{(E_x + iE_y)(D - \omega\omega_B) + (E_x - iE_y)(D + \omega\omega_B)}{D^2 - \omega^2\omega_B^2}\right] \tag{3.20}$$

Finally it simplifies to

$$x(t) = \frac{e}{m_e}\left(\frac{DE_x - i\omega\omega_B E_y}{D^2 - \omega^2\omega_B^2}\right) \tag{3.21}$$

Similarly for the y component,

$$y(t) = \frac{ie}{2m_e}\left[\frac{-(E_x + iE_y)}{D + \omega\omega_B} + \frac{E_x - iE_y}{D - \omega\omega_B}\right] = \frac{ie}{2m_e}\left[\frac{-(E_x + iE_y)(D - \omega\omega_B) + (E_x - iE_y)(D + \omega\omega_B)}{D^2 - \omega^2\omega_B^2}\right] \tag{3.22}$$

This simplifies to

$$y(t) = \frac{e}{m_e}\left(\frac{i\omega\omega_B E_x + DE_y}{D^2 - \omega^2\omega_B^2}\right) \tag{3.23}$$

But these last expressions really aren't totally enlightening. Yes they tell you the motion. No, they don't give much insight. However, these do show that the induced dipole moment $\mathbf{d} = e\mathbf{r}$ is not parallel to the applied field, instead, the relation involves a matrix:

$$\mathbf{d} = e\mathbf{r} = e\begin{bmatrix} x(t) \\ y(t) \end{bmatrix} = \frac{e^2}{m_e(D^2 - \omega^2\omega_B^2)}\begin{bmatrix} D & -i\omega\omega_B \\ i\omega\omega_B & D \end{bmatrix} \cdot \begin{bmatrix} E_x \\ E_y \end{bmatrix} \tag{3.24}$$

The 2x2 array (along with pre-factors) is the microscopic polarizability for one electron, $\mathbf{d}/\mathbf{E}$, so in fact, this calculation does show how that matrix relation arises. Note that the terms on the diagonal are the same, and the off-diagnonal terms are not complex conjugate of each other, but they are of opposite signs. When the DC magnetic field is zero, the matrix returns to diagonal form, and becomes equivalent to a scalar. Further, the response gets large if the optical frequency ω matches the cyclotron frequency ω_B, especially in the limit of no damping and no binding ($\omega_0 = 0$).

IF the applid field, however, only had one of the eigen components present, say, the $\hat{u}_1$ comonent, then the solution is very simple: the solution for $\mathbf{r}$ is directly proportional to that applied field component E_1. It would imply a separate polarizability for the two different eigen solutions. These solutions are present only when the applied field is rotating, as in a wave of circular polarization. See this as follows. Look at the Cartesian components in time. For the λ_1 solution, the space and time dependent field is

$$\mathbf{E}(\mathbf{r}, t) = \mathrm{Re}\left\{\frac{E_0}{\sqrt{2}}(\hat{x} - i\hat{y})e^{i(kz - \omega t)}\right\} = \frac{E_0}{\sqrt{2}}\left[\hat{x}\cos(kz - \omega t) + \hat{y}\sin(kz - \omega t)\right] \tag{3.25}$$

When viewed looking back towards the source of these waves, at a fixed point in space, the electric vector rotates clockwise with time. If you point your right thumb towards the source, your right hand fingers curl the same way as $\mathbf{E}$ is rotating, which is why it is called a wave with **right circular polarization**. However, its angular momentum points opposite to its wave vector. So it has negative helicity, $h = \hat{k} \cdot \hat{L} = -1$. Also, if you point your right thumb along $\hat{k}$, your right-hand fingers curl in the sense that $\mathbf{E}$ does through space, at fixed tme. The amount of induced electric dipole for this wave is

$$d_1 = er_1 = \frac{e^2}{m_e\lambda_1}E_1 = \frac{e^2/m_e}{D + \omega\omega_B}E_1. \tag{3.26}$$

This means the microscopic polarizability for right circular polarization is

$$\alpha_1 \longrightarrow \alpha_R = \frac{e^2/m_e}{D + \omega\omega_B} \tag{3.27}$$

I use an R subscript to indicate that it applies only to right circular polarization. Note that in the limit of zero binding (free electrons, $\omega_0 = 0$), the parameter D becomes

$$D = -\omega(\omega + i\gamma) \tag{3.28}$$

Then the corresponding result for this polarizability is

$$\alpha_R = -\frac{e^2/m_e}{\omega(\omega + i\gamma - \omega_B)} \tag{3.29}$$

The negative sign shows that the induced electric dipoles are opposite to the applied field, no matter what the sign of the charges e. There may be a phase shift, however, due to the presence of the complex term with γ. The behavior of α_R with frequency is shown in Fig. 1.

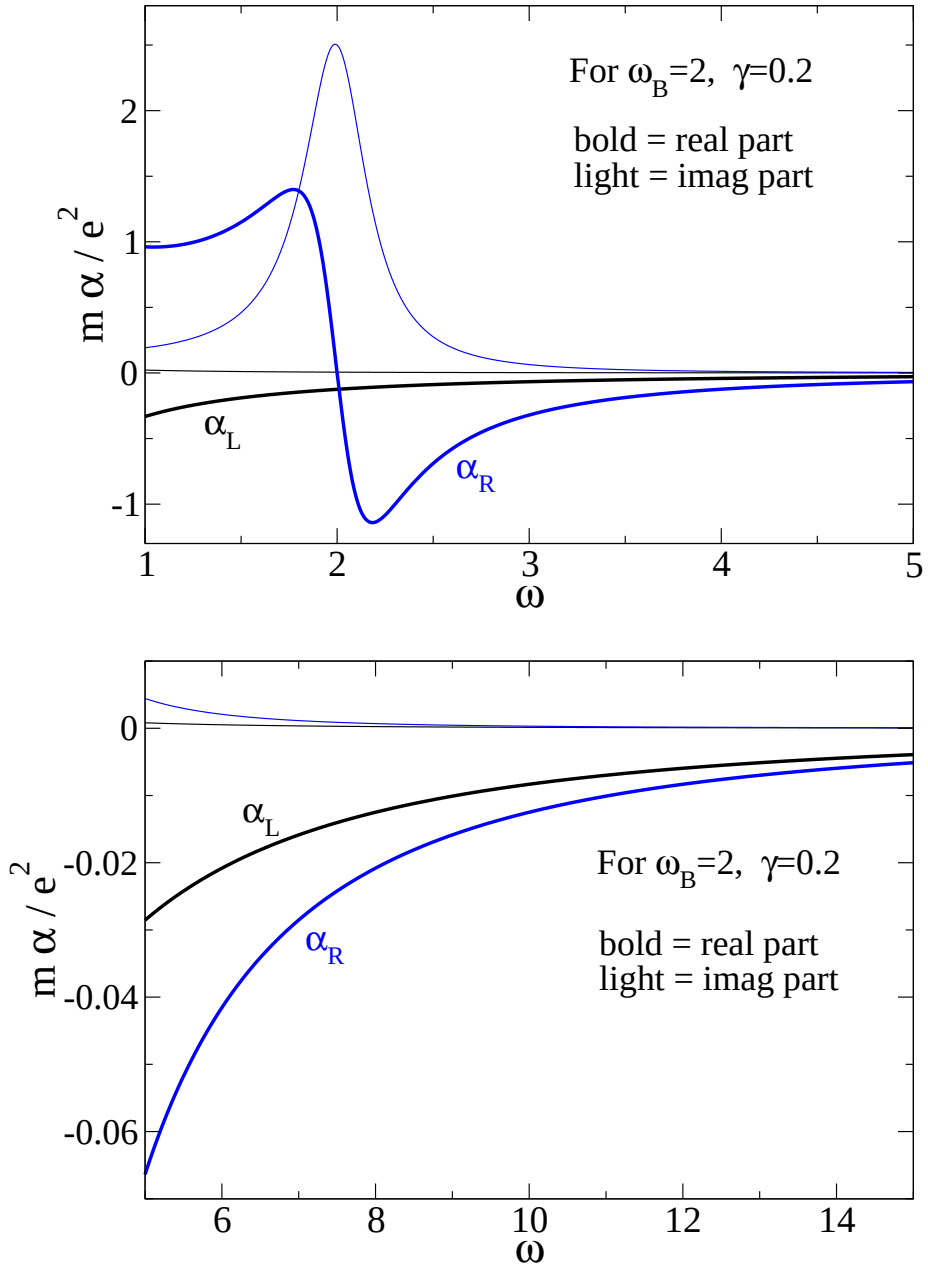

Figure 1: The microscopic polarizabilities versus frequency, showing the differences that might be expected for the two circular polarizations. The real parts are bold curves, the imaginary parts are the finer curves. The magnetic frequency $\omega_B = 2$ is set at a very large value so that the differences can be enhanced. The damping parameter is $\gamma = 0.2$. Note that the polarizability for right circular polarization is affected the most.

On the other hand, the other eigensolution corresponds to circular motion in the opposite direction, because it gives

$$\mathbf{E}(\mathbf{r},t) = \mathrm{Re}\left\{\frac{E_0}{\sqrt{2}}(\hat{x}+i\hat{y})e^{i(kz-\omega t)}\right\} = \frac{E_0}{\sqrt{2}}\left[\hat{x}\cos(kz-\omega t) - \hat{y}\sin(kz-\omega t)\right] \tag{3.30}$$

Now you can point your left thumb back towards the source, then your left hand fingers curl in the sense that **E** rotates with time at a fixed point in space. This wave has **left circular polarization**, and its angular momentum is parallel to its wave vector, hence the helicity is positive, $h = \hat{k}\cdot\hat{L} = +1$. By analogy, the microscopic polarizability is now different,

$$\alpha_2 \longrightarrow \alpha_L = \frac{e^2/m_e}{D - \omega\omega_B} \tag{3.31}$$

Again, the subscript L indicates that this applies only to left circular polarization. Because this is different from the other polarization, it leads to a different speed of propagation for the two different polarizations, if one analyzes Maxwell's equations with the complex dielectric function that results. In the limit of zero binding, with the limiting value of D substituted, there results

$$\alpha_L = -\frac{e^2/m_e}{\omega(\omega + i\gamma + \omega_B)} \tag{3.32}$$

This is still generally negative, regardless of the sign of the charges. Also keep in mind that the optical frequency is typically much greater than the magnetic frequency ω_B. The only difference from α_R is that the sign on the magnetic frequency is reversed. We will see that this is generally true for all the formulas. When switching from a formula for right circular polarization to the equivalent one for left circular polarization, change the sign on ω_B. The polarizabilities for the two polarizations are compared in Fig. 1, for an unrealistically high value of the magnetic frequency, so that their differences can be noted. One sees that α_R is affected much more by the magnetic field than α_L is affected.

3.2 Classical dielectric function with a DC magnetic field

The resulting dielectric permittivity tensor $\tilde{\epsilon}$ is hinted at in the previous part, see the result (3.24) for the induced dipole moment of one electron. The resulting electric dipole moment per unit volume, for N electrons in volume V, is the electric polarization

$$\mathbf{P} = \frac{N}{V}\mathbf{d} = \tilde{\chi}\cdot\mathbf{E}, \qquad \tilde{\epsilon} = \mathbf{1} + 4\pi\tilde{\chi}. \tag{3.33}$$

This implicitly defines the susceptibility, which then gives the dielectric function. One can see here the matrix for the transverse suscpetibility, for $n = N/V$ electrons per unit volume, is

$$\tilde{\chi} = \frac{ne^2}{m_e(D^2 - \omega^2\omega_B^2)}\begin{bmatrix} D & -i\omega\omega_B \\ i\omega\omega_B & D \end{bmatrix} = \begin{bmatrix} \chi_{xx} & \chi_{xy} \\ -\chi_{xy} & \chi_{xx} \end{bmatrix} = \begin{bmatrix} \chi_{xx} & i\mathcal{X}_{xy} \\ -i\mathcal{X}_{xy} & \chi_{xx} \end{bmatrix} \tag{3.34}$$

There are only two numbers needed to define the matrix, the diagonal and off-diagonal elements:

$$\begin{aligned} \chi_{xx} &= \frac{ne^2 D}{m_e(D^2 - \omega^2\omega_B^2)} = \frac{ne^2}{m_e}\cdot\frac{\omega_0^2 - \omega^2 - i\omega\gamma}{[\omega_0^2 - \omega^2 - i\omega\gamma]^2 - \omega^2\omega_B^2} \\ \chi_{xy} &= \frac{-ine^2\,\omega\omega_B}{m_e(D^2 - \omega^2\omega_B^2)} = \frac{ne^2}{m_e}\cdot\frac{-i\omega\omega_B}{[\omega_0^2 - \omega^2 - i\omega\gamma]^2 - \omega^2\omega_B^2} \equiv i\mathcal{X}_{xy} \end{aligned} \tag{3.35}$$

The factor of i is taken in this definition because it simplifies later results. Then it is clear that the dielectric tensor has a similar structure,

$$\tilde{\epsilon} = \mathbf{1} + 4\pi\tilde{\chi} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} \\ -\epsilon_{xy} & \epsilon_{xx} \end{bmatrix} = \begin{bmatrix} \epsilon_{xx} & i\mathcal{E}_{xy} \\ -i\mathcal{E}_{xy} & \epsilon_{xx} \end{bmatrix} \tag{3.36}$$

The elements are obviously defined as

$$\epsilon_{xx} = 1 + 4\pi\chi_{xx} = 1 + \frac{4\pi ne^2 D}{m_e(D^2 - \omega^2\omega_B^2)} = 1 + \frac{4\pi ne^2}{m_e} \cdot \frac{\omega_0^2 - \omega^2 - i\omega\gamma}{[\omega_0^2 - \omega^2 - i\omega\gamma]^2 - \omega^2\omega_B^2}$$
$$\epsilon_{xy} = i\mathcal{E}_{xy} = 4\pi\chi_{xy} = \frac{-4\pi ne^2\, i\omega\omega_B}{m_e(D^2 - \omega^2\omega_B^2)} = \frac{4\pi ne^2}{m_e} \cdot \frac{-i\omega\omega_B}{[\omega_0^2 - \omega^2 - i\omega\gamma]^2 - \omega^2\omega_B^2} \tag{3.37}$$

For future reference, also give the result when the binding frequency is not present (free electrons).

$$\epsilon_{xx} = 1 - \frac{4\pi ne^2}{m_e\omega} \cdot \frac{\omega + i\gamma}{(\omega + i\gamma)^2 - \omega_B^2}$$
$$\epsilon_{xy} = i\mathcal{E}_{xy} = -i\frac{4\pi ne^2}{m_e\omega} \cdot \frac{\omega_B}{(\omega + i\gamma)^2 - \omega_B^2} \tag{3.38}$$

One can see that the diagonal part (ϵ_{xx}) goes to the correct limit when $\omega_B = 0$. The off-diagonal part (ϵ_{xy}) is approximately proportional to the magnetic field at weak field strength.

The off-diagonal elements go to zero when the magnetic field is turned off. When it is turned on, the permittivity tensor causes an anisotropic response to the electric field. Note, however, that this works in a simple way, if the applied electric field is expanded in the eigenvectors of $\tilde{\epsilon}$. But we already know those eigenvectors. They are actually the $\hat{u}_1$ and $\hat{u}_2$ vectors found for the M matrix. Check this! The eigenvalue problem is

$$\begin{bmatrix} \epsilon_{xx} & i\mathcal{E}_{xy} \\ -i\mathcal{E}_{xy} & \epsilon_{xx} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \end{bmatrix} = \lambda \begin{bmatrix} E_x \\ E_y \end{bmatrix}. \tag{3.39}$$

The determinant needed to get the eigenspectrum of $\tilde{\epsilon}$ is

$$D' = (\epsilon_{xx} - \lambda)^2 - (-i\mathcal{E}_{xy})(i\mathcal{E}_{xy}) = (\epsilon_{xx} - \lambda)^2 - \mathcal{E}_{xy}^2 = 0 \tag{3.40}$$

The eigenvalues are found as

$$\lambda = \epsilon_{xx} \pm \mathcal{E}_{xy} \quad \Longrightarrow \quad \lambda_1 = \epsilon_{xx} + \mathcal{E}_{xy}, \quad \lambda_2 = \epsilon_{xx} - \mathcal{E}_{xy}. \tag{3.41}$$

Then one sees that for each choice of eigenvalue we get it eigenvector. Change the notation slightly:

$$\lambda_1 \;=\; \epsilon_R = \epsilon_{xx} + \mathcal{E}_{xy}: \quad E_y = -iE_x, \quad \hat{u}_R = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{y}), \quad \text{(right circular)}$$
$$\lambda_2 \;=\; \epsilon_L = \epsilon_{xx} - \mathcal{E}_{xy}: \quad E_y = +iE_x, \quad \hat{u}_L = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{y}). \quad \text{(left circular)} \tag{3.42}$$

The eigenvalues themselves determine how light propagates. They determine the complex wave vectors for a given frequency, for the two independent circular polarizations. Generally, the off-diagonal term is small, because it is roughly proportional to an applied magnetic field. But that small correction leads to differences in the propagation of the two polarizations, which is what causes the Faraday rotation. The wave vectors for the two polarizations are

$$k_R \;=\; \frac{\omega}{c}\sqrt{\mu\epsilon_R} = \frac{\omega}{c}\sqrt{\mu(\epsilon_{xx} + \mathcal{E}_{xy})}$$
$$k_L \;=\; \frac{\omega}{c}\sqrt{\mu\epsilon_L} = \frac{\omega}{c}\sqrt{\mu(\epsilon_{xx} - \mathcal{E}_{xy})} \tag{3.43}$$

Without saying how B points, one cannot say which wave vector is larger, besides, they are complex. But the important thing is that these two components will gradually get out of phase as a wave propagates; they have slightly different phase velocities and wave lengths.

3.3 Matrix algebra for circular polarizations

The unit vectors for right and left circular polarizations already appeared twice. Here I summarize their properties and the transformations between linear and circular polarization bases.

The right and left circular basis vectors are repeated here, along with the reverse tranform,

$$\begin{aligned} \hat{u}_R &= \frac{1}{\sqrt{2}}(\hat{x} - i\hat{y}), \qquad & \hat{x} &= \frac{1}{\sqrt{2}}(\hat{u}_R + \hat{u}_L), \\ \hat{u}_L &= \frac{1}{\sqrt{2}}(\hat{x} + i\hat{y}), \qquad & \hat{y} &= \frac{i}{\sqrt{2}}(\hat{u}_R - \hat{u}_L). \end{aligned} \tag{3.44}$$

As already mentioned, either basis can be used to express the transverse components of an electric field (in an EM wave).

$$\mathbf{E} = E_x\hat{x} + E_y\hat{y} = E_R\hat{u}_R + E_L\hat{u}_L. \tag{3.45}$$

Because the basis vectors are complex, they have interesting algebraic properties that must be kept in mind when finding components. The normalization scalar products are

$$\hat{u}_R^* \cdot \hat{u}_R = \hat{u}_L^* \cdot \hat{u}_L = \hat{u}_R \cdot \hat{u}_L = 1, \qquad \hat{u}_R^* \cdot \hat{u}_L = \hat{u}_R \cdot \hat{u}_L^* = \hat{u}_R \cdot \hat{u}_R = \hat{u}_L \cdot \hat{u}_L = 0. \tag{3.46}$$

Then applying either $\hat{u}_R^*$ or $\hat{u}_L^*$ onto the electric field expression pulls out the desired circular polarization component:

$$E_R = \hat{u}_R^* \cdot \mathbf{E} = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{y})^* \cdot (E_x\hat{x} + E_y\hat{y}) = \frac{1}{\sqrt{2}}(E_x + iE_y) \tag{3.47}$$

$$E_L = \hat{u}_L^* \cdot \mathbf{E} = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{y})^* \cdot (E_x\hat{x} + E_y\hat{y}) = \frac{1}{\sqrt{2}}(E_x - iE_y) \tag{3.48}$$

Can go the other way obviously by scalar products with $\hat{x}$ and $\hat{y}$,

$$E_x = \hat{x} \cdot \mathbf{E} = \hat{x} \cdot (E_R\hat{u}_R + E_L\hat{u}_L) = \frac{1}{\sqrt{2}}(E_R + E_L) \tag{3.49}$$

$$E_y = \hat{y} \cdot \mathbf{E} = \hat{y} \cdot (E_R\hat{u}_R + E_L\hat{u}_L) = \frac{-i}{\sqrt{2}}(E_R - E_L) \tag{3.50}$$

The relations can be expressed using matrices. Let me call the matrix that gives the circular components in terms of the Cartesian components, matrix T. One has

$$\begin{pmatrix} E_R \\ \\ E_L \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} E_x \\ \\ E_y \end{pmatrix}, \qquad \text{or} \qquad E' = T \cdot E \tag{3.51}$$

In the last form, the prime indicates the column vector of circular polarization components, and unprimed is the column vector of Cartesian components. One can see that the T-matrix is composed from the R/L components of the Cartesian basis vectors, as column vectors:

$$T = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} x_R & y_R \\ \\ x_L & y_L \end{pmatrix} = \begin{pmatrix} \hat{x} & \hat{y} \end{pmatrix}. \tag{3.52}$$

The inverse transformation matrix can be seen to be composed from the Cartesian components of the right/left basis vectors, as column vectors:

$$\begin{pmatrix} E_x \\ \\ E_y \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \\ \frac{-i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} E_R \\ \\ E_L \end{pmatrix}, \qquad \text{or} \qquad E = T^{-1} \cdot E' \tag{3.53}$$

The inverse matrix is

$$T^{-1} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \\ \frac{-i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} u_{R,x} & u_{L,x} \\ \\ u_{R,y} & u_{L,y} \end{pmatrix} = \begin{pmatrix} \hat{u}_R & \hat{u}_L \end{pmatrix}. \tag{3.54}$$

The matrix T is unitary, its inverse is its Hermitian conjugate (the complex conjugate of its transpose), $T^{-1} = \tilde{T}^*$. The determinant of T is $-i$, complex but of unit magnitude.

Now one wants to know how the dielectric tensor changes with this transformation. The dielectric function gives the electric displacement, as a column vector of Cartesian components, as $D = \epsilon E$. Can apply the transformation into this equation as follows:

$$D' = TD = T\epsilon E = T\epsilon T^{-1} TE = (T\epsilon T^{-1})(TE) = \epsilon' E', \qquad \text{where } \epsilon' = T\epsilon T^{-1}. \tag{3.55}$$

The matrix ϵ' is the dielectric function as represented in the circular polarization components. This is a usual similarity transformation. One can check exactly what comes out here, using the matrices:

$$\epsilon' = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \\ \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \epsilon_{xx} & i\mathcal{E}_{xy} \\ \\ -i\mathcal{E}_{xy} & \epsilon_{xx} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \\ \frac{-i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \tag{3.56}$$

This becomes

$$\epsilon' = \frac{1}{2} \begin{pmatrix} 1 & i \\ \\ 1 & -i \end{pmatrix} \begin{pmatrix} \epsilon_{xx} + \mathcal{E}_{xy} & \epsilon_{xx} - \mathcal{E}_{xy} \\ \\ -i(\epsilon_{xx} + \mathcal{E}_{xy}) & i(\epsilon_{xx} - \mathcal{E}_{xy}) \end{pmatrix} = \begin{pmatrix} \epsilon_{xx} + \mathcal{E}_{xy} & 0 \\ \\ 0 & \epsilon_{xx} - \mathcal{E}_{xy} \end{pmatrix} \tag{3.57}$$

The array is diagonal, as expected, and the diagonal elements are just $\epsilon_R = \epsilon_{xx} + \mathcal{E}_{xy} = \epsilon_{xx} - i\epsilon_{xy}$ and $\epsilon_L = \epsilon_{xx} - \mathcal{E}_{xy} = \epsilon_{xx} + i\epsilon_{xy}$, for the two independent (and somehow, fundamental) circular polarizations. These were the eigenvalues already encountered for the dielectric matrix. Transformation to circular polarization components brings the matrix to diagonal form, as it should! The circular states are the eigenstates, and propagate unchanged. On the other hand, the linear polarization states are superpositions of these two different eigenstates, hence, a linear polarization state evolves as it propagates, because the eigenstates interfere with each other.

3.4 Faraday Rotation

Suppose an incident wave enters a medium, travelling in the z-direction, and polarized in the x-direction. It can be considered as a linear combination of equal amounts of right and left polarizations. This is represented by the mathematics,

$$\mathbf{E}_{\rm inc} = E_{\rm inc}\hat{x} = E_{\rm inc}\,\frac{1}{\sqrt{2}}(\hat{u}_R + \hat{u}_L) \tag{3.58}$$

That is the wave at a point $z = 0$. After it propagates some distance z, over a time interval t, each part gets a phase shift by $e^{i(kz-\omega t)}$, using the appropriate wave vector for each polarization. The result arriving at a receiver at position z is

$$\begin{aligned} \mathbf{E}(z) &= \frac{E_{\rm inc}}{\sqrt{2}} \left[\hat{u}_R e^{i(k_R z - \omega t)} + \hat{u}_L e^{i(k_L z - \omega t)} \right] \\ &= \frac{E_{\rm inc}}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} \left[(\hat{x} - i\hat{y}) e^{ik_R z} + (\hat{x} + i\hat{y}) e^{ik_L z} \right] e^{-i\omega t} \\ &= \frac{1}{2} E_{\rm inc} \left[(e^{k_R z} + e^{k_L z})\hat{x} + \frac{1}{i}(e^{k_R z} - e^{k_L z})\hat{y} \right] e^{-i\omega t} \end{aligned} \tag{3.59}$$

This shows the amount of light still polarized along $\hat{x}$, versus the amount that now is polarized along $\hat{y}$. It helps to make some definitions or notation,

$$\overline{k} \equiv \frac{1}{2}(k_R + k_L), \qquad \Delta k \equiv k_R - k_L$$
$$k_R = \overline{k} + \frac{1}{2}\Delta k, \qquad k_L = \overline{k} - \frac{1}{2}\Delta k. \tag{3.60}$$

Then the signal becomes

$$\begin{aligned} \mathbf{E}(z) &= \frac{1}{2}E_{\rm inc}\left[\frac{1}{2}(e^{i\frac{\Delta k}{2}z} + e^{-i\frac{\Delta k}{2}z})\hat{x} + \frac{1}{2i}(e^{i\frac{\Delta k}{2}z} - e^{-i\frac{\Delta k}{2}z})\hat{x}\right] e^{i\overline{k}z}e^{-i\omega t} \\ &= E_{\rm inc}\left[\hat{x}\cos\frac{\Delta k}{2}z + \hat{y}\sin\frac{\Delta k}{2}z\right] e^{i(\overline{k}z-\omega t)} \end{aligned} \tag{3.61}$$

One can see from this that the electric field is now polarized at angle $\frac{\Delta k}{2}z$ to the x-axis. This is the simple calculation, assuming that the wave vectors are real. The Faraday rotation angle is then

$$\theta = \frac{\Delta k}{2}z = \frac{1}{2}(k_R - k_L)\, z. \tag{3.62}$$

Another way this is sometimes written would be in terms of the indices of refraction for the two polarizations, $n_R = \sqrt{\mu\epsilon_R}$ and $n_L = \sqrt{\mu\epsilon_L}$,

$$\theta = \frac{\omega}{2c}(n_R - n_L)\, z. \tag{3.63}$$

The farther the wave travels in the medium, the greater is the rotation. This happens because a linear polarization state is not an eigenstate of the EM field. Only the circular polarization states are the eigenstates, and they propagate unchanged.

One would like to know, most importantly, how the rotation of the polarization depends on the applied magnetic field. Do an expansion of the wave vectors, assuming the off-diagonal part of the dielectric tensor is small, and ϵ_{xx} and $\mathcal{E}_{xy}$ are real (this is not exactly true, I will correct this later):

$$\begin{aligned} \theta &= \frac{z}{2}(k_R - k_L) = \frac{z}{2}\frac{\omega}{c}\sqrt{\mu}\left[\sqrt{\epsilon_{xx} + \mathcal{E}_{xy}} - \sqrt{\epsilon_{xx} - \mathcal{E}_{xy}}\right] \\ &\approx \frac{z}{2}\frac{\omega}{c}\sqrt{\mu\epsilon_{xx}}\left[\left(1 + \frac{1}{2}\frac{\mathcal{E}_{xy}}{\epsilon_{xx}}\right) - \left(1 - \frac{1}{2}\frac{\mathcal{E}_{xy}}{\epsilon_{xx}}\right)\right] = \frac{\omega}{2c}\sqrt{\frac{\mu}{\epsilon_{xx}}}\,\mathcal{E}_{xy}\, z. \end{aligned} \tag{3.64}$$

Since $\mathcal{E}_{xy}$ is approximately proportional to the magnetic field, for small fields, the Faraday rotation is also proportional to the magnetic field strength along the propagation direction of the light. The approximate expression could be found from using the results for ϵ.

In the more general case where the wave vectors are complex, because there is absorption, one can show that not only is there a Faraday rotation, but also an ellipticity is generated in the polarization. This means that the polarization is not circular when it arrives at a receiver. Instead, the ratio of its semi-minor axis b to semi-major axis a is different from 1. The ratio is characterized by an ellipticity angle $\chi = \tan^{-1}(b/a)$. Then, one gets a complex rotation angle, where the real part is the usual Faraday rotation θ, and the imaginary part is the ellipticity angle χ. The relation becomes

$$\theta + i\chi = \frac{\Delta k}{2}\, z = \frac{1}{2}(\Delta k' + i\Delta k'')\, z \tag{3.65}$$

The prime and double prime indicate the real and imaginary parts. Those also can be translated into the real and imaginary parts of the indices of refraction. To prove this is an excercise in the plane geometry of ellipses, which I will not do here! It is still true, however, that this leads to

$$\theta + i\chi \approx \frac{\omega}{2c}\sqrt{\frac{\mu}{\epsilon_{xx}}}\,\mathcal{E}_{xy}\, z. \tag{3.66}$$

To apply it requires inserting and evaluating with the real and imaginary parts of the dielectric functions.

All of this has been classical mechanics. The rest of these notes is concerned with how dielectrics in a magnetic field work in the quantum world.

4 Quantum electron dynamics with a DC magnetic field

An electron in a uniform DC magnetic field plus an applied optical field will have a Hamiltonian as discussed previously

$$H = \frac{1}{2m_e}\left[\mathbf{p} - \frac{e}{c}\mathbf{A}_{\rm tot}(\mathbf{r},t)\right]^2 + e\phi(\mathbf{r},t) + U(\mathbf{r}). \tag{4.1}$$

Now, however, the vector potential must include both that due to the optical field and that due to the DC magnetic field. Further, for simplicity, we take the scalar potential as zero (Coulomb gauge for the optical field). The crystal potential $U(\mathbf{r})$ leads to states in bands, however, we try to ignore that for the time being. This will lead to something analogous to the classical treatment just discussed (quasi-free electrons).

I can consider the vector potential as a sum of DC part $\mathbf{A}$ plus AC part $\tilde{\mathbf{A}}$:

$$\mathbf{A}_{\rm tot} = \mathbf{A} + \tilde{\mathbf{A}} \tag{4.2}$$

Then each of these can interact with the momentum operator, as well as with each other when the square is taken. I'll ignore those quadratic interaction terms, but keep the term due to squaring the DC vector potential. The reason is, we suppose the DC magnetic field is much much stronger than that in the light waves. The DC field leads to the so-called **Landau levels** which can resemble classical cyclotron motion. They have an energy scaled dependent on $\bar{\mathbf{B}}$ and we really want to take them into account. The optical field here will be first treated as a classical time-dpendent field. So the Hamiltonian to currently consider is

$$H = \frac{1}{2m_e}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 - \frac{e}{m_e c}\tilde{\mathbf{A}}\cdot\mathbf{p}. \tag{4.3}$$

The first term is considered the original Hamiltonian H_0, the second term is a perturbation.

4.1 Landau Levels

One wants to understand the eigen states of the system before the optical field is applied. It is assumed that the DC magnetic field B points along the z-axis. Then its vector potential only needs to depend on x and y coordinates, at most. It makes sense to write H_0 using the dynamic momentum operator,

$$H_0 = \frac{1}{2m_e}\vec{\pi}^2, \qquad \vec{\pi} = \mathbf{p} - \frac{e}{c}\mathbf{A}. \tag{4.4}$$

This operator is very interesting because its components do not commute with each other! That is because the vector potential depends on position. One gets commutators

$$[\pi_x, \pi_y] = [p_x - \frac{e}{c}A_x, p_y - \frac{e}{c}A_y] = -\frac{e}{c}\left([p_x, A_y] + [A_x, p_y]\right) \tag{4.5}$$

In the coordinate represention, the momentum operator is $\mathbf{p} = -i\hbar\vec{\nabla}$, so the action on some arbitrary wave function ψ is

$$\begin{aligned}[p_x, A_y]\psi &= (-i\hbar\partial_x)(A_y\psi) - (A_y)(-i\hbar\partial_x\psi) \\ &= (-i\hbar)\left[(\partial_x A_y)\psi + A_y(\partial_x\psi) - A_y(\partial_x\psi)\right] = -i\hbar(\partial_x A_y)\psi\end{aligned} \tag{4.6}$$

The other one is

$$\begin{aligned}[A_x, p_y]\psi &= A_x(-i\hbar\partial_y\psi) - (-i\hbar\partial_y)(A_x\psi) \\ &= (-i\hbar)\left[A_x(\partial_y\psi) - (\partial_y A_x)\psi - A_x(\partial_y\psi)\right] = i\hbar(\partial_y A_x)\psi\end{aligned} \tag{4.7}$$

Then the commutator of two components of $\vec{\pi}$ is

$$[\pi_x, \pi_y] = -\frac{e}{c}(-i\hbar)[\partial_x A_y - \partial_y A_x] = \frac{ie\hbar}{c}(\vec{\nabla}\times\mathbf{A})_z = i\hbar\frac{eB}{c} \tag{4.8}$$

Note that in fact, the combination eB/m_ec is the classical cyclotron frequency,

$$\omega_B = \frac{eB}{m_e c} \tag{4.9}$$

So the basic commutator here is

$$[\pi_x, \pi_y] = i\hbar m_e \omega_B. \tag{4.10}$$

This is curiously very much like the fundamental canonical commutator $[x, p_x] = i\hbar$, except for the scale proportional to the applied magnetic field. Further, this Hamiltonian bears a very close mathematical resemblance to that of a simple harmonic oscillator:

$$H_0 = \frac{1}{2m_e}(\pi_x^2 + \pi_y^2); \qquad H_{SHM} = \frac{1}{2m_e}(p_x^2 + m_e^2\omega^2 x^2). \tag{4.11}$$

This means that the electron in B_z can be quantized just the same way that a harmonic oscillator is quantized. The easiest and best approach is to re-arrange H_0 so it can be written in terms of creation and annihilation operators. Based on the structure, try the following (operator version of taking the square root):

$$H_0 = \frac{1}{2m_e} \cdot \frac{1}{2}\left[(\pi_x + i\pi_y)(\pi_x - i\pi_y) + (\pi_x - i\pi_y)(\pi_x + i\pi_y)\right] \tag{4.12}$$

Then this is symmetrized, and introduce creation and annihilation operators that must be scaled correctly to give a unit commutator,

$$a = N_0(\pi_x + i\pi_y), \quad a^\dagger = N_0(\pi_x - i\pi_y), \quad [a, a^\dagger] = 1. \tag{4.13}$$

N_0 is the normalization factor, and is found by applying (4.8):

$$[a, a^\dagger] = N_0^2[\pi_x + i\pi_y,\ \pi_x - i\pi_y] = N_0^2\left(-i[\pi_x, \pi_y] + i[\pi_y, \pi_x]\right) = N_0^2(-2i)\left(i\hbar\frac{e}{c}B_z\right) = 1. \tag{4.14}$$

This gives

$$N_0 = \sqrt{\frac{c}{2\hbar eB}} \implies a = \sqrt{\frac{c}{2\hbar eB}}(\pi_x + i\pi_y), \quad a^\dagger = \sqrt{\frac{c}{2\hbar eB}}(\pi_x - i\pi_y). \tag{4.15}$$

The factors on the creation/annihilation operators involve the cyclotron frequency and take the same form as those on the momentum in the SHO.

$$a = \sqrt{\frac{1}{2m_e\hbar\omega_B}}\ (\pi_x + i\pi_y), \quad a^\dagger = \sqrt{\frac{1}{2m_e\hbar\omega_B}}\ (\pi_x - i\pi_y). \tag{4.16}$$

The inverse relations are

$$\pi_x = \sqrt{\frac{m_e\hbar\omega_B}{2}}\ (a + a^\dagger), \quad \pi_y = \frac{1}{i}\sqrt{\frac{m_e\hbar\omega_B}{2}}\ (a - a^\dagger), \tag{4.17}$$

Then the Hamiltonian is

$$H_0 = \frac{1}{4m_e} \cdot (2m_e\hbar\omega_B)(aa^\dagger + a^\dagger a) = \frac{1}{2}\hbar\omega_B(aa^\dagger + a^\dagger a). \tag{4.18}$$

It can also be expressed in terms of the usual number operator, $a^\dagger a$, via the commutation relation, as

$$H_0 = \hbar\omega_B\left(a^\dagger a + \frac{1}{2}\right). \tag{4.19}$$

The quantized states of this Hamiltonian are the Landau levels. Since the eigenvalues of the number operator are positive integers (and 0), the energy levels are just like those of a harmonic oscillator,

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_B, \quad n = 0, 1, 2, 3, ... \tag{4.20}$$

The derivation implicitly assumed the product $eB > 0$. Normally we would be interested in electrons, then, it would make sense here for the magnetic field pointing in the $-\hat{z}$ direction. If you did do the problem of a negative charge with $\mathbf{B}$ in the positive $\hat{z}$ direction, you'll find it useful to swap π_x and π_y in the definition of the creation/annihilation operators, and see that the sign of ω_B is negative, and there results $H_0 = -\hbar\omega_B\left(a^\dagger a + \frac{1}{2}\right)$. So the most general result is to put absolute value on ω_B, and then (4.19) works for any choice of sign of charge or direction of $\mathbf{B}$.

4.1.1 Landau Levels and Constants of the Motion

I don't want to discuss all possible aspects of Landau levels, just those ideas I need to talk about their effect on the dielectric function $\epsilon(\omega)$. Because they can have a role due to transitions between them, we need also to discuss their degeneracy. This is not so obvious. The states of a 1D harmonic oscillator are non-degenerate. But here, the system is two-dimensional, yet the Hamiltonian appears to be like a 1D Hamiltonian now. It's as if a dimension was lost, but it's not actually lost, it's just that these levels have a degeneracy. It can be seen because there are constants of the motion associated with an arbitrary choice of the center of the cyclotron motion. This is probably easiest to see from looking at the classical problem. A classical electron affected just by a magnetic field has dynamics from

$$m_e\dot{v}_x = \frac{e}{c}v_y B_z, \qquad m_e\dot{v}_y = -\frac{e}{c}v_x B_z \tag{4.21}$$

This is the same as writing

$$\dot{v}_x = \omega_B v_y, \qquad \dot{v}_y = -\omega_B v_x \tag{4.22}$$

And the combination of the equations gives usual harmonic motion:

$$\ddot{v}_x = -\omega_B^2 v_x, \qquad \ddot{v}_y = -\omega_B^2 v_y \tag{4.23}$$

An integration as follows gives two constants of the motion (two integration constants):

$$\int dt\ \dot{v}_x = \omega_B \int dt\ v_y \implies v_x(t) = \omega_B(y(t) - Y) \implies Y = y(t) - \frac{v_x(t)}{\omega_B}. \tag{4.24}$$

$$\int dt\ \dot{v}_y = -\omega_B \int dt\ v_x \implies v_y(t) = \omega_B(x(t) - X) \implies X = x(t) + \frac{v_y(t)}{\omega_B}. \tag{4.25}$$

These integration constants X and Y don't change during the cyclotron motion. Indeed, the solution for the velocities is found easily. Try harmonic functions:

$$v_x(t) = v_1\cos\omega_B t + v_2\sin\omega_B t, \implies \dot{v}_x = \omega_B v_y = \omega_B(-v_1\sin\omega_B t + v_2\cos\omega_B t) \tag{4.26}$$

Then it is easy to see that the constants here are just $v_1 = v_x(0)$ and $v_2 = v_y(0)$. The solution for velocity and position is then

$$\begin{array}{ll} v_x(t) = v_x(0)\cos\omega_B t + v_y(0)\sin\omega_B t, & v_y(t) = -v_x(0)\sin\omega_B t + v_y(0)\cos\omega_B t, \\ x(t) = \frac{1}{\omega_B}[v_x(0)\sin\omega_B t - v_y(0)\cos\omega_B t] + c_1, & y(t) = \frac{1}{\omega_B}[v_x(0)\cos\omega_B t + v_y(0)\sin\omega_B t] + c_2. \end{array} \tag{4.27}$$

Try to evaluate the above constants of integration in terms of the initial velocities and these new integration constants c_1 and c_2. One gets

$$\begin{aligned} Y = y(t) - \frac{v_x(t)}{\omega_B} &= \frac{1}{\omega_B}[v_x(0)\cos\omega_B t + v_y(0)\sin\omega_B t] + c_2 \\ &- \frac{1}{\omega_B}[v_x(0)\cos\omega_B t + v_y(0)\sin\omega_B t] = c_2. \end{aligned} \tag{4.28}$$

$$\begin{aligned} X = x(t) + \frac{v_y(t)}{\omega_B} &= \frac{1}{\omega_B}[v_x(0)\sin\omega_B t - v_y(0)\cos\omega_B t] + c_1 \\ &+ \frac{1}{\omega_B}[-v_x(0)\sin\omega_B t + v_y(0)\cos\omega_B t] = c_1. \end{aligned} \tag{4.29}$$

Of course, the point $(X, Y) = (c_1, c_2)$ is the average position, which is just the center of the cyclotron orbit! It does not change with time, it is a constant of the motion. In addition to this, the size of the orbit is determined by the initial velocity components. Consider the deviation of the position from its average:

$$\begin{aligned}\rho^2 &= [x(t) - X]^2 + [y(t) - Y]^2 \\ &= \frac{1}{\omega_B^2}\left\{[v_x(0)\sin\omega_B t - v_y(0)\cos\omega_B t]^2 + [v_x(0)\cos\omega_B t + v_y(0)\sin\omega_B t]^2\right\} \\ &= \frac{v_x^2(0) + v_y^2(0)}{\omega_B^2}, \quad \Longrightarrow \quad |\mathbf{v}(0)| = \omega_B \rho. \end{aligned} \tag{4.30}$$

It shows that the initial speed determines the size (and energy) of the orbit.

Now how to find the equivalent conserved objects like X and Y for the quantum problem? The simplest approach is to construct the corresponding quantum operators, and see their properties. But be careful: the velocity is connected to the kinetic momentum $\vec{\pi}$, not to the canonical momentum $\mathbf{p}$. Replacing velocity by kinetic momentum over mass, one can define new quantum operators,

$$X = x + \frac{\pi_y}{m_e\omega_B}, \qquad Y = y - \frac{\pi_x}{m_e\omega_B}. \tag{4.31}$$

Check the commutator between them:

$$\begin{aligned}[X, Y] = \left[x + \frac{\pi_y}{m_e\omega_B},\ y - \frac{\pi_x}{m_e\omega_B}\right] &= \frac{1}{m_e\omega_B}\left(-[x, \pi_x] + [\pi_y, y] - \frac{1}{m_e\omega_B}[\pi_y, \pi_x]\right) \\ &= \frac{1}{m_e\omega_B}\left[-i\hbar - i\hbar - \frac{1}{m_e\omega_B}(-i\hbar m_e\omega_B)\right] = \frac{-i\hbar}{m_e\omega_B} \end{aligned} \tag{4.32}$$

This is similar to the non-commutation of $\vec{\pi}_x$ and $\vec{\pi}_y$, except that the sign is negative, and, the magnetic field is in the denominator! This non-commutation gets weaker with increasing magnetic field. This also shows that these objects cannot be simultaneously specified to arbitrary precision.

Check also some other commutation relations. Try these with the kinetic momentum.

$$[X, \pi_x] = \left[x + \frac{\pi_y}{m_e\omega_B},\ \pi_x\right] = [x, \pi_x] + \frac{1}{m_e\omega_B}[\pi_y, \pi_x] = i\hbar + \frac{1}{m_e\omega_B}(-i\hbar m_e\omega_B) = 0. \tag{4.33}$$

$$[X, \pi_y] = \left[x + \frac{\pi_y}{m_e\omega_B},\ \pi_y\right] = [x, \pi_y] + \frac{1}{m_e\omega_B}[\pi_y, \pi_y] = 0. \tag{4.34}$$

Then the other two like this are also zero: $[Y, \pi_y] = [Y, \pi_x] = 0$. So X and Y are new operators that can be specified independently of the kinetic momenta. Furthermore, since they commute with the kinetic momenta, they commute with the Hamiltonian, so they are constants of the motion. They lead to the degeneracy of the Landau levels.

Based on their mutual commutator, X and Y can be combined into another kind of creation and annihilation operators. Consider the obvious combinations that form the squared central position of a cyclotron orbit, denoted with Δ^2:

$$\Delta^2 = X^2 + Y^2 = \frac{1}{2}\left[(X - iY)(X + iY) + (X + iY)(X - iY)\right] \propto (bb^\dagger + b^\dagger b) \tag{4.35}$$

Then the new operators are

$$b = M_0(X - iY), \qquad b^\dagger = M_0(X + iY) \tag{4.36}$$

The choice of signs is based on the negative sign in the result, $[X, Y] = -i\hbar/m_e\omega_B$. M_0 is the normalization to be chosen so that $[b, b^\dagger] = 1$. Let's determine that:

$$[b, b^\dagger] = M_0^2[X - iY, X + iY] = iM_0^2([X, Y] - [Y, X]) = iM_0^2(-2i\hbar/m_e\omega_B) = 1. \tag{4.37}$$

This leads to $M_0 = \sqrt{m_e\omega_B/2\hbar}$, and the creation/annihilation operators are

$$b = \sqrt{\frac{m_e\omega_B}{2\hbar}}(X - iY), \qquad b^\dagger = \sqrt{\frac{m_e\omega_B}{2\hbar}}(X + iY). \tag{4.38}$$

What do they do for us? For one thing, they determine the location of the center of the cyclotron motion, which is the operator Δ^2. It can be expressed

$$\Delta^2 = X^2 + Y^2 = \frac{1}{2}\frac{2\hbar}{m_e\omega_B}\left(bb^\dagger + b^\dagger b\right) = \frac{2\hbar}{m_e\omega_B}\left(b^\dagger b + \frac{1}{2}\right). \tag{4.39}$$

This isn't a Hamiltonian, yet it resembles one. The $b^\dagger$ operator will raise the amount of Δ^2 in the system, and b reduces it. The minimum is the zero point value seen here, $\Delta^2 \geq \hbar/m_e\omega_B$, the same number as that appearing in the commutator of X and Y. As (X, Y) classically is the center of the cyclotron motion, one can see that different values of this position will all have the same energy, hence there is great degeneracy. But the size of $2\hbar/m_e\omega_B$ determines the scale of that degeneracy. Also, it's seen that all the Landau levels will have the same degeneracy, because they all have the same choices for possible centers.

4.1.2 What about angular momentum?

Before figuring out the amount of degeneracy, consider what else is physically related to b and $b^\dagger$. Classical cyclotron motion is clearly associated with an angular momentum. Look at the angular momentum for the quantum problem. But again, it seems a little tricky, because there is the canonical momentum and the kinetic momentum, and each could be used to construct an angular momentum. This is really confusing and for certain problems those things are the same, for other problems they are different. But generally, canonical momentum is not physical (or kinetic) momentum, rather, it is more of a device for calculations.

Consider an angular momentum based on the kinetic momentum,

$$\tilde{\mathbf{L}} = \mathbf{r} \times \vec{\pi}, \qquad \tilde{L} = \tilde{L}_z = x\pi_y - y\pi_x. \tag{4.40}$$

Only the z component is important for this effectively 2D problem. Check if it commutes with the Hamiltonian (maybe, based on the rotational symmetry in operator $\vec{\pi}$), via the following:

$$\begin{aligned}[\tilde{L}, \pi_x] = [x\pi_y - y\pi_x, \pi_x] &= [x\pi_y, \pi_x] - [y\pi_x, \pi_x] = x[\pi_y, \pi_x] + [x, \pi_x]\pi_y - [y, \pi_x]\pi_x \\ &= x(-i\hbar m_e\omega_B) + (i\hbar)\pi_y - 0 = i\hbar(-m_e\omega_B x + \pi_y).\end{aligned} \tag{4.41}$$

And the square,

$$\begin{aligned}[\tilde{L}, \pi_x^2] = \pi_x[\tilde{L}, \pi_x] + [\tilde{L}, \pi_x]\pi_x &= \pi_x[i\hbar(-m_e\omega_B x + \pi_y)] + [i\hbar(-m_e\omega_B x + \pi_y)]\pi_x \\ &= i\hbar[-m_e\omega_B(x\pi_x + \pi_x x) + (\pi_x\pi_y + \pi_y\pi_x)]\end{aligned} \tag{4.42}$$

$$\begin{aligned}[\tilde{L}, \pi_y] = [x\pi_y - y\pi_x, \pi_y] &= [x\pi_y, \pi_y] - [y\pi_x, \pi_y] = [x, \pi_y]\pi_y - y[\pi_x, \pi_y] - [y, \pi_y]\pi_x \\ &= 0 - y(i\hbar m_e\omega_B) - (i\hbar)\pi_x = -i\hbar(m_e\omega_B y + \pi_x).\end{aligned} \tag{4.43}$$

$$\begin{aligned}[\tilde{L}, \pi_y^2] = \pi_y[\tilde{L}, \pi_y] + [\tilde{L}, \pi_y]\pi_y &= \pi_y[-i\hbar(m_e\omega_B y + \pi_x)] + [-i\hbar(m_e\omega_B y + \pi_x)]\pi_y \\ &= i\hbar[-m_e\omega_B(y\pi_y + \pi_y y) - (\pi_x\pi_y + \pi_y\pi_x)]\end{aligned} \tag{4.44}$$

So somewhat surprisingly, the total of these is not zero, and this $\tilde{L}$ does not commute with H_0:

$$[\tilde{L}, \pi_x^2 + \pi_y^2] = -i\hbar m_e\omega_B(x\pi_x + \pi_x x + y\pi_y + \pi_y y) \neq 0. \tag{4.45}$$

Instead, try the usual (canonical) angular momentum. Let

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}, \qquad L = L_z = xp_y - yp_x. \tag{4.46}$$

Let me use the basic fact about the momentum operator in coordinate representation, that is

$$[p_x, f(x)] = -i\hbar\frac{\partial f}{\partial x} = -i\hbar\partial_x f = p_x f \tag{4.47}$$

and the fact that, for example, $\pi_x = p_x - (e/c)A_x$. Then the first commutator we need is

$$\begin{aligned}
[L, \pi_x] &= [xp_y - yp_x, \pi_x] = [xp_y, \pi_x] - [yp_x, \pi_x] \\
&= x[p_y, \pi_x] + [x, \pi_x]p_y - y[p_x, \pi_x] - [y, \pi_x]p_x \\
&= x(-i\hbar\frac{-e}{c}\partial_y A_x) + (i\hbar)p_y - y(-i\hbar\frac{-e}{c}\partial_x A_x) - 0p_x \\
&= i\hbar p_y - i\hbar\frac{-e}{c}(x\partial_y - y\partial_x)A_x = i\hbar p_y - \frac{e}{c}(LA_x)
\end{aligned} \tag{4.48}$$

The operation rotated p_x into p_y and affected the vector potential That is also the expected action of the angular momentum operator in the coordinate representation. Continuing,

$$[L, \pi_x^2] = \pi_x[L, \pi_x] + [L, \pi_x]\pi_x = i\hbar(\pi_x p_y + p_y\pi_x) - \frac{e}{c}[\pi_x(LA_x) + (LA_x)\pi_x]. \tag{4.49}$$

Doing some similar algebra for π_y we have

$$\begin{aligned}
[L, \pi_y] &= [xp_y - yp_x, \pi_y] = [xp_y, \pi_y] - [yp_x, \pi_y] \\
&= x[p_y, \pi_y] + [x, \pi_y]p_y - y[p_x, \pi_y] - [y, \pi_y]p_x \\
&= x(-i\hbar\frac{-e}{c}\partial_y A_y) + 0p_y - y(-i\hbar\frac{-e}{c}\partial_x A_y) - (i\hbar)p_x \\
&= -i\hbar p_x - i\hbar\frac{-e}{c}(x\partial_y - y\partial_x)A_y = -i\hbar p_x - \frac{e}{c}(LA_y)
\end{aligned} \tag{4.50}$$

Then with the squared,

$$[L, \pi_y^2] = \pi_y[L, \pi_y] + [L, \pi_y]\pi_y = -i\hbar(\pi_y p_x + p_x\pi_y) - \frac{e}{c}[\pi_y(LA_y) + (LA_y)\pi_y]. \tag{4.51}$$

Put it all together,

$$\begin{aligned}
[L, \pi_x^2 + \pi_y^2] &= i\hbar \cdot \frac{-e}{c}\left[A_x p_y + p_y A_x - A_y p_x - p_x A_y\right] \\
&\quad -\frac{e}{c}[\pi_x(LA_x) + (LA_x)\pi_x + \pi_y(LA_y) + (LA_y)\pi_y].
\end{aligned} \tag{4.52}$$

At this point, I can't get a simple result. This is too much algebra without thinking.

4.1.3 Choices of vector potential

The difficulty is, that the Hamiltonian, in general, is not rotationally invariant, because of the presence of the vector potential. Hence the algebra above is not simple. The both weird and beautiful thing about this problem, is that this dependence on the vector potential means there are different solutions to the problem, depending on the choice of the gauge. The simplest would be to choose a gauge that is rotationally invariant. Let me consider that.

The (uniform) magnetic field is derived from the vector potential, and in circular coordinates, the equations needed is

$$B_z = B = (\vec{\nabla} \times \mathbf{A})_z = \frac{1}{r}\left[\frac{\partial}{\partial r}(rA_\phi) - \frac{\partial}{\partial\phi}A_r\right] \tag{4.53}$$

There is an infinite family of solutions. Two of the simplest are either to choose a solution where only A_ϕ is present or where only A_r is present. Suppose you tried $A_\phi = 0$, then solve

$$B = -\frac{1}{r}\frac{\partial}{\partial\phi}A_r \qquad \Longrightarrow A_r = -Br\phi + C. \tag{4.54}$$

This is not rotationally invariant, although it gives a uniform magnetic field. Try instead with $A_r = 0$, and solve

$$B = \frac{1}{r}\frac{\partial}{\partial r}(rA_\phi) \qquad \Longrightarrow A_\phi = \frac{1}{2}Br + C. \tag{4.55}$$

This is "better" in the sense that it is invariant under rotations around the origin. Drawn out, the vector field looks like a whirlpool, with longer arrows farther from the origin. But really, it is just another arbitrary choice that will give the uniform magnetic field we want. Usually it might be quoted in Cartesian coordinates. Then we have the "symmetric gauge",

$$\begin{aligned} A_x &= A_r\cos\phi - A_\phi\sin\phi = -\frac{1}{2}Br\sin\phi = -\frac{1}{2}By \\ A_y &= A_r\sin\phi + A_\phi\cos\phi = +\frac{1}{2}Br\cos\phi = +\frac{1}{2}Bx \end{aligned} \tag{4.56}$$

Also note the action of the canonical angular momentum on this. In circular coordinates, the angular momentum operator is $L = L_x = -i\hbar(\partial/\partial\phi)$. Then it is interesting that

$$LA_\phi = 0, \qquad LA_x = -i\hbar\left(\frac{1}{2}Br\cos\phi\right) = i\hbar A_y, \qquad LA_y = -i\hbar\left(\frac{1}{2}Br\sin\phi\right) = -i\hbar A_x, \tag{4.57}$$

So even though the original A_ϕ is a zero eigenfunction of L, the Cartesian components are not. In fact, one can form some linear combinations, that are other eigenfunctions of L, namely,

$$L\cdot(x+iy) = -i\hbar\frac{\partial}{\partial\phi}(r\cos\phi + ir\sin\phi) = -i\hbar\frac{\partial}{\partial\phi}(re^{+i\phi}) = +\hbar(re^{+i\phi}) = +\hbar(x+iy). \tag{4.58}$$

$$L\cdot(x-iy) = -i\hbar\frac{\partial}{\partial\phi}(r\cos\phi - ir\sin\phi) = -i\hbar\frac{\partial}{\partial\phi}(re^{-i\phi}) = -\hbar(re^{-i\phi}) = -\hbar(x-iy). \tag{4.59}$$

There are also asymmetric choices for the vector potential, for example, one with only an A_x component is sometimes a popular choice:

$$\mathbf{A} = (A_x, A_y) = (-By, 0), \qquad \text{then } B_z = (\partial_x A_y - \partial_y A_x) = B. \tag{4.60}$$

The other simple choice is one with only an A_y component,

$$\mathbf{A} = (A_x, A_y) = (0, Bx), \qquad \text{then } B_z = (\partial_x A_y - \partial_y A_x) = B. \tag{4.61}$$

Or, you could even choose a vector potential that only has a component perpendicular to an axis at angle β to the x-axis. This would be a rotation of one of these last choices, like

$$\begin{aligned} \mathbf{A} = (A_x, A_y) &= (-B(\cos\beta)[y\cos\beta + x\sin\beta], -B(-\sin\beta)[y\cos\beta + x\sin\beta]) \\ &= -B([y\cos^2\beta + x\sin\beta\cos\beta],\ [-x\sin^2\beta - y\sin\beta\cos\beta]) \end{aligned} \tag{4.62}$$

This was performed by rotating the vector *and* rotating the coordinates. Check the field it produces:

$$B_z = (\partial_x A_y - \partial_y A_x) = -B\left(-\sin^2\beta - \cos^2\beta\right) = B. \tag{4.63}$$

In fact, there are extra "un-needed terms" after the rotation. But for example, if you remove the un-needed terms, and say, put the angle $\beta = 45°$, then this vector potential becomes the same as that in the symmetric gauge. But *with* the un-needed terms, it is another form for $\mathbf{A}$ that does not look like a whirlpool, but rather, a set of parallel arrows whose length increases away from the line at angle β to the x-axis.

Just for curiousity, what do you get if you do this same β-rotation of the vector potential of the symmetric gauge? There results under the same operations, for example, to be more specific how the rotation is done,

$$\begin{aligned} A_{x'}(x', y') &= A_x\cos\beta + A_y\sin\beta = \frac{B}{2}(-y\cos\beta + x\sin\beta) \\ &= \frac{B}{2}(-[y'\cos\beta + x'\sin\beta]\cos\beta + [x'\cos\beta - y'\sin\beta]\sin\beta) = \frac{-B}{2}y'. \end{aligned} \tag{4.64}$$

$$A_{y'}(x',y') = -A_x\sin\beta + A_y\cos\beta = \frac{B}{2}\left(y\sin\beta + x\cos\beta\right)$$
$$= \frac{B}{2}\left(\left[y'\cos\beta + x'\sin\beta\right]\sin\beta + \left[x'\cos\beta - y'\sin\beta\right]\cos\beta\right) = \frac{B}{2}x'. \qquad (4.65)$$

This is what is meant by rotationally invariant. The form of the potential in the rotated coordinates is unchanged from the original coordinates.

These different choices of vector potential all give the same magnetic field. They can give different wave functions for the Landau levels, although once expectation values of real problems are taken, the results should not depend on the specific choice of gauge.

4.1.4 Connection between angular momentum and b, $b^\dagger$?

We know from the form of (4.39) that b and $b^\dagger$ control the squared position of the center of the motion. Here I consider a commutation relation between canonical L and b or $b^\dagger$, just to see what comes out. To do that, it is easiest to consider a particular gauge. First suppose we are in the symmetric gauge. Look at the expressions,

$$b = M_0(X - iY) = M_0\left\{x + \frac{\pi_y}{m_e\omega_B} - i\left(y - \frac{\pi_x}{m_e\omega_B}\right)\right\} = M_0\left\{x - iy + \frac{i}{m_e\omega_B}(\pi_x - i\pi_y)\right\} \quad (4.66)$$

$$b^\dagger = M_0(X + iY) = M_0\left\{x + \frac{\pi_y}{m_e\omega_B} + i\left(y - \frac{\pi_x}{m_e\omega_B}\right)\right\} = M_0\left\{x + iy - \frac{i}{m_e\omega_B}(\pi_x + i\pi_y)\right\} \quad (4.67)$$

The commutators of L with $x \pm iy$ were already found. We also have

$$[L, \pi_x - i\pi_y] = i\hbar p_y - \frac{e}{c}(LA_x) - i\left[-i\hbar p_x - \frac{e}{c}(LA_y)\right] = -\hbar(p_x - ip_y) - \frac{e}{c}L\cdot(A_x - iA_y) \quad (4.68)$$

$$[L, \pi_x + i\pi_y] = i\hbar p_y - \frac{e}{c}(LA_x) + i\left[-i\hbar p_x - \frac{e}{c}(LA_y)\right] = +\hbar(p_x + ip_y) - \frac{e}{c}L\cdot(A_x + iA_y) \quad (4.69)$$

Now one sees that these linear combinations of components of $\mathbf{A}$ could give simple results, if, for example, they were eigenfunctions of L. Imagine if that is enforced. The best choice would be

$$L\cdot(A_x - iA_y) = -\hbar(A_x - iA_y), \qquad L\cdot(A_x + iA_y) = +\hbar(A_x + iA_y), \qquad (4.70)$$

because these will give back the kinetic momentum components on the RHS of (4.69) and (4.68). But these linear combinations are the same as

$$A_x - iA_y = (A_r\cos\phi - A_\phi\sin\phi) - i(A_r\sin\phi + A_\phi\cos\phi) = (A_r - iA_\phi)e^{-i\phi} \qquad (4.71)$$

$$A_x + iA_y = (A_r\cos\phi - A_\phi\sin\phi) + i(A_r\sin\phi + A_\phi\cos\phi) = (A_r + iA_\phi)e^{+i\phi} \qquad (4.72)$$

The first will have eigenvalue $-\hbar$ and the second will have eigenvalue $+\hbar$, if the combinations $(A_r \pm iA_\phi)$ are independent of ϕ. The simplest way to accomplish that would be to choose $A_r = 0$, then we are forced to the symmetric gauge with $A_\phi \propto r$. So for the symmetric gauge, relations (4.70) hold, and there results commutators

$$[L, \pi_x - i\pi_y] = -\hbar(\pi_x - i\pi_y), \qquad [L, \pi_x + i\pi_y] = +\hbar(\pi_x + i\pi_y). \qquad (4.73)$$

Finally, the commutators with these creation/annihlation operators are now determined, in the symmetric gauge,

$$[L, b] = -\hbar b, \qquad [L, b^\dagger] = +\hbar b^\dagger. \qquad (4.74)$$

These then show that b destroys one quantum of angular momentum, while $b^\dagger$ creates one quantum of angular momentum. For instance, if the state $|l\rangle$ has L-eigenvalue of $l\hbar$, then for the state $b^\dagger|l\rangle$,

$$L(b^\dagger|l\rangle) = (Lb^\dagger - b^\dagger L + b^\dagger L)|l\rangle = (+\hbar b^\dagger + b^\dagger L)|l\rangle = (l+1)\hbar(b^\dagger|l\rangle). \qquad (4.75)$$

So $b^\dagger|l\rangle$ is the raised state with one more quantum of angular momentum. Similarly, $b\,|l\rangle$ is the lowered state with more less quantum of angular momentum. Therefore, one sees also that for this gauge, changing the angular momentum is associated with changing Δ^2. But these do not involve a change in the energy.

What about one of the non-symmetric gauges, like (4.60), where there is only an x-component to the vector potential? With $\mathbf{A} = (-By, 0)$, one has

$$L \cdot (A_x - iA_y) = L \cdot (A_x + iA_y) = L \cdot (-By) = L \cdot (-Br\sin\phi) = -i\hbar(-Br\cos\phi) = i\hbar Bx. \quad (4.76)$$

This doesn't give a simple commutation relation between L and b or $b^\dagger$. This leads one to believe, that the properties to do with the canonical angular momentum for this problem, are not physically too important, because of this gauge dependence.

4.1.5 Relation between a, b, and L operators?

Now I assume the discussion only concerns the symmetric gauge, so that the action of b and $b^\dagger$ is to reduce or increase the angular momentum. Also, by the above derivations, we can see immediately that a and $a^\dagger$ not only change the energy, but they also change the angular momentum. Since $a \propto (\pi_x + i\pi_y)$ is a positive angular momentum eigenfunction and $a^\dagger \propto (\pi_x - i\pi_y)$ is a negative angular momentum eigenfunction [the result (4.73)], one can see that

$$[L, a] = +\hbar a, \qquad [L, a^\dagger] = -\hbar a^\dagger. \quad (4.77)$$

This is in contrast to the action with the b and $b^\dagger$ operators, which I repeat here:

$$[L, b] = -\hbar b, \qquad [L, b^\dagger] = +\hbar b^\dagger. \quad (4.78)$$

This is somehow very curious. If there was a ground state of a of zero angular momentum, then by acting with $a^\dagger$ on that state to raise the energy, its action of lowering L would bring it to a negative angular momentum component along z. On the other hand that original ground state of a could be acted upon by the $b^\dagger$ operator, raising its L_z without changing its energy. It means there are multiple ground states of the a operator, that differ in their angular momenta, which is equivalent to differing in their squared radius, Δ^2. When they get acted on by $a^\dagger$, their energy is raised while their L is lowered to a more negative value. But because there are many different states of different L_z for the same energy, there is degeneracy. However, the energy of the system is not dependent on its canonical angular momentum.

Keep in mind, however, based on their construction, the a and b operators commute as follows:

$$[a, b] = [a, b^\dagger] = [a^\dagger, b] = [a^\dagger, b^\dagger] = 0. \quad (4.79)$$

But of course, within each family,

$$[a, a^\dagger] = [b, b^\dagger] = 1. \quad (4.80)$$

To summarize this, both the a and b operators change angular momentum. But only the a operators change the energy, without changing Δ^2, while only the b operators change Δ^2, without changing the energy.

4.1.6 Counting the degeneracy

Consider some eigenstate of the Hamiltonian, i.e., and eigenstate of the number operator $a^\dagger a$, denoted as $|n\rangle$, with energy $E_n = \hbar\omega_B(n + 1/2)$. We can already see that this enough enough to fully specify the state, because there are many such states, with different eigenvalues corresponding to the Δ^2 number operator, $b^\dagger b$. We originally solved this problem as if the system is infinitely extended in the x and y directions. If that is the case, then Δ^2 has no upper limit. But in a real system, there will be a limit, because Δ^2 cannot be larger than the size of the system squared. So without actually trying to solve exactly for the states in a finite system, one can still estimate their degeneracy.

For greatest simplicity in this, suppose the system is circular, of radius R. Then it can be roughly expected that there is a limit on the expectation value of the operator Δ^2, according to

$$\langle \Delta^2 \rangle < R^2, \quad \text{or} \quad \left\langle \frac{2\hbar}{m_e \omega_B}(b^\dagger b + 1/2) \right\rangle < R^2. \tag{4.81}$$

Suppose the eigenvalue of the number operator $b^\dagger b$ is n_b. Then ignoring the factor of $1/2$. this shows that the maximum value for n_b is on the order of

$$n_{b,\max} \approx \frac{m_e \omega_B R^2}{2\hbar} = \frac{R^2}{r_0^2}, \qquad r_0 \equiv \sqrt{\frac{2\hbar}{m_e \omega_B}}. \tag{4.82}$$

This is then the estimate of the degeneracy of any energy eigenstate. The parameter r_0 is the scale of the squared radus operator Δ^2. It is very interesting to express the degeneracy in terms of the magnetic flux $\Phi_B = \int dS \cdot B$ passing through the cross section of the system.

$$n_{b,\max} \approx \frac{m_e \frac{eB}{m_e c} \pi R^2}{2\pi\hbar} = \frac{e}{2\pi\hbar c} \cdot (\pi R^2 B) = \frac{e}{hc} \cdot \Phi_B = \frac{\Phi_B}{\Phi_0}. \tag{4.83}$$

This is written in terms of the fundamental quantum of magnetic flux!

$$\Phi_0 \equiv \left(\frac{hc}{e}\right)_{(\text{CGS})} = \left(\frac{h}{e}\right)_{(\text{SI})} \approx 4.136 \times 10^{-15} \text{ Tm}^2. \tag{4.84}$$

Note that for SI units the cyclotron frequency needed to be substituted as $\omega_B = eB/m_e$. It is clear that for even small magnetic field strength, the degeneracy is going to be very large. It corresponds vaguely to having the center of the cyclotron motion in many differeny locations in the system. With stronger magnetic field, there is even greater degeneracy.

What is the effect of this degeneracy, in general? We are talking about electrons, which are fermions. Therefore, including spin, only two electrons can be placed into any fundamental Landau level, specified by the quantum numbers n and n_b. However, each Landau energy level (specified by only n), when degeneracy is included, can hold an enormous number ($n_{b,\max}$) of electrons. Therefore, if the system has few electrons, in some sense, a large fraction of them can be in the lowest energy Landau levels. This can lead to interesting behavior, that changes with the strength of the magnetic field, as the degeneracy is changed. At very strong magnetic field, most electrons can be allowed to stay in the lowest energy level. As the magnetic field becomes weaker, the electrons are forced to populate higher energy Landau levels. Obviously, these effects will be more apparent at low temperature, where the tendency will be to populate only the lowest energy levels. Higher temperature would already cause the higher Landau levels to be thermally populated and smear out the interesting quantum effects. This behavior leads to the "quantum Hall effects", but I will not delve into the details of that here.

The existence of the flux quantum Φ_0, and its appearance in this problem, is intriguing. The result suggests that at very weak magnetic field, the electron's wave function is very spread out, trying to fill up a large area of the system. An individual electron (for each choice of spin, up or down) is "allowed" to spread out over an area through which one quantum of flux passes. At stronger magnetic field, the electron has to fill a much smaller area. It is as if each electron has to stay close to one "line" of the magnetic field passing through the system. The electrons get squeezed closer together as the magnetic field strength is increased.

4.1.7 Landau level state and wave functions

The actual wave functions of electrons in Landay levels will depend on the choice of the gauge for the vector potential. Even so, it is interesting to see their form in some situations. Here I use the symmetric gauge. Some expressions for the general state vectors can also be found, that don't necessarily depend on the gauge.

Suppose state vectors are written as $|n, n_b\rangle$, where n is the eigenvalue of $a^\dagger a$ and determines the energy, and n_b is the eigenvalue of $b^\dagger b$ and determines squared radius Δ^2. Because the destruction operator has a lowest energy eigenstate, use it to define a ground state, specified by energy quantum number $n = 0$, and Δ^2 quantum number n_b:

$$a|0, n_b\rangle = 0 \tag{4.85}$$

Of course, this ground state has degeneracy and is not unique. Thus the presence of the second quantum number n_b, the eigenvalue of $b^\dagger b$, which plays no role in determining the energy. Suppose in fact one starts with also $n_b = 0$. Then application of $b^\dagger$ will keep the energy fixed, but raise the Δ^2 and the angular momentum. This can be done a number of times, and make use of the basic identity, as would be found for any harmonic oscillator operator,

$$b^\dagger|n, n_b\rangle = \sqrt{n_b + 1}\,|n, n_b + 1\rangle \tag{4.86}$$

This follows from the basic commutation relations, and the fact that $b^\dagger$ is a raising operator. Doing this repeatedly on the state with $n_b = 0$, one will have

$$|n, n_b\rangle = \frac{(b^\dagger)^{n_b}}{\sqrt{n_b!}}|n, 0\rangle \tag{4.87}$$

or more specifically, the different ground states (with $n = 0$) can be found this way by acting on the ground state of smallest Δ^2, that has $n_b = 0$,

$$|0, n_b\rangle = \frac{(b^\dagger)^{n_b}}{\sqrt{n_b!}}|0, 0\rangle \tag{4.88}$$

Further, the other creation operator can also be applied to raise instead the energy, thus a general state vector can be obtained from this lowest ground state:

$$|n, n_b\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}\frac{(b^\dagger)^{n_b}}{\sqrt{n_b!}}|0, 0\rangle \tag{4.89}$$

The operators $a^\dagger$ and $b^\dagger$ commute, so the order here is unimportant.

The wave functions give more physical insight, perhaps. In the coordinate representation the a operator can be expressed

$$a = \frac{\pi_x + i\pi_y}{\sqrt{2m_e\hbar\omega_B}} = \frac{1}{\sqrt{2m_e\hbar\omega_B}}\left\{p_x + ip_y - \frac{e}{c}(A_x + iA_y)\right\} \tag{4.90}$$

Now consider some different coordinate systems. The problem has some circular symmetry, especially in the symmetric gauge. And these kinds of combinations also tend to help. Recall some different transformations, just for the record. To go to polar coordinates, we need

$$(x, y) = (r\cos\phi, r\sin\phi), \qquad (r, \phi) = (\sqrt{x^2 + y^2}, \tan^{-1}(y/x)) \tag{4.91}$$

To transform the derivatives, we need

$$\begin{aligned}
\frac{\partial r}{\partial x} &= \frac{x}{r} = \cos\phi, \qquad & \frac{\partial \phi}{\partial x} &= \frac{-y/x^2}{y^2/x^2} = \frac{-y}{x^2 + y^2} = \frac{-\sin\phi}{r}, \\
\frac{\partial r}{\partial y} &= \frac{y}{r} = \sin\phi, \qquad & \frac{\partial \phi}{\partial y} &= \frac{1/x}{y^2/x^2} = \frac{x}{x^2 + y^2} = \frac{\cos\phi}{r}.
\end{aligned} \tag{4.92}$$

Then there are the relations,

$$\begin{aligned}
\partial_x = \frac{\partial}{\partial x} &= \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \phi}{\partial x}\frac{\partial}{\partial \phi} = \cos\phi\frac{\partial}{\partial r} - \frac{\sin\phi}{r}\frac{\partial}{\partial \phi} \\
\partial_y = \frac{\partial}{\partial y} &= \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial \phi}{\partial y}\frac{\partial}{\partial \phi} = \sin\phi\frac{\partial}{\partial r} + \frac{\cos\phi}{r}\frac{\partial}{\partial \phi}
\end{aligned} \tag{4.93}$$

Using polar coordinates, this is fairly simple, because

$$p_x + ip_y = -i\hbar(\partial_x + i\partial_y) = -i\hbar e^{i\phi}\left(\partial_r + \frac{i}{r}\partial_\phi\right) \tag{4.94}$$

Now with the vector potential of the symmetric gauge applied, there also is

$$A_x + iA_y = \frac{-B}{2}(y - ix) = \frac{iB}{2}(x + iy) = \frac{iB}{2}re^{i\phi}. \tag{4.95}$$

So the destruction operator can be written some different ways, for instance,

$$a = \frac{1}{\sqrt{2m_e\hbar\omega_B}}\left\{p_x + ip_y - \frac{ieB}{2c}(x + iy)\right\} = \frac{e^{i\phi}}{\sqrt{2m_e\hbar\omega_B}}\left\{-i\hbar\left(\partial_r + \frac{i}{r}\partial_\phi\right) - \frac{ieB}{2c}r\right\} \tag{4.96}$$

4.1.8 Ground state wave functions

The last is not so pretty, however, consider it applied to a wave function ψ, which gives zero. The ground states are its solutions:

$$\left\{\partial_r + \frac{i}{r}\partial_\phi + \frac{eB}{2\hbar c}r\right\}\psi(r,\phi) = 0. \tag{4.97}$$

A circularly symmetric solution would be a good place to start, with $\partial_\phi\psi = 0$. Then the equation is easy to integrate,

$$\frac{d\psi}{dr} = -\frac{eB}{2\hbar c}r\psi \quad\Longrightarrow\quad \frac{d\psi}{\psi} = -\frac{eB}{2\hbar c}r\,dr \quad\Longrightarrow\quad \psi(r) = Ce^{-\frac{eB}{4\hbar c}r^2}. \tag{4.98}$$

That is a beautiful solution that is localized over a radius of the order of $r_0 = \sqrt{2\hbar c/eB}$. With greater magnetic field, ψ gets more strongly localized, as was suggested earlier based on the degeneracy arguments. Another way to write this length scale is $\sqrt{2\hbar/m_e\omega_B}$, it is the same as the scale r_0 that determines the squared radius operator Δ^2. Because ψ is circularly symmetric, it has zero angular momentum. Get the constant for normalization:

$$\int d^2r\ |\psi|^2 = C^2\int_0^\infty 2\pi r\,dr\ e^{-\frac{r^2}{r_0^2}} = C^2\pi r_0^2\int_0^\infty d(\frac{r^2}{r_0^2})e^{-\frac{r^2}{r_0^2}} = C^2\pi r_0^2 = 1 \quad\Longrightarrow\quad C = \frac{1}{\sqrt{\pi}\,r_0}. \tag{4.99}$$

So this normalized ground state is

$$\psi_0 = \frac{1}{\sqrt{\pi}\,r_0}\exp\left\{-\frac{r^2}{2r_0^2}\right\}, \qquad r_0 = \sqrt{\frac{2\hbar c}{eB}}. \tag{4.100}$$

Based on the differential equation (4.97) for $a\psi = 0$, there should also be solutions with azimuthal dependence on ϕ varying as $e^{il\phi}$, where l is an integer (the quantum number for the angular momentum). So with the separation of $\psi(r,\phi) = e^{il\phi}\psi_l(r)$, other ground states must satisfy

$$\left\{\frac{d}{dr} - \frac{l}{r} + \frac{eB}{2\hbar c}r\right\}\psi_l(r) = 0, \qquad \text{or} \quad \left\{\frac{d}{d\rho} - \frac{l}{\rho} + \rho\right\}\psi_l(\rho) = 0, \quad \rho = \frac{r}{r_0}. \tag{4.101}$$

Luckily, this equation is very easy to solve! Since we know the solution when $l = 0$, try a slight modification with an unknown power s:

$$\psi_l(\rho) = C\rho^s e^{-\rho^2/2}, \qquad \text{then} \quad \frac{d\psi_l}{d\rho} = \left(\frac{s}{\rho} - \rho\right)\psi_l. \tag{4.102}$$

Inserted into the ODE, the function works exactly if $s = l$. Now get the normalization also,

$$\int d^2r\ |\psi|^2 = C^2\int_0^\infty 2\pi r_0^2\,\rho\,d\rho\ \rho^{2l}e^{-\rho^2} = C^2\pi r_0^2\int_0^\infty du\ u^l e^{-u} = C^2\pi r_0^2(l!) = 1 \tag{4.103}$$

The variable $u = \rho^2$ was used, as well as the basic integral that will be used various times,

$$\int_0^\infty du\ u^l e^{-u} = l! \tag{4.104}$$

Then this normalization constant is

$$C = \frac{1}{\sqrt{\pi(l!)}\ r_0}. \tag{4.105}$$

Then the general ground state wave function that corresponds to the state vector $|0, l\rangle$ is

$$\psi_l(\rho,\phi) = \frac{1}{\sqrt{\pi(l!)}\ r_0}\ e^{il\phi}\rho^l e^{-\rho^2/2}, \qquad \psi_l(r,\phi) = \frac{1}{\sqrt{\pi(l!)}\ r_0^{l+1}}\ e^{il\phi} r^l e^{-r^2/2r_0^2}. \tag{4.106}$$

The solution is valid only if $l \geq 0$. Its angular momentum is clearly $+l\hbar$. Then there are no negative angular momentum ground states! If desired, one could have obtained ψ_l from applying the coordinate representation of operator $b^\dagger$ onto ψ_0. I'll assume that all works out; this way was much simpler.

The probability of finding the electron at some scaled radius ρ is proportional to $2\pi\rho d\rho\ |\psi_l|^2$. A short calculation shows where this peaks:

$$\frac{d}{d\rho}\left[\rho\ |\psi_l|^2\right] \propto \frac{d}{d\rho}\left[\rho^{2l+1}e^{-\rho^2}\right] = \left[(2l+1)\rho^{2l} - 2\rho\rho^{2l+1}\right]e^{-\rho^2} = \rho^{2l}\left[2l+1-2\rho^2\right]e^{-\rho^2} = 0 \tag{4.107}$$

Thus the most likely place to find the electron is at

$$\rho_{\max} = \sqrt{l+\frac{1}{2}}, \qquad \text{or} \quad r_{\max} = \sqrt{l+\frac{1}{2}}\, r_0. \tag{4.108}$$

This increases with the canonical angular momentum in the state.

What about some of the **ground state properties** or **expectation values**? Look at the value of its squared radius. Its center is clearly at the origin. So r^2 can be averaged, which should be the same as doing the average of Δ^2. By design, however, we should have

$$\Delta^2|0,l\rangle = r_0^2(b^\dagger b + 1/2)|0,l\rangle = r_0^2(l+1/2)|0,l\rangle. \tag{4.109}$$

That is, it is an eigenstate, and the eigenvalue is $(l+1/2)r_0^2$. Check if that works out by the more elementary approach, actually calculating

$$\langle r^2\rangle = \int d^2r\ \psi_l^* r^2 \psi_l = \int 2\pi r\, dr\ r^2 \frac{r^{2l}e^{-r^2/r_0^2}}{\pi(l!)r_0^{2(l+1)}} = \frac{r_0^2}{l!}\int_0^\infty du\ u^{l+1}e^{-u} = \frac{r_0^2}{l!}(l+1)! = (l+1)r_0^2. \tag{4.110}$$

Curiously, this is not the same as the eigenvalue of Δ^2. However, we could also check whether indeed this is an eigenstate of Δ^2. This takes more work. Look at the definition,

$$\Delta^2 = X^2 + Y^2 = \left(x + \frac{\pi_y}{m_e\omega_B}\right)^2 + \left(y - \frac{\pi_x}{m_e\omega_B}\right)^2 \tag{4.111}$$

The squares can be easily expanded because the operators inside them commute. Then we get some interesting parts,

$$\Delta^2 = (x^2+y^2) + \frac{1}{m_e^2\omega_B^2}(\pi_x^2+\pi_y^2) + \frac{2}{m_e\omega_B}\left[(xp_y - yp_x) - \frac{e}{c}(xA_y - yA_x)\right] \tag{4.112}$$

The first factor is just r^2, the second is related to the energy operator, so ψ is an eigenfunction of that, the third part is the angular momentum operator, and again ψ is one of its eigenfunctions. But the last part is, in the symmetric gauge,

$$xA_y - yA_x = x\left(\frac{B}{2}x\right) - y\left(\frac{-B}{2}y\right) = \frac{B}{2}(x^2+y^2) = \frac{B}{2}r^2. \tag{4.113}$$

Then the total for the squared radius operator is

$$\Delta^2 = r^2 + \frac{1}{m_e^2\omega_B^2}(2m_eH_0) + \frac{2}{m_e\omega_B}\left[L - \frac{e}{c}\cdot\frac{B}{2}r^2\right] = \frac{2}{m_e\omega_B^2}\left(H_0 + \omega_B L\right). \tag{4.114}$$

The dependence on coordinate r^2 cancelled internally. Write this in dimensionless format,

$$\Delta^2 = \frac{2\hbar}{m_e\omega_B}\left(\frac{H_0}{\hbar\omega_B} + \frac{L}{\hbar}\right) = r_0^2\left(\frac{H_0}{\hbar\omega_B} + \frac{L}{\hbar}\right). \tag{4.115}$$

Now the state with wave function ψ_l found above has the minimum energy eigenvalue, $H_0\psi_l = (\hbar\omega_B/2)\psi_l$, and it angular momentum eigenvalue is $l\hbar$. So it is indeed an eigenfunction (or eigenstate) of Δ^2, and that eigenvalue is

$$\Delta^2 = r_0^2\left(\frac{\hbar\omega_B/2}{\hbar\omega_B} + \frac{l\hbar}{\hbar}\right) = (l + 1/2)r_0^2. \tag{4.116}$$

So indeed, the expectation of r^2 is actually different (and larger) than the eigenvalue of Δ^2 for these states. But they measure different things. $\langle r^2\rangle$ is the spread of the probability for the electron around the origin, while Δ^2 relates to the its center position (X, Y) for the cyclotron motion. Regardless of which average is looked at, it increases linearly with l, the angular momentum. One might also consider further at a later point, how to construct other ground states where X and Y are somehow separately controlled (probably by some linear combinations of the states found here).

From the Hamiltonian and the original expression (4.39) for Δ^2, compared with these last results, we can find the following for the angular momentum,

$$\frac{\Delta^2}{r_0^2} = a^\dagger a + \frac{1}{2} + \frac{L}{\hbar} = b^\dagger b + \frac{1}{2} \quad\Longrightarrow\quad L = \hbar\left(b^\dagger b - a^\dagger a\right). \tag{4.117}$$

Thus here is the explicit demonstration that the angular momentum is determined by the number of "b-quanta" (this is n_b) minus the number of "a-quanta" (this is n). Starting from the ground states, and then acting with $a^\dagger$ to go to excited states, involves going towards more negative angular momentum. Also the angular momentum eigenvalue is then

$$l = n_b - n. \tag{4.118}$$

The number eigenvalues n_b and n are both greater than or equal to zero. So one sees an interesting result, that the angular momentum can only be positive in the ground state ($n = 0$). To get a negative angular momentum (clockwise motion in the xy-plane for a positive electron) requires $n > 0$, i.e., an excited state.

Some good questions to ask at this point are: Is there motion of the electron in the ground states? In which direction? Does it agree with the direction for classical cyclotron motion? Does the motion correspond to an electric current? Do the ground states with higher l (or higher n_b) have a higher current? To answer these, one needs to consider the velocity operator, which is $\mathbf{v} = \vec{\pi}/m_e$. Expand it out to get the components, in the symmetric gauge,

$$v_x = \frac{1}{m_e}\left[p_x - \frac{e}{c}\left(\frac{-B}{2}y\right)\right], \qquad v_y = \frac{1}{m_e}\left[p_y - \frac{e}{c}\left(\frac{+B}{2}x\right)\right]. \tag{4.119}$$

Due to the symmetry of the solution, it would make sense to look instead at the velocity components in circular coordinates. Let me just check the transformation carefully. The transformation is based on the transformation of the unit vectors,

$$\begin{aligned} \hat{r} &= \hat{x}\cos\phi + \hat{y}\sin\phi, & \hat{x} &= \hat{r}\cos\phi - \hat{\phi}\sin\phi, \\ \hat{\phi} &= -\hat{x}\sin\phi + \hat{y}\cos\phi, & \hat{y} &= \hat{r}\sin\phi + \hat{\phi}\cos\phi. \end{aligned} \tag{4.120}$$

Any vector can be expanded in either system,

$$\mathbf{v} = v_x\hat{x} + v_y\hat{y} = v_r\hat{r} + v_\phi\hat{\phi} \tag{4.121}$$

So then transforming from Cartesian to circular,

$$\begin{aligned}\mathbf{v} &= v_x\left(\hat{r}\cos\phi - \hat{\phi}\sin\phi\right) + v_y\left(\hat{r}\sin\phi + \hat{\phi}\cos\phi\right) \\ &= \left(v_x\cos\phi + v_y\sin\phi\right)\hat{r} + \left(-v_x\sin\phi + v_y\cos\phi\right)\hat{\phi}. \end{aligned} \tag{4.122}$$

So the radial and azimuthal components can be read off this last line. Now applying these, together with $x = r\cos\phi$ and $y = r\sin\phi$,

$$\begin{aligned} v_r &= \frac{1}{m_e}\left[\cos\phi\ \pi_x + \sin\phi\ \pi_y\right] \\ &= \frac{1}{m_e}\left[\cos\phi\left(p_x + \frac{eB}{2c}y\right) + \sin\phi\left(p_y - \frac{eB}{2c}x\right)\right] = \frac{1}{m_e}\left[\cos\phi\ p_x + \sin\phi\ p_y\right] \\ &= \frac{-i\hbar}{m_e}\left[\cos\phi\left(\cos\phi\ \partial_r - \frac{\sin\phi}{r}\partial_\phi\right) + \sin\phi\left(\sin\phi\ \partial_r + \frac{\cos\phi}{r}\partial_\phi\right)\right] = \frac{-i\hbar}{m_e}\frac{\partial}{\partial r} = \frac{p_r}{m_e}. \end{aligned} \tag{4.123}$$

$$\begin{aligned} v_\phi &= \frac{1}{m_e}\left[-\sin\phi\ \pi_x + \cos\phi\ \pi_y\right] \\ &= \frac{1}{m_e}\left[-\sin\phi\ \left(p_x + \frac{eB}{2c}y\right) + \cos\phi\left(p_y - \frac{eB}{2c}x\right)\right] = \frac{1}{m_e}\left[\left(-\sin\phi\ p_x + \cos\phi\ p_y\right) - \frac{eB}{2c}r\right] \\ &= \frac{-i\hbar}{m_e}\left[-\sin\phi\left(\cos\phi\ \partial_r - \frac{\sin\phi}{r}\partial_\phi\right) + \cos\phi\left(\sin\phi\ \partial_r + \frac{\cos\phi}{r}\partial_\phi\right)\right] - \frac{eB}{2m_ec}r. \\ &= \frac{-i\hbar}{m_e r}\frac{\partial}{\partial\phi} - \frac{eB}{2m_ec} = \frac{p_\phi}{m_e} - \frac{eB}{2m_ec} = \frac{1}{m_e}\left(\frac{1}{r}L_z - \frac{eB}{2c}r\right). \end{aligned} \tag{4.124}$$

Here the obvious radial and azimuthal momentum operators come out, as could be expected, but there is an extra azimuthal contribution due to the vector potential. Furthermore, to apply these, however, one needs to remember that the physical current is real, and the quantum probability current is determined from the real part of a product. So the electric current density components in the ground states (4.106) found above are given by

$$J_r = \mathrm{Re}\{\psi^*(ev_r)\psi\}, \qquad J_\phi = \mathrm{Re}\{\psi^*(ev_\phi)\psi\}. \tag{4.125}$$

Look first at the radial component, which naively might be expected to be zero, because classically one would think there is just some orbital cyclotron motion of the electron. I can get the radial derivative from the differential equation for ψ_l, and find

$$v_r\psi_l = \frac{-i\hbar}{m_e}\frac{\partial\psi_l}{\partial r} = \frac{-i\hbar}{m_e}\left(\frac{l}{r} - \frac{eB}{2\hbar c}r\right)\psi_l \tag{4.126}$$

Combining with ψ^* gives

$$\psi_l^* v_r\psi_l = \frac{-i\hbar}{m_e}\left(\frac{l}{r} - \frac{eB}{2\hbar c}r\right)|\psi_l|^2. \tag{4.127}$$

OK, the result is pure imaginary. There is then no radial current density in any of the ground states. Naive intuition was correct. Now for the azimuthal component, the ground states are eigenstates of L, so this is simple:

$$v_\phi\psi_l = \frac{1}{m_e}\left(\frac{l\hbar}{r} - \frac{eB}{2c}r\right)\psi_l. \tag{4.128}$$

Then the result for this component is indeed nonzero:

$$J_\phi = \mathrm{Re}\{\psi_l^*(ev_\phi)\psi_l\} = \frac{e}{m_e}\left(\frac{l\hbar}{r} - \frac{eB}{2c}r\right)|\psi_l|^2 = \frac{e\hbar}{m_e r_0}\left(l - \frac{r^2}{r_0^2}\right)\frac{r_0}{r}|\psi_l|^2. \tag{4.129}$$

This is a remarkable result! Near the origin, the current density is in the positive sense (for $l > 0$). [The positive sense is counterclockwise when viewed looking down onto the usual xy-plane, with

the z-axis and magnetic field towards the observer.] But beyond the radius $r > \sqrt{l}\, r_0$, the current flows in the negative sense around the origin. This negative sense is what is expected for a classical electron (positively charged) with the magnetic field in the positive z-direction. So over most of the area of the xy-plane the current goes in the same direction as in the classical system. It is somehow forced to go "backwards" over a small region near the origin with an area of about $\pi l r_0^2$. Obviously, for $l = 0$, the current only flows around in the expected negative azimuthal direction. But it is very curious that all of these different configurations end up having identical energies.

Obviously for large enough radius the current is practically zero, due to the exponential factor. The functional dependence on radius can be summarized:

$$J_\phi(\rho) = \frac{e\hbar}{m_e r_0}\left(l-\rho^2\right)\frac{1}{\rho}\frac{\rho^{2l}e^{-\rho^2}}{\pi(l!)r_0^2} = \frac{e\hbar}{\pi(l!)m_e r_0^3}\left(l-\rho^2\right)\rho^{2l-1}e^{-\rho^2}. \tag{4.130}$$

Consider the current direction at the most probable radius to find the electron. That is at the radius $\rho^2 = l + 1/2$. At that point, it is seen that the current flows in the negative sense, as expected from classical considerations.

These ground states should create a magnetic dipole, due to the circulating current. That is defined by the current times the area it encircles ($(1/c)i\pi r^2$, scaled by c in CGS units). This can be found here, by summing over the circular current contributions at each radius. This current "density" has dimensions of current per length. The current travels in the $\hat{\phi}$ direction, perpendicular to $\hat{r}$. So the element of current is $di = J_\phi dr$. Then the total magnetic dipole μ_l in one of the ground state wave functions is

$$\begin{aligned}
\mu_l &= \frac{1}{c}\int di\ \pi r^2 = \int dr\ \frac{J_\phi}{c}\pi r^2 = \int_0^\infty dr\ \pi r^2 \frac{e\hbar}{\pi(l!)m_e c r_0^3}\left(l-\rho^2\right)\rho^{2l-1}e^{-\rho^2}. \\
&= \frac{e\hbar}{(l!)m_e c}\int_0^\infty d\rho\ \left(l-\rho^2\right)\rho^{2l+1}e^{-\rho^2} = \frac{e\hbar}{2m_e c(l!)}\int_0^\infty du\ (l-u)u^l e^{-u} \qquad (4.131) \\
&= \frac{e\hbar}{2m_e c(l!)}[l(l!) - (l+1)!] = -\frac{e\hbar}{2m_e c}. \qquad (4.132)
\end{aligned}$$

(The transformation $u = \rho^2$ was used to do the integrations.) That's also an amazing result: it doesn't depend on which ground state l, and the value is exactly negative one Bohr magneton (μ_B), the atomic unit of orbital magnetic moment. This value of μ would usually be associated with an electron moving with an orbital angular momentum of $\hbar$. The negative here is the sign expected for the direction of the classical cyclotron motion in the clockwise sense.

4.1.9 Excited state wave functions

There are some different ways to find the excited states. One way is to apply the raising operator $a^\dagger$ to any of the ground states, a number of times equal to the energy excitation quanta that are desired. The expression for that is somewhat complicated:

$$a^\dagger = \frac{\pi_x - i\pi_y}{\sqrt{2m_e\hbar\omega_B}} = \frac{1}{\sqrt{2m_e\hbar\omega_B}}\left\{p_x - ip_y - \frac{e}{c}(A_x - iA_y)\right\} = \frac{e^{-i\phi}}{\sqrt{2m_e\hbar\omega_B}}\left\{-i\hbar\left(\partial_r - \frac{i}{r}\partial_\phi\right) + \frac{ieB}{2c}r\right\} \tag{4.133}$$

Applying this many times to any function could be tedious. It may actually be simpler to find the excited states by solving Schrodinger's equation. Using the symmetric gauge, it is simple to write the Hamiltonian out,

$$H_0 = \frac{\vec{\pi}^2}{2m_e} = \frac{1}{2m_e}\left\{-\hbar^2(\partial_x^2 + \partial_y^2) + \frac{i\hbar eB}{c}(x\partial_y - y\partial_x) + \left(\frac{eB}{2c}\right)^2(x^2+y^2)\right\}. \tag{4.134}$$

The first operator is the Laplacian, ∇^2. The operator in the middle is the angular momentum. The last part is just squared radius. It is clear, for this gauge, that H_0 commutes with $L = L_z$. So the eigenstates will have again an index l related to the angular momentum, and a separated form like

$\psi(r,\phi) = e^{il\phi}\psi_{nl}(r)$. Here the radial w.f. can depend on two indices, one that determines the energy and the other for the angular momentum.

This is probably easyist to look at in circular coordinates, where we want to solve $H_0\psi = E\psi$,

$$\left[\frac{-\hbar^2}{2m_e}\left(\partial_r^2 + \frac{1}{r}\partial_r + \frac{1}{r^2}\partial_\phi^2\right) - \frac{eB}{2m_e c}L_z + \frac{e^2B^2}{8m_e c^2}r^2\right]\psi = E\psi \tag{4.135}$$

The angular momentum is $L = l\hbar$. This also appears as part of the Laplacian. Further, the energy is known to be $E = E_n = \hbar\omega_B(n + 1/2)$. If needed, this can be helpful for finding the wave functions.

For just the radial wave function, there results,

$$\left[\frac{-\hbar^2}{2m_e}\left(\partial_r^2 + \frac{1}{r}\partial_r - \frac{l^2}{r^2}\right) - \frac{eBl\hbar}{2m_e c} + \frac{e^2B^2}{8m_e c^2}r^2\right]\psi = E\psi \tag{4.136}$$

It is put into a convenient dimensionless form by multiplying by $4/\hbar\omega_B$, and using the variable $\rho = r/r_0$, where $r_0 = \sqrt{2\hbar/m_e\omega_B}$:

$$\left[-\partial_\rho^2 - \frac{1}{\rho}\partial_\rho + \frac{l^2}{\rho^2} - 2l + \rho^2\right]\psi = \frac{4E}{\hbar\omega_B}\psi = 4\epsilon\psi \tag{4.137}$$

Here ϵ is introduced as the energy in units of $\hbar\omega_B$. The asymptotics of this equation call for a solution varying as $\psi \sim e^{-\rho^2/2}$ for large radius. This suggests making a transformation to a different form,

$$\begin{aligned} \psi &= f(\rho)e^{-\rho^2/2}, \quad \psi' = (f' - \rho f)e^{-\rho^2/2}, \quad \psi'' = (f'' - 2\rho f' - f + \rho^f)e^{-\rho^2/2}, \\ \psi'' &+ \frac{1}{\rho}\psi' = \left[f'' + (\frac{1}{\rho} - 2\rho)f' + (\rho^2 - 2)f\right]e^{-\rho^2/2} \end{aligned} \tag{4.138}$$

With that, the asymptotic dependence is removed, and the ODE becomes

$$-f'' + \left(2\rho - \frac{1}{\rho}\right)f' + \frac{l^2}{\rho^2}f = (4\epsilon + 2l - 2)f \tag{4.139}$$

Although it may look intimidating, this is actually a fun equation to solve. A single power of ρ does not work. But a power series in ρ sounds like a good idea. Let that be

$$f(\rho) = \sum_k a_k\rho^k, \qquad f' = \sum_k a_k k\rho^{k-1}, \qquad f'' = \sum_k a_k k(k-1)\rho^{k-2} \tag{4.140}$$

This produces in the ODE

$$\sum_k a_k\left[(-k^2 + k - k + l^2)\rho^{k-2} + 2k\rho^k\right] = \sum_k a_k[4\epsilon + 2l - 2]\rho^k \tag{4.141}$$

Shifting $k \to k + 2$ on the term with ρ^{k-2}, this leads to a recursion relation for the coefficients,

$$\left[l^2 - (k+2)^2\right]a_{k+2} = 2[2\epsilon + l - 1 - k]a_k. \tag{4.142}$$

This recursion could go in either direction: towards higher k or towards lower k. But for that to work, the terms in the brackets can't be zero. Of course, if one of them goes to zero, it leads to a terminatin of the recursion, and an end to the series. This is a good thing when it happens, because it will lead to constrants on the solution that determine both the energy eigenvalues and the limitations on the allowed k. Also, it is clear, k always jumps by 2. So the solution either has all even or all odd powers of ρ. However, one thing to be aware of: in the end, the solution for ψ cannot have negative powers of ρ, which would diverge at the origin.

Angular momentum parameter l is already some chosen integer (positive or negative). Look at the bracket on the LHS of (4.142). It will go to zero at index value $k = l - 2$ and $k = -l - 2$. These two solutions means we need to be a little careful.

Positive angular momentum solutions. Suppose first that l is positive, then the important solution is $k = l - 2$ (the other is a negative power, not allowed). The equation then says $a_{l-2} = 0$. That is one end of the series. This means the first nonzero coefficient is for $k = k_{\min} = l$. So the first nonzero term in the series has to be $a_l \neq 0$. For a state of angular momentum $\hbar l$, the lowest power of ρ is ρ^l. That is consistent with the ground state solutions (4.106) already determined earlier.

Now consider iterating to larger values of k. That iteration will terminate when the bracket on the RHS of (4.142) is zero, at some particular $k = k_{\max}$, which gives

$$2\epsilon + l - 1 - k_{\max} = 0 \quad \Longrightarrow \quad \epsilon = \frac{1}{2}\left(k_{\max} - l + 1\right). \tag{4.143}$$

This is basically what was wanted. l is already chosen and $k_{\max}$ is another integer that differs from l by an even integer (k is incremented in steps of 2). Check that this works correctly if $l = 0$: The energy is found to be $\epsilon = (k_{\max} + 1)/2$. But $k_{\max}$ has to be an even integer, so the correct energy levels will indeed come out. For the general case, suppose there are n "steps" of the iteration (incrementing k by 2) to generate $a_{k_{\max}}$ starting from a_l. Then write this as

$$k_{\max} = k_{\min} + 2n = l + 2n \tag{4.144}$$

where n is a positive integer, and including zero. This gives the dimensionless energy as

$$\epsilon = \frac{1}{2}(l + 2n - l + 1) = n + \frac{1}{2} \tag{4.145}$$

which is the expected result.

Negative angular momentum solutions. Now what if l is a negative number? Then the termination on the LHS of (4.142) is due to $k = -l - 2$. The first nonzero term should now be $k_{\min} = -l$, which is a positive power. The first term in the power series is $a_{-l}\rho^{-l}$, but because $l < 0$ there is no divergence at the origin. These states cannot be ground states, but still one can determine their wave functions via the power series. Their solution can be found almost the same as that for positive l. But there is one caveat. The minimum index can be written $k_{\min} = -l = |l|$. The maximum iteration index is then

$$k_{\max} = k_{\min} + 2n = |l| + 2n \tag{4.146}$$

Then for the negative l solutions, the energy formula is different than for positive l:

$$\epsilon = \frac{1}{2}(k_{\max} - l + 1) = \frac{1}{2}(|l| + 2n - l + 1) = n + |l| + \frac{1}{2} \tag{4.147}$$

The formula, however, is the same as that for the positive angular momentum solutions, if we rename $n + |l|$ as the principal quantum number "n", and, make the stipulation that this new n must be at least as large as $|l|$, ie, $\epsilon = n + 1/2$, with $n \geq |l|$. This is an interesting restriction only on the **negative angular momentum** states. However, one can see it makes sense, if really the new n is $n = n_b + |l|$, meaning, the original n that counted the steps of the iteration was actually n_b, and then the principle quantum number is related to l by the expected relation, $n = n_b - l \to n_b + |l|$.

Now this all shows that the energy levels come out as one would like:

$$\epsilon = \frac{1}{2}\left(|l| + 2n - l + 1\right) \to n + \frac{1}{2} \quad \Longrightarrow \quad E_n = \hbar\omega_B\left(n + \frac{1}{2}\right). \tag{4.148}$$

That the energy levels come out correct is a good check of the solution. Indeed, there is no *explicit* dependence on l. But there is an *implicit* dependence on l, because the negative l states must have $n \geq |l|$. This is a really subtle and interesting point.

The construction of the wave functions is summarized as follows.

1. Choose l, it could even be negative. But if it is negative, the state being constructed cannot be a groud state.

2. Choose the number of energy quanta to put into the system, $n \geq -l$ (see pt. 4 below). The power series will start with the term $a_{|l|}\rho^{|l|}$ and end with the term $a_{|l|+2n}\rho^{|l|+2n}$.

3. Generate the expansion coefficients starting from $a_l = 1$ by iterating the recursion relation, which can be expressed as

$$a_{k+2} = \frac{-2[2n+l-k]}{(k+2)^2 - l^2}\, a_k = \frac{-2[k_{\max}-k]}{(k+2)^2 - l^2}\, a_k. \tag{4.149}$$

   The terms oscillate in sign.

4. From the series that is formed, normalize the wave function. The wave function that results corresponds to the state vector $|n,l\rangle$ introduced earlier. The value for the squared central position will be

$$\Delta^2 = r_0^2 \left(n + l + \frac{1}{2}\right) \tag{4.150}$$

   The number of "a-quanta" is n and the number of "b-quanta" is $n+l$. This looks like another constraint, $n + l \geq 0$. Or, in fact, one needs to choose $n \geq -l$ to get allowed states. But this has no bearing on the positive l states, and is the same as the constraint found for the negative l states, $n > |l|$. In other words, if it is a negative angular momentum state, it has to have a number of energy quanta at least as large as the number of negative angular momentum quanta.

Example: $n = 1$ for any l. The solutions for negative l look technically the same as those for positive l, the only difference being what values of n can be chosen. For $n = 1$, the only allowed choice of negative l is $l = -1$. For any value of l the beginning term is $k_{\min} = |l|$. The first term is $a_{|l|}\rho^{|l|}$. There is only one iteration step, which will generate $a_{|l|+2}\rho^{|l|+2}$. With $k = |l|$ and $k_{\max} = |l| + 2$, that iteration gives

$$a_{|l|+2} = \frac{-2 \times 2}{(|l|+2)^2 - l^2} a_{|l|} = \frac{-4a_{|l|}}{2(|l|+2)} = \frac{-2a_{|l|}}{|l|+2}. \tag{4.151}$$

Then the solution for the radial w.f. becomes

$$\psi(r) = a_{|l|}\left(1 - \frac{2}{|l|+2}\rho^2\right)\rho^{|l|}e^{-\rho^2/2} \tag{4.152}$$

and the total w.f. would be $\psi = \psi(r)e^{il\phi}$. To get it normalized one has the integral,

$$I = \int 2\pi r_0^2\, \rho\, d\rho\; a_{|l|}^2 \left(1 - \frac{4}{|l|+2}\rho^2 + \frac{4}{(|l|+2)^2}\rho^4\right)\rho^{2|l|}e^{-\rho^2} = 1. \tag{4.153}$$

With $u = \rho^2$, this is

$$\begin{aligned} I &= \pi r_0^2 a_{|l|}^2 \int_0^\infty du\; \left(1 - \frac{4}{|l|+2}u + \frac{4}{(|l|+2)^2}u^2\right) u^{|l|}e^{-u} \\ &= \pi r_0^2 a_{|l|}^2 \left[|l|! - \frac{4}{|l|+2}(|l|+1)! + \frac{4}{(|l|+2)^2}(|l|+2)!\right] = \pi r_0^2 a_{|l|}^2 |l|! = 1 \\ a_{|l|} &= \frac{1}{\sqrt{\pi|l|!}\; r_0}. \end{aligned} \tag{4.154}$$

Then the normalized w.f. for the $n = 1, l \geq -1$ excited states is

$$\psi(\rho,\phi) = \frac{e^{il\phi}}{\sqrt{\pi|l|!}\; r_0}\left[1 - \frac{2\rho^2}{|l|+2}\right]\rho^{|l|}e^{-\rho^2/2}, \quad \text{for } \; l \geq -1. \tag{4.155}$$

Apparently w.f.s for higher n can be found the same way, and it just becomes a matter of tedious calculations. Probably with some more elegant mathematics, the solutions could be analyzed and organized into a simpler format, in terms of some standard polynomials.

To check some property of the solution, look at its current density and then its net magnetic dipole moment. The current density is given from (4.129), which becomes in this case

$$\begin{aligned} J_\phi &= \frac{e\hbar}{m_e r_0}\left(l-\rho^2\right)\frac{1}{\rho}|\psi_l|^2 = \frac{e\hbar}{m_e r_0}\left(l-\rho^2\right)\frac{\rho^{2|l|-1}e^{-\rho^2}}{\pi(|l|!)r_0^2}\left[1-\frac{2\rho^2}{|l|+2}\right]^2 \\ &= \frac{e\hbar}{\pi|l|!m_e r_0^3}\rho^{2|l|-1}e^{-\rho^2}\left(l-\rho^2\right)\left[1-\frac{4\rho^2}{|l|+2}+\frac{4\rho^4}{(|l|+2)^2}\right] \\ &= \frac{e\hbar}{\pi|l|!m_e r_0^3}\rho^{2|l|-1}e^{-\rho^2}\left[l-\left(1+\frac{4|l|}{|l|+2}\right)\rho^2+\left(\frac{4}{|l|+2}+\frac{4|l|}{(|l|+2)^2}\right)\rho^4-\frac{4}{(|l|+2)^2}\rho^6\right] \end{aligned} \tag{4.156}$$

Do a little more arranging of the part in brackets,

$$J_\phi \sim [...] = l-\left(1+\frac{4|l|}{|l|+2}\right)\rho^2+\frac{8(|l|+1)}{(|l|+2)^2}\rho^4-\frac{4}{(|l|+2)^2}\rho^6 \tag{4.157}$$

Multiplication by $\pi r^2/c$ and integration over radius gives the magnetic dipole moment,

$$\mu_l = \int dr\ \frac{J_\phi}{c}\pi r^2 = \frac{e\hbar}{m_e c|l|!}\int_0^\infty d\rho\ \rho^{2|l|+1}e^{-\rho^2}[...] = \frac{e\hbar}{2m_e c|l|!}\int_0^\infty du\ u^{|l|}e^{-u}[...] \tag{4.158}$$

It's ugly and I hope there isn't an error. Somehow some magic cancellations might occur. All the integrals are of the standard form (4.104), giving different factorials,

$$\mu_l = \frac{e\hbar}{2m_e c\,|l|!}\left\{l|l|!-\left(1+\frac{4|l|}{|l|+2}\right)(|l|+1)!+\frac{8(|l|+1)}{(|l|+2)^2}(|l|+2)!-\frac{4}{(|l|+2)^2}(|l|+3)!\right\} \tag{4.159}$$

Some cancellations take place in the braces,

$$\begin{aligned} \{...\}\div|l|! &= l-(|l|+1)-4|l|\frac{|l|+1}{|l|+2}+8\frac{(|l|+1)^2}{|l|+2}-4(|l|+3)\frac{|l|+1}{|l|+2} \\ &= l-|l|-1-4\frac{|l|+1}{|l|+2}[|l|-2(|l|+1)+|l|+3] \\ &= l-|l|-1-4\frac{|l|+1}{|l|+2}. \end{aligned} \tag{4.160}$$

Then the result for the magnetic dipole in first excited states ($n=1, l\geq 0$) is

$$\mu_l = \frac{e\hbar}{2m_e c}\left\{l-|l|-1-4\ \frac{|l|+1}{|l|+2}\right\} \tag{4.161}$$

I am not sure of this result, it does not have any beautiful simple form. It can be summarized also as

$$\mu_l = \begin{cases} -\left(1+4\ \frac{l+1}{l+2}\right)\frac{e\hbar}{2m_e c}, & \text{for } l\geq 0, \\ -\frac{17}{3}\frac{e\hbar}{2m_e c}, & \text{for } l=-1. \end{cases} \tag{4.162}$$

This is so weird I doubt that is correct. It does give, however, $-3\mu_B$ for $l=0$, and no more than $-5\mu_B$ at large l. It is interesting, though, that all these values are negative, which might be encouraging.

4.2 AC fields acting on Landau levels?

The point of these calculations is to understand how EM waves induce electric (and magnetic) polarization into the electron system, in the presence of the DC magnetic field. Thus, the next step is to see the effect of an AC field on the electrons in Landau levels. The AC field to consider is the oscillating optical electric field due to an electromagnetic wave passing through the system.

Before proceeding on that program, let me consider the degeneracy of the Landau levels–how large is it, typically, in an experimental situation where Faraday rotation might be measured? How many electrons can occupy each level? This is important for the counting of state occupancy, when given a certain number density of electrons as in an electron gas.

Let's suppose the DC magnetic field strength is 1.0 tesla. Then the cyclotron frequency in SI units is

$$\omega_B = \frac{eB}{m_e} = \frac{(1.602 \times 10^{-19}\mathrm{C})(1.0\,\mathrm{T})}{9.11 \times 10^{-31}\mathrm{kg}} = 1.76 \times 10^{11}\,\mathrm{rad/s}. \tag{4.163}$$

This corresponds to a frequency $f = \omega_B/2\pi = 28$ GHz, well below optical frequencies. Then the Landau length scale r_0 is

$$r_0 = \sqrt{\frac{2\hbar}{m_e\omega_B}} = \sqrt{\frac{6.626 \times 10^{-34}\mathrm{Js}/\pi}{(9.11 \times 10^{-31}\mathrm{kg})(1.76 \times 10^{11}\,\mathrm{rad/s})}} = 36\text{ nm}. \tag{4.164}$$

This is much larger than I expected! If the magnetic field were smaller, this size would be even bigger. For instance, at $B = 0.1$ T, using the alternative form in SI units,

$$r_0 = \sqrt{\frac{2\hbar}{eB}} = \sqrt{\frac{6.626 \times 10^{-34}\mathrm{Js}/\pi}{(1.602 \times 10^{-19}\mathrm{C})(0.1\,\mathrm{T})}} = 115\text{ nm}. \tag{4.165}$$

This is much larger than the typical size of nanoparticles that I might be interested in.

The degeneracy of any Landau level is $n_{b,\max} \approx (R/r_0)^2$, for a system of radius R. Suppose the system is a particle with a radius of 1000 nm, in the 1.0 T field. The degeneracy is then about $(1000/36)^2 \approx 800$. Many electrons could squeeze into each level. On the other hand, suppose the system is a nanoparticle with a radius of only 10 nm, then, the degeneracy comes out $(10/36)^2 \approx 0.08$; what does that mean?? It could only mean that the system constrains the electrons so much, that the effects of the boundaries are important. The sense of Landau levels as discussed in these notes would not really apply, it seems. Then what? Further, the size of r_0 is much much greater than the electron displacements expected due to moderate sized electric fields in an optical pulse (on the order of 10^{-14} m for 500 nm wavelength light of electric field amplitude 1.0 MV/m). If the Landau level wavefunction does not fit into the system, then these solutions are incorrect. So there has to be some different theory for the effects of the DC magnetic field in this situation.

4.3 Magnetic states in confined cylindrical geometry

So for the moment consider this situation of a nanometer-sized system, much smaller than r_0 for the given applied DC magnetic field. Then the Landau ground state wavefunction does not fit into the system, it does not apply. Instead, what are the states when the boundary condition is that the wave function goes to zero at the boundary of the system? Let me assume a circular system of radius R. Essentially, this is a cylindrical particle. It could still have a long dimension along the z-axis, parallel to the magnetic field. That may not be totally realistic, however, it can give some idea of the differences encountered, compared to using the Landau levels in an unconstrained geometry.

One can start from the differential equation (4.135) used to find the excited Landau levels. The critical assumption to make is that the scaled radius $\rho = r/r_0 \ll 1$. Then the term in r^2 in the potential an be ignored. Taking the wave function in the separated form, $\psi(\rho,\phi) = e^{il\phi}\psi(\rho)$, the angular momentum is $L = l\hbar$, and the radial equation is reduced to

$$\left[\frac{-\hbar^2}{2m_e}\left(\partial_r^2 + \frac{1}{r}\partial_r + \frac{(il)^2}{r^2}\right) - \frac{eBl\hbar}{2m_e c}\right]\psi = E\psi \tag{4.166}$$

With some re-arranging this becomes Bessel's equation, following these steps,

$$\frac{-\hbar^2}{2m_e}\left(\partial_r^2 + \frac{1}{r}\partial_r - \frac{l^2}{r^2}\right)\psi = \left(E + \frac{eBl\hbar}{2m_e c}\right)\psi \tag{4.167}$$

Move things around some more,

$$\frac{1}{\frac{2m_e}{\hbar^2}\left(E+\frac{eBl\hbar}{2m_ec}\right)}\left(\partial_r^2+\frac{1}{r}\partial_r-\frac{l^2}{r^2}\right)\psi=-\psi \tag{4.168}$$

Define a new position variable,

$$x=\alpha r, \qquad \alpha=\sqrt{\frac{2m_e}{\hbar^2}\left(E+\frac{eBl\hbar}{2m_ec}\right)} \tag{4.169}$$

Then the equation is indeed Bessel's equation:

$$\left(\partial_x^2+\frac{1}{x}\partial_x-\frac{l^2}{x^2}+1\right)\psi=0 \tag{4.170}$$

The solutions that are finite at the origin are the Bessel functions of the first kind, $J_l(x)$. To get the wave function to go to zero at the system boundary, $r=R$, one needs to do

$$J_l(\alpha R)=0 \qquad \Longrightarrow \quad \alpha=\frac{x_{ln}}{R},\ n=1,2,3,... \tag{4.171}$$

So the α must be chosen based on the zeros of the Bessel functions, where x_{ln} is the n^{th} zero of $J_l(x)$. Then once α is determined for some particular solution, it allows calculation of the energy,

$$\alpha^2=\frac{x_{ln}^2}{R^2}=\frac{2m_e}{\hbar^2}\left(E+\frac{eBl\hbar}{2m_ec}\right) \quad \Longrightarrow \quad E_{l,n}=-\frac{eBl\hbar}{2m_ec}+\frac{\hbar^2x_{ln}^2}{2m_eR^2}. \tag{4.172}$$

For the solution to be valid, the energy must be greater than 0. It seems this could put a restriction on the size of l for a chosen n, but that is hard to see by inspection. One can see from the assumption of $r<R\ll r_0$, the following

$$R^2\ll\frac{2\hbar c}{eB} \quad \Longrightarrow \quad \frac{\hbar^2}{2m_eR^2}\gg\frac{\hbar^2\cdot eB}{2m_e\cdot 2\hbar c}=\frac{1}{4}\hbar\omega_B \tag{4.173}$$

The energy and the wave function can be written also as

$$E_{l,n}=\frac{\hbar^2x_{ln}^2}{2m_eR^2}-\frac{l}{2}\hbar\omega_B, \qquad \psi_{ln}=Ce^{il\phi}J_l\left(x_{ln}\frac{r}{R}\right). \tag{4.174}$$

This means that the energy has to be larger than (approximately)

$$E_{l,n}\gg\frac{1}{4}\hbar\omega_Bx_{ln}^2-\frac{l}{2}\hbar\omega_B=\left(\frac{x_{ln}^2}{2}-l\right)\frac{\hbar\omega_B}{2} \tag{4.175}$$

For small l this will be easily satisfied, and the only question might concern large values of l. For example, if $l=50$, probably the first root of $J_{50}(x)$ is not as large as 10?? It would require a value of $x_{ln}>10$ for the energy result to be positive. This could imply a minimum value of n for any chosen l, which seems reasonable, based on the solutions found for the excited Landau levels.

The energy can be written in a better format, for example, using $r_0^2=2\hbar/m_e\omega_B$,

$$E_{l,n}=\frac{\hbar^2x_{ln}^2}{2m_er_0^2}\left(\frac{r_0}{R}\right)^2-\frac{l}{2}\hbar\omega_B=\left[\frac{x_{ln}^2}{2}\left(\frac{r_0}{R}\right)^2-l\right]\frac{\hbar\omega_B}{2}. \tag{4.176}$$

This solution makes better sense when the magnetic field is weaker and then r_0/R is larger. But even at the example parameters for $B=1.0$ T, we might have $r_0/R\approx 36/10$, and energies given by

$$E_{l,n}=\left(6.5x_{ln}^2-l\right)\frac{\hbar\omega_B}{2}. \tag{4.177}$$

Now to check the validity of these solutions and the energies, I could try an approximate asymptotic expression for the zeros of $J_l(x)$. I am not sure of its accuracy for large l, but it should be good for large n. Based on the asymptotic formula,

$$J_l(x) \approx \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{l\pi}{2} - \frac{\pi}{4}\right), \quad x \gg \left|l^2 - \frac{1}{4}\right|, \tag{4.178}$$

then the zeros can be approximated from the zeros of the cosine, which occur when its argument is an odd integer times $\pi/2$, i.e., $(2n-1)\pi/2$, for the different roots, $n = 1, 2, 3...$ So there results

$$x_{ln} = \left[(2n-1) + l + \frac{1}{2}\right]\frac{\pi}{2}, \quad n = 1, 2, 3... \tag{4.179}$$

Check the case mentioned above, $l = 50$; the formula gives $x_{50,1} \approx 81$. That is much greater than the "10" we had wanted, so that solution should be good.

Now the worst case to test should be when l is large, and we want to see if the first root, $n = 1$, will give a positive energy. So put $n = 1$. The energy is dependent on $x_{ln}^2 - 2l$. I have

$$x_{l1}^2 = \left(\frac{3}{2} + l\right)^2 \left(\frac{\pi}{2}\right)^2 > 2l^2. \tag{4.180}$$

That is certainly true (for positive l) by ignoring the 3/2 and approximating $(\pi/2)^2 \approx 2$. Then this gives a good bound on the energies for all the positive l states,

$$E_{l,1} > \left(x_{l1}^2 - 2l\right)\frac{\hbar\omega_B}{4} > 2l(l-1)\frac{\hbar\omega_B}{4} > 0. \tag{4.181}$$

In fact, for any l this gives a number greater than or equal to zero. It is a reasonably good demonstration that the solutions found work for all choices of l and all $n \geq 1$. It does have the weakness, however, of depending on the asymptotoic form of the Bessel functions and their roots.

4.4 Magnetic states in confined spherical geometry?

One could even better, try to solve the same problem (igonoring again the r^2 term in the potential) with a spherical boundary of radius R. This is more realistic for a spherical nanoparticle. The differential equation is nearly the same, just with the Laplacian for polar spherical coordinates, while the z-component of angular momentum is still the same formula, $L_z = -i\hbar\partial_\phi$. But it helps to use a known fact from QM, that the KE depends on

$$\mathbf{p}^2 = p_r^2 + \frac{\vec{L}^2}{r^2}, \qquad p_r^2 = -\frac{\hbar^2}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right). \tag{4.182}$$

So the KE term depends only on the magnitude of the angular momentum, and the Schrodinger equation is

$$\left\{\frac{-\hbar^2}{2m_e}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\vec{L}^2}{2m_e r^2} - \frac{eB}{2m_e c}L_z\right\}\psi = E\psi \tag{4.183}$$

Now in this case, the solutions can be written using the eigenfunctions of $\vec{L}^2$ and L_z, which are the spherical harmonics $Y_{lm}(\theta,\phi)$, with eigenvalues $l(l+1)\hbar^2$ and $m\hbar$, respectively. So the solutions can be written $\psi = Y_{lm}(\theta,\phi)\psi(r)$, where the radial equation is

$$\left\{\frac{-\hbar^2}{2m_e}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{l(l+1)\hbar^2}{2m_e r^2} - \frac{eBm\hbar}{2m_e c}\right\}\psi(r) = E\psi(r) \tag{4.184}$$

I can do a similar re-arrangement as that done for the cylindrical problem,

$$\frac{1}{\frac{2m_e}{\hbar^2}\left(E + \frac{eBm\hbar}{2m_e c}\right)}\left\{-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{l(l+1)}{r^2}\right\}\psi(r) = \psi(r) \tag{4.185}$$

This suggests a new radial variable,

$$x = \alpha r, \qquad \alpha = \sqrt{\frac{2m_e}{\hbar^2}\left(E + \frac{eBm\hbar}{2m_e c}\right)}. \tag{4.186}$$

Then the differential equation becomes

$$\left\{\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\frac{\partial}{\partial x}\right) - \frac{l(l+1)}{x^2} + 1\right\}\psi(x) = 0 \tag{4.187}$$

Conveniently, this is also an equation whose solution is known (because we removed the potential). It can also be expressed as

$$\left\{\frac{\partial^2}{\partial x^2} + \frac{2}{x}\frac{\partial}{\partial x} - \frac{l(l+1)}{x^2} + 1\right\}\psi(x) = 0 \tag{4.188}$$

If the "2" was a 1 it would be Bessel's equation. But that can be arranged. It helps to transform to a rescaled radial wave function by $\psi(x) = u(x)/\sqrt{x}$. Then there are the derivatives,

$$\frac{\partial}{\partial x}\frac{u}{\sqrt{x}} = \frac{1}{\sqrt{x}}\left[u' - \frac{1}{2x}u\right], \qquad \frac{\partial^2}{\partial x^2}\frac{u}{\sqrt{x}} = \frac{1}{\sqrt{x}}\left[u'' - \frac{1}{x}u' + \frac{1}{2}\cdot\frac{3}{2}\cdot\frac{u}{x^2}\right] \tag{4.189}$$

$$\begin{aligned}\left[\frac{\partial^2}{\partial x^2} + \frac{2}{x}\frac{\partial}{\partial x}\right]\frac{u}{\sqrt{x}} &= \frac{2}{x}\cdot\frac{1}{\sqrt{x}}\left[u' - \frac{1}{2x}u\right] + \frac{1}{\sqrt{x}}\left[u'' - \frac{1}{x}u' + \frac{1}{2}\cdot\frac{3}{2}\cdot\frac{u}{x^2}\right] \\ &= \frac{1}{\sqrt{x}}\left[u'' + \frac{1}{x}u' - \frac{1}{4x^2}u\right]\end{aligned} \tag{4.190}$$

The transformation changes the 2 into a 1, but adds an extra term. Now the differential equation has become

$$u'' + \frac{1}{x}u' - \frac{1}{4x^2}u - \frac{l(l-1)}{x^2}u + u = 0 \tag{4.191}$$

The factors $\frac{1}{4} + l^2 + l = (l + \frac{1}{2})^2$. Then this is a Bessel equation at a half integer order, $\nu = l + \frac{1}{2}$:

$$u'' + \frac{1}{x}u' - \frac{(l+\frac{1}{2})^2}{x^2}u + u = 0 \tag{4.192}$$

So the solutions are basically

$$\psi(x) = \frac{1}{\sqrt{x}}\, J_{l+\frac{1}{2}}(x), \tag{4.193}$$

which are the spherical Bessel functions, except for a constant of $\sqrt{\pi/2}$. That statement is not too enlightening, as I like to see how things behave in terms of something more concrete. If in fact, one went instead to the more usual transformation, $\psi(x) = f(x)/x$, then the needed derivatives are

$$\psi' = \frac{1}{x}\left[f' - \frac{1}{x}f\right], \qquad \psi'' = \frac{1}{x}\left[f'' - \frac{2}{x}f' + \frac{2}{x^2}f\right] \tag{4.194}$$

$$\frac{2}{x}\psi' + \psi'' = \frac{2}{x}\cdot\frac{1}{x}\left[f' - \frac{1}{x}f\right] + \frac{1}{x}\left[f'' - \frac{2}{x}f' + \frac{2}{x^2}f\right] = \frac{1}{x}f'' \tag{4.195}$$

Then the differential equation is really simple:

$$f'' + \left(1 - \frac{l(l+1)}{x^2}\right)f = 0 \tag{4.196}$$

This is an ODE whose solutions $\psi = f/x$ are some spherical Bessel functions. These may not be the usual spherical Bessel functions in scattering theory, because there the solution should be finite

at large x, whereas here, we want solutions finite at $x \to 0$. At $l = 0$ one sees the solutions for $f(x)$ are $\sin x$ and $\cos x$ functions. What about for general l? The power series solution works well here, because it results in a finite series. But it helps to first take out the oscillatory behaviour. So let $f(x) = e^{isx} g(x)$, where $s = \pm 1$. Then with $f' = e^{isx}(g' + isg')$, and $f'' = e^{isx}(g'' + 2isg' - g)$, there results now,

$$g'' + 2isg' - \frac{l(l+1)}{x^2} g = 0. \tag{4.197}$$

Although it seems we are going in circles, that got rid of the term with just f or g. Now look for solutions finite at the origin, the center of the nanoparticle. Do a power series, which is always fun, ha ha, In this case, it requires negative powers to get a simple solution!

$$g = \sum_k a_k x^{-k}, \qquad g' = -\sum_k a_k\, k x^{-k-1}, \qquad g'' = \sum_k a_k\, k(k+1) x^{-k-2}, \tag{4.198}$$

Shifting the indices so that all are the same powers, x^{-k-2}, the recursion relation is

$$a_k k(k+1) - 2isa_{k+1}(k+1) - l(l+1)a_k = 0 \tag{4.199}$$

This can be expressed as

$$a_{k+1} = \frac{k(k+1) - l(l+1)}{2is(k+1)} a_k. \tag{4.200}$$

The numerator goes to zero when $k = l$, which defines the end of the series. That would imply $a_{l+1} = 0$. This suggests that a_l and all coefficients at lower indexes are non-zero. They can be built up, starting from assuming $a_0 = 1$.

For $l = 0$, one can choose $a_0 = 1/2$, and the solutions for ψ are just $\psi = e^{\pm ix}/2x$. One can form linear combinations, which obvious could be $\cos x/x$ and $\sin x/x$, only the latter is finite at the origin. But it will have zeros determined by the sine, which makes fitting the desired boundary condition very easy, I think.

For $l = 1$, select $a_0 = -1/2$, then a_2 and above will be zero, but

$$a_1 = \frac{-2}{2is} a_0 = isa_0, \qquad \psi_s = \frac{e^{isx}}{x}\left(1 + \frac{is}{x}\right) a_0, \quad s = \pm 1. \tag{4.201}$$

By themselves these diverge at the origin, however, their difference is

$$\psi = \psi_- - \psi_+ = \frac{i\sin x}{x} + \frac{i\cos x}{x^2} \tag{4.202}$$

and their sum is

$$\psi = \psi_- + \psi_+ = -\frac{\cos x}{x} + \frac{\sin x}{x^2} \tag{4.203}$$

The sum is both imaginary, and divergent at the origin–not a solution desired for the NP problem. The difference is an acceptable solution, in fact, it is the usual spherical Bessel function $j_1(x)$.

Try one more, at $l = 2$, with $a_0 = -1/2$. The iterations give

$$a_1 = \frac{-2(3)}{2is} a_0 = 3isa_0, \qquad a_2 = \frac{1(2) - 2(3)}{2is(2)} a_1 = isa_1 = -3a_0. \tag{4.204}$$

Then the solutions are

$$\psi_s = \frac{e^{isx}}{x}\left(1 + \frac{3is}{x} - \frac{3}{x^2}\right) a_0, \quad s = \pm 1. \tag{4.205}$$

Their difference is

$$\psi = \psi_- - \psi_+ = \frac{i\sin x}{x} + \frac{3i\cos x}{x^2} - \frac{3i\sin x}{x^3} \tag{4.206}$$

and their sum is

$$\psi = \psi_- + \psi_+ = -\frac{\cos x}{x} + \frac{3\sin x}{x^2} + \frac{3\cos x}{x^3} \tag{4.207}$$

Now this is curious. In this case, the difference is divergent at the origin, due to the last term. The sum is convergent at the origin, and is proportional to the spherical Bessel function $j_2(x)$.

Obviously the mathematicians have categorized these functions,so I don't need to derive more on that here. In the end what we will use, is that the solutions regular at the origin at the set of spherical Bessel functions, $\psi(x) \sim j_l(x)$. These are also expressed as

$$j_l(x) = \sqrt{\frac{\pi}{2x}}\, J_{l+\frac{1}{2}}(x). \tag{4.208}$$

Then the wave functions for the energy eigenstates are

$$\psi(r,\theta,\phi) = C\, j_l(\alpha r)\, Y_{lm}(\theta,\phi), \qquad \text{with} \;\; j_l(\alpha R) = 0. \tag{4.209}$$

The boundary condition at the surface of the sphere, $r = R$, will select the correct values of α that fits the solution into the sphere. That will relate to the zeros of the Bessel functions, $\alpha R = x_{ln},\ n = 1, 2, 3...$, similar to the problem solved in cylindrical coordinates. In this case, of course, the zeros of the spherical Bessel functions need to be used. Then the relation between α and energy can be inverted and gives the energy eigenvalues, very similar to the cylindrical problem,

$$E_{l,m,n} = \frac{\hbar^2\alpha^2}{2m_e} - \frac{eBm\hbar}{2m_ec} = \frac{\hbar^2 x_{ln}^2}{2m_eR^2} - \frac{eBm\hbar}{2m_ec} \tag{4.210}$$

With the definition of the Landau length $r_0^2 = 2\hbar/m_e\omega_B$, and $\omega_B = eB/m_ec$, this is also arranged as

$$E_{l,m,n} = \frac{\hbar^2 x_{ln}^2}{2m_er_0^2}\left(\frac{r_0}{R}\right)^2 - \frac{m}{2}\hbar\omega_B = \left[\frac{x_{ln}^2}{2}\left(\frac{r_0}{R}\right)^2 - m\right]\frac{\hbar\omega_B}{2} \tag{4.211}$$

The similarity to the solution in cylindrical coordinates is somewhat surprising. Now I have an extra quantum index, but only because I had left out a longitudinal quantum index for the KE associated with p_z in the cylindrical problem. My belief at this point, is that all the possible choices of l, m, n will give acceptable solutions with energies greater than zero, as long as the system is smaller than the Landau length, $R < r_0$. To go much further here, seems to require some numerical evaluations.

One could ask, however, if the creation/annihilation operator algebra works in the confined geometry. At this point, I don't know the answer to that question–except that it certainly does not give the correct energy eigenvalues, without some kind of modification. One would need to account for the dropping of the r^2 term in the potential, due to $\mathbf{A}^2$ being ignored here.

One can check the ground state energy for this problem. I will guess that is associated with an $l = 0$ state, only because then there is only left the p_x^2 and p_y^2 KE terms. If $l = 0$ then the only choice for the azimuthal number is $m = 0$. Then there is no angular dependence and the actual wave function will look like

$$\psi_{0,0,1}(r,\theta,\phi) = C\,\frac{\sin\alpha r}{r}. \tag{4.212}$$

The zeros occur where $\alpha R = x = n\pi,\ n = 1, 2, 3....$ The energies in the set of spherically symmetric states are

$$E_{0,0,n} = \frac{n^2\pi^2}{4}\left(\frac{r_0}{R}\right)^2\hbar\omega_B. \tag{4.213}$$

The lowest choice for an eigenstate is $x = x_{01} = \pi$. So the ground state energy is

$$E_{0,0,1} = \frac{\pi^2}{4}\left(\frac{r_0}{R}\right)^2\hbar\omega_B. \tag{4.214}$$

Consider a setup where $r_0 \approx 115$ nm (at $B = 0.10$ T) and the particle size is $R = 11.5$ nm. Then the spacing of these energy levels is determined by the factor $(\pi^2/4)\times 10^2 \times \hbar\omega_B = 250\,\hbar\omega_B$. In these units, this looks large. It is a situation where the quantum confinement effects are overpowering the magnetic field effects. For a real electron living in electron bands, it is not totally clear how the effects of confinement and the local potential responsible for the bands work together to produce the total energy. This calculation suggests that also the general theory for the bands must be modified

slightly, and the confinement potential could become large in nanoparticles. However, that depends on the actual numerical values for the band energies and $\hbar\omega_B$. The latter is not very large at 0.10 T, being only $\hbar\omega_B \approx (1.054\times10^{-34}\text{J s})(1.76\times10^{10}\text{rad/s})/(1.602\times10^{-19}\text{J/eV}) = 1.2\times10^{-5}$ eV. The band energies, will be from tenths of eV to eV, hence they still dominate the dynamics. Furthermore, the confinement energy does not actually depend on B, see expression (4.210). So in the end, it will probably not significantly affect magneto-optical properties like the Faraday rotation. That will still be determined just by the term coupling B to the angular momentum quantum number m.

If I go to the limit where these solutions should start to break down, that is when the system radius is equal to the Landau length, $R = r_0$. There the ground state energy becomes

$$E_{0,0,1} = \frac{\pi^2}{4}\hbar\omega_B \approx 2.5\hbar\omega_B. \tag{4.215}$$

That is good, because we should not get a result less than $0.5\hbar\omega_B$, or there would be something really wrong. This shows that the approximations used are reasonable.

For comparison, consider $l = 1$ states. Now one can have $m = 0, \pm1$, leading to energy shifts of $\pm0.5\hbar\omega_B$. For the wave function $\psi \sim j_1(x)$, the first few zeros are at

$$x_{1n} \approx 4.49,\ 7.73,\ 10.9,\ 14.1,\ 17, 2.... \tag{4.216}$$

which I got from a calculator at http://keisan.casio.com/has10/SpecExec.cgi. In this case, the lowest state of the $l = 1$ family will be

$$E_{1,1,1} = \left[\frac{4.49^2}{2}\left(\frac{r_0}{R}\right)^2 - 1\right]\frac{\hbar\omega_B}{2} \approx \left[10.1\left(\frac{r_0}{R}\right)^2 - 1\right]\frac{\hbar\omega_B}{2} \tag{4.217}$$

For $R = r_0$, this gives $E_{1,1,1} \approx 9.6\hbar\omega_B$. So it is higher than the lowest $l = 0$ state.

One could also, ask, shouldn't the energy levels change by $\pm\hbar\omega_B$? It is a reasonable question, but the difficulty is that there are different effects producing the total energy, not just a magnetic effect. The confinement causes the energy levels and spacing to change dramatically. Also, my way of writing the energy in units of $\hbar\omega_B$ is misleading. In fact, the confinement term does not depend on B, as already mentioned, and the magnetic term is $-m\hbar\omega_B/2$. The magnetic spacing is actually $\hbar\omega_B/2$. The real curiousity might the factor of 1/2 here! However, that actually makes sense, because the same factor of 1/2 appears in the definition of the Bohr magneton, $\mu_B = e\hbar/2mc$, and this magnetic emergy is just $-\vec{\mu}\cdot\mathbf{B} = -\frac{eL_z}{2m}B_z = -m\mu_B B$. Indeed, in the usual Landau levels of an infinite system, this term due to L_z is cancelled by another term, so the total energy appears mostly independent of L_z (except for the constraints between n and l when $l < 0$ there).

4.4.1 A classical particle in a confined geometry?

For comparison, what if a classical charge e were confined to move around inside a small sphere or cylinder? What would be the typical energy? This may not be a well-defined question, since we know at some level that classical mechanics will break down in small systems. But it could be good for a comparison of the order of magnitude of the energy.

The classical Larmour frequency is still $\omega_B = eB/mc$. With $v = \omega_B r$, the kinetic energy of the particle in a cyclotron orbit of radus r is $E = \frac{1}{2}mv^2 = \frac{1}{2}m\omega_B^2 r^2$. But now the radius can't be larger than the particle. Consider a particle of radius 10 nm in the 0.10 T magnetic field. The Larmor angular frequency for an electron is $\omega_B = 1.76\times10^{10}$ rad/s. If it were in an orbit of 5 nm radius, its speed is only 88 m/s! Then its kinetic energy is only 3.5×10^{-27} J, which is ridiculously small.

On the other hand,the QM energy unit would be considerably larger, $\hbar\omega_B = 1.9\times10^{-24}$ J. It is clear a classical description would not be valid. The de Broglie wavelength would be on the order of $h/mv \approx 8\times10^{-6}$ m. One can forget about any kind of semi-classical limit here. Then a comparison with classical mechanics is not of much use. Still, it was interesting to see how the numbers work out. Further, it gives some credence to the widely spaced energy levels that come out if cases like this, with $R/r_0 \approx 115/10 \approx 11$.

4.5 An adequate theory for coupling to the DC magnetic field?

It is shown already that the concept of Landau levels does not apply if the system is too small. Still, the primary effect of the applied DC magnetic field is to cause splittings of the orbital angular momentum states, labeled by the quantum index m. The fact that the band states are getting confined is true, but not so important in terms of their dependence on magnetic field. The splitting into subbands due to confinement occurs even in the absence of B, see (4.210). These splittings are two separate effects. Since I am mainly interested in Faraday rotation effects, I can ignore the confinement effects on the energy bands. That just gives a set of subbands, still, the important perturbation on them due to the DC magnetic field is

$$\Delta E_m = -\vec{\mu}_L \cdot \mathbf{B} = -m\mu_B B, \qquad \vec{\mu}_L = \frac{e}{2m_e c}\vec{L}. \tag{4.218}$$

This involves the orbital angular momentum and the component of its related magnetic dipole moment $\vec{\mu}_L$ along the DC magnetic field. The component of $\vec{\mu}_L$ along $\mathbf{B}$ is just $m\mu_B$, where $\mu_B = \frac{e\hbar}{2m_e c}$ is the Bohr magneton, the atomic unit of orbital angular momentum. This term comes directly from the cross term of squaring $\mathbf{p} - \frac{e}{c}\mathbf{A}$ in the KE. It is already included intrinsically in the Landau level Hamiltonian.

In the paper on "Faraday effect in semi-conductors," by Boswara, Howard, and Lidiard[2] they have included an energy for Landau levels, $\hbar\omega_B(n + 1/2)$, and also, the above term. That is wrong! That would be counting this interaction twice, it does not make sense. In what I want to do here, I am already going to forget about the Landau levels, because they do not apply in nano particles, but I do need to include this orbital angular momentum term. It will be the term most responsible for causing Faraday rotation, I believe.

So in the end, after much study of Landau levels and confined states, I will not really need any of that to make a simplified QM model for the Faraday rotation. The simplified model has electrons in band states, together with this angular momentum coupling. I think spin can be ignored, because the transitions caused by the optical field do not couple to spin. The transitions do couple to L_z, because the photon carries $\pm\hbar$ of angular momentum along the propagation direction, which is the z-direction in the Faraday setup. That means, as stated in BWL, that the electronic transitions needed must follow the transition rule $\Delta m = \pm 1$. These correspond to either right or left handed circularly polarized photons. I'll clarify the polarizations later.

There may also arise questions about the degeneracy of certain terms involving transitions, and/or counting of initial and final states. That counting should be associated with any corresponding counting of the density of states for initial final levels of an electron. I will apply the theory for the dielectric function as developed in the previous set of notes, especially as concerns band-to-band transitions. However, the response of free conduction electrons should not need the interband theory. It may be very simple and comparable to the plasma response encountered earlier, as caused only by the oscillating vector potential of the optical field.

If the sets of subbands caused by confinement were taken into account, supposing they are orthonormal, there would not be any allowed transitions from one to the other. Then, we can suppose we are doing a theory where all electrons considered are in the lowest of the confined subband states. If we consider transitions from valence to conduction band, still, suppose they are both in the lowest of the confined bands. Really, this means ignoring the energy structure due to geometric confinement. The only sense of the geometric confinement, is that the Landau energy levels are not used at all. The splitting due to geometric confinement is likely to be large compared to the magnetic splitting, hence, it should make sense to ignore it.

5 Quantum dielectric function with DC magnetic field

The paper BWL finds expressions for the Faraday rotation angle in terms of B. Instead, here I want to get the dielectric function $\epsilon(\omega)$ and its dependence on B, a result that I will use in more complex

[2] Proc. Royal Soc. London, Series A, Mathematical and Sciences, Vol. **269**, No. 1336 pp. 125-141 (Aug. 21, 1962), also at http://www.jstor.org/stable/2414441

geometry situations. Thus I want the bulk ϵ but I do not want the bulk Verdet function or Faraday angle directly at this point.

In part A of *Dielectrics* the response theory via density matrix was used to get ϵ mainly from averaging of the electric polarization operator $\hat{\mathbf{P}} = n\mathbf{d} = ne\mathbf{r}$, and also from the current density operator, $\hat{\mathbf{J}} = ne\mathbf{v}$, for $n = N/V$ electrons per unit volume, and velocity operator

$$\mathbf{v} = \frac{1}{m_e}\left[\mathbf{p} - \frac{e}{c}\left(\mathbf{A} + \tilde{\mathbf{A}}\right)\right] \tag{5.1}$$

The first vector potential is of the DC magnetic field, and the second is the oscillating optical field, which is the perturbation. When this is averaged, it gives the current density averaged over the whole volume of the system. Once we know the part of $\mathbf{J}$ that oscillates at the same frequency as the optical source, it can be used to get the dielectric function. The electric polarization and the susceptibility and associated current density are related to the electric field by

$$\mathbf{P} = \tilde{\chi}(\omega)\cdot\mathbf{E}, \qquad \mathbf{J} = -i\omega\mathbf{P}. \tag{5.2}$$

Then there is a direct connection between the current density and electric field, which ends up giving the susceptibility and permittivity,

$$\mathbf{J} = -i\omega\tilde{\chi}(\omega)\cdot\mathbf{E}, \qquad \tilde{\epsilon}(\omega) = 1 + 4\pi\tilde{\chi}(\omega). \tag{5.3}$$

Thus the approach generally rests on finding the current density, then getting the susceptibility, including the damping constant, from the symbolic division,

$$\tilde{\chi}(\omega) = \frac{\mathbf{J}}{-i\omega\mathbf{E}}. \tag{5.4}$$

The main steps of finding the dielectric function from the current density are summarized here. The DC vector potential here will not produce a current oscillating at frequency ω. Therefore it may be OK to ignore it in the calculation of $\mathbf{J}$. In any case, based on finding the averaged current density, that averaging via the perturbation of the density matrix by $\tilde{\mathbf{A}}$ gives an expression,

$$\mathbf{J} = \langle ne\mathbf{v}\rangle = \mathrm{Tr}\{ne\mathbf{v}(\hat{\rho}_0 + \hat{\rho}_1)\} = ne\left(\mathrm{Tr}\{\hat{\rho}_0\mathbf{v}\} + \mathrm{Tr}\{\hat{\rho}_1\mathbf{v}\}\right) = \mathbf{J}_0 + \mathbf{J}_1. \tag{5.5}$$

The unperturbed density matrix $\hat{\rho}_0$ is associated with the Hamiltonian that includes the normal KE, the band's potential, and the DC magnetic field,

$$H_0 = \frac{\mathbf{p}^2}{2m_e} + U(\mathbf{r}) - \frac{e}{m_e c}\mathbf{A}\cdot\mathbf{p} \tag{5.6}$$

The last term, in the symmetric gauge, is the same as $-\vec{\mu}_L\cdot\mathbf{B} = -m\mu_B B$ that was mentioned earlier. These states are labeled by a band index b, a wave vector $\mathbf{k}$, and the angular momentum quantum number m, and have energies E_i. The DC field enters in these energies.

The perturbation is the AC EM field, as it interacts with momentum and with the DC vector potential! The term in the Hamiltonian is

$$H_1 = -\frac{e}{m_e c}\tilde{\mathbf{A}}\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right) \equiv -\frac{e}{m_e c}\tilde{\mathbf{A}}\cdot\vec{\pi}, \qquad \tilde{\mathbf{A}} = \mathbf{A}_q e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}. \tag{5.7}$$

Here I am using $\vec{\pi}$ as an operator containing the DC vector potential but not the AC part. The corresponding variation caused in the density matrix is

$$\hat{\rho}_1 = \sum_{fi}\frac{(w_i - w_f)|f\rangle\langle f|H_1|i\rangle\langle i|}{\hbar(\omega + i\gamma) + (E_i - E_f)} \tag{5.8}$$

The factor γ is a somewhat artificial damping constant, written here as a frequency, introduced for convergence. It is supposed to represent the slow turning on of the perturbation for times $t < 0$.

Alternatively, its presence means the solution is found with the retarded Green's function. It has to be the same γ that is damping the electron motion in the expression connecting $\mathbf{J}$ and $\mathbf{E}$.

One can see that terms depending on the square of the vector potential (and cross terms between $\mathbf{A}$ and $\tilde{\mathbf{A}}$) are ignored. Ignoring the square of the DC vector potential is exactly the same as the approximation we made that the system is very small compared to the Landau length. Ignoring the square of the AC vector potential means that nonlinear optical terms are excluded. It is useful to express the perturbation in terms of its electric field, in the Coulomb gauge,

$$\mathbf{E} = -\frac{1}{c}\frac{\partial \tilde{\mathbf{A}}}{\partial t} = \frac{i(\omega + i\gamma)}{c}\tilde{\mathbf{A}} \quad \Rightarrow \quad H_1 = -\frac{e}{i(\omega + i\gamma)m_e}\,\mathbf{E}\cdot\vec{\pi}. \tag{5.9}$$

Note: I included the imaginary damping part of the frequency here. It is said to represent the turning on of the perturbation for negative times. The damping in the system is phenomenological and causes a phase shift between the applied field and the response of the current. This factor of γ is needed here if the results are intended to agree with the classical physics calculatons. Further, it is needed so that results from averaging of electric polarization agree with those from averaging the current density.

This means the required matrix elements of the perturbation are

$$\langle f|H_1|i\rangle = -\frac{e}{i(\omega + i\gamma)m_e}\langle f|(E_x\hat{\pi}_x + E_y\hat{\pi}_y)e^{i\mathbf{q}\cdot\mathbf{r}}|i\rangle \tag{5.10}$$

Generally one will do the dipole approximation and take $e^{i\mathbf{q}\cdot\mathbf{r}} \approx 1$.

5.1 The averaged polarization

For polarization averaging as was done in Part A, the calculation is fairly simple, but remember it does not seem to include the plasma current term, curiously. We want the following statistical average:

$$\mathbf{P} = \langle ne\mathbf{r}\rangle = \mathrm{Tr}\left\{\hat{\rho}_1\, ne\mathbf{r}\right\}. \tag{5.11}$$

This is equivalent to a matrix product followed by summing over both indices,

$$\mathbf{P} = ne\sum_{fi}\hat{\rho}_{1,fi}\mathbf{r}_{if}. \tag{5.12}$$

Even with the DC magnetic field, this calculation is the same as without it. The effect of B is only to change the energy levels. Inserting the required matrix elements, this is

$$\mathbf{P} = ne\sum_{fi}\frac{(w_i - w_f)\langle f|\hat{H}_1|i\rangle}{\hbar(\omega + i\gamma) + (E_i - E_f)}\langle i|\hat{\mathbf{r}}|f\rangle \tag{5.13}$$

We can transform into velocity matrix elements, or equivalently, matrix elements of the $\vec{\pi}$ kinetic momentum operator. Try the usual trick. Look at the commutator of $\mathbf{r}$ with the Hamiltonian,

$$[H_0, x] = \left[\frac{p_x^2}{2m_e}, x\right] - \frac{eB}{2m_e c}[L_z, x] = \frac{-i\hbar}{m_e}p_x - \frac{eB}{2m_e c}(i\hbar y) \tag{5.14}$$

That can be simplified to

$$[H_0, x] = \frac{-i\hbar}{m_e}\left(p_x + \frac{eB}{2c}y\right) = \frac{-i\hbar}{m_e}\left(p_x - \frac{e}{c}A_x\right) = \frac{-i\hbar}{m_e}\hat{\pi}_x = -i\hbar\hat{v}_x. \tag{5.15}$$

That's very good, it shows the velocity operator! (As it should.) Check the same for the y-component,

$$[H_0, y] = \left[\frac{p_y^2}{2m_e}, y\right] - \frac{eB}{2m_e c}[L_z, y] = \frac{-i\hbar}{m_e}p_y - \frac{eB}{2m_e c}(-i\hbar x) \tag{5.16}$$

This one simplifies to

$$[H_0, y] = \frac{-i\hbar}{m_e}\left(p_y - \frac{eB}{2m_e c}x\right) = \frac{-i\hbar}{m_e}\left(p_y - \frac{e}{c}A_y\right) = \frac{-i\hbar}{m_e}\hat{\pi}_y = -i\hbar\hat{v}_y. \tag{5.17}$$

It means that one really should include the vector potential terms, and then the matrix elements are much easier! This even includes the effects of correctly averaging the vector potential over the volume of the system. For example, between two states we have

$$\langle f|\hat{\pi}_x|i\rangle = \langle f|\frac{im_e}{\hbar}[H_0, x]|i\rangle = \frac{im_e}{\hbar}(E_f - E_i)\langle f|x|i\rangle \tag{5.18}$$

The same can be done for y, and for z it works too although there is no A_z. So the momentum m.e.s become dipole m.e.s and *vice-versa*. The matrix elements needed can be expressed from

$$\langle f|\hat{\pi}|i\rangle = im_e\omega_{fi}\ \langle f|\,\mathbf{r}\,|i\rangle, \qquad \omega_{fi} \equiv \frac{E_f - E_i}{\hbar}. \tag{5.19}$$

Also, instead of $\vec{\pi}$, one can use $\vec{\pi} = m_e\mathbf{v}$,

$$\langle f|\mathbf{v}|i\rangle = i\omega_{fi}\ \langle f|\,\mathbf{r}\,|i\rangle, \tag{5.20}$$

Now we have all that is needed to get the polarization averaging expression. One gets in terms of the $\hat{\pi}$ variables,

$$\mathbf{P} = ne\sum_{fi}\frac{(w_i - w_f)\langle f|\frac{ie}{(\omega+i\gamma)m_e}\mathbf{E}\cdot\vec{\pi}|i\rangle}{\hbar\omega + i\gamma + (E_i - E_f)}\cdot\frac{\hbar\langle i|\vec{\pi}|f\rangle}{im_e(E_i - E_f)} \tag{5.21}$$

This is usually expressed using the transition frequencies,

$$\mathbf{P} = \frac{ne^2}{\hbar(\omega+i\gamma)m_e^2}\sum_{fi}\frac{(w_i - w_f)}{\omega_{if}}\frac{\langle i|\vec{\pi}|f\rangle\langle f|\mathbf{E}\cdot\vec{\pi}|i\rangle}{\omega + i\gamma + \omega_{if}} \tag{5.22}$$

Instead, in terms of the velocity it is simpler, but nearly the same.

$$\mathbf{P} = \frac{ne^2}{\hbar(\omega+i\gamma)}\sum_{fi}\frac{(w_i - w_f)}{\omega_{if}}\frac{\langle i|\mathbf{v}|f\rangle\langle f|\mathbf{E}\cdot\mathbf{v}|i\rangle}{\omega + i\gamma + \omega_{if}} \tag{5.23}$$

Factoring out the electric field, the result for the susceptibility components is the same expression as found in the absence of the DC magnetic field, using either the $\vec{\pi}$ or velocity operator, from **polarization averaging**,

$$\chi_{ab} = \frac{ne^2}{m_e^2\hbar(\omega+i\gamma)}\sum_{fi}\frac{(w_i - w_f)}{\omega_{if}}\frac{\langle i|\hat{\pi}_a|f\rangle\langle f|\hat{\pi}_b|i\rangle}{\omega + i\gamma + \omega_{if}} \tag{5.24}$$

$$\chi_{ab} = \frac{ne^2}{\hbar(\omega+i\gamma)}\sum_{fi}\frac{(w_i - w_f)}{\omega_{if}}\frac{\langle i|\hat{v}_a|f\rangle\langle f|\hat{v}_b|i\rangle}{\omega + i\gamma + \omega_{if}}. \tag{5.25}$$

Note that there does not appear to be the plasmon term. Or, perhaps it is hiding in there?!

It is convenient to write this in a form with dimensionless factors times a dimensionless sum, like

$$\chi_{ab} = \frac{-ne^2}{m_e\omega(\omega+i\gamma)} \times S_{ab}, \tag{5.26}$$

$$S_{ab} = \frac{-\omega}{m_e\hbar}\sum_{fi}\frac{(w_i - w_f)}{\omega_{if}}\frac{\langle i|\hat{\pi}_a|f\rangle\langle f|\hat{\pi}_b|i\rangle}{\omega + i\gamma + \omega_{if}} \tag{5.27}$$

$$S_{ab} = \frac{-m_e\omega}{\hbar}\sum_{fi}\frac{(w_i - w_f)}{\omega_{if}}\frac{\langle i|\hat{v}_a|f\rangle\langle f|\hat{v}_b|i\rangle}{\omega + i\gamma + \omega_{if}} \tag{5.28}$$

Eventually we need the susceptibilities and permittivities for left and right circular polarizations. These susceptibilities come from the combinations,

$$\chi_R = \chi_{xx} - i\chi_{xy}, \quad \chi_L = \chi_{xx} + i\chi_{xy}. \tag{5.29}$$

We can see that each polarization needs a slightly different sum,

$$S_R = \frac{-\omega}{m_e\hbar}\sum_{fi}\frac{(w_i - w_f)}{\omega_{if}}\frac{\langle i|\hat{\pi}_x|f\rangle\langle f|\hat{\pi}_x - i\hat{\pi}_y|i\rangle}{\omega + i\gamma + \omega_{if}} \tag{5.30}$$

$$S_L = \frac{-\omega}{m_e\hbar}\sum_{fi}\frac{(w_i - w_f)}{\omega_{if}}\frac{\langle i|\hat{\pi}_x|f\rangle\langle f|\hat{\pi}_x + i\hat{\pi}_y|i\rangle}{\omega + i\gamma + \omega_{if}}. \tag{5.31}$$

There appears an assymetry here between x and y indices. But we know $\chi_{xx} = \chi_{yy}$. So we should be able to arrange this differently, if desired. We could have done $\chi_R = \chi_{yy} - i\chi_{xy}$ or even $\chi_R = \chi_{yy} + i\chi_{yx}$, and similarly to get χ_L. If we did a symmetrical sum:

$$\chi_R = \frac{1}{2}\left[\chi_{xx} + \chi_{yy} - i\left(\chi_{xy} - \chi_{yx}\right)\right], \tag{5.32}$$

the matrix element factors would be

$$\begin{aligned} \ldots &= \langle i|\hat{\pi}_x|f\rangle\langle f|\hat{\pi}_x|i\rangle + \langle i|\hat{\pi}_y|f\rangle\langle f|\hat{\pi}_y|i\rangle - i\langle i|\hat{\pi}_x|f\rangle\langle f|\hat{\pi}_y|i\rangle + i\langle i|\hat{\pi}_y|f\rangle\langle f|\hat{\pi}_x|i\rangle \\ &= \langle i|(\hat{\pi}_x + i\hat{\pi}_y)|f\rangle\langle f|(\hat{\pi}_x - i\hat{\pi}_y)|i\rangle = \left|\langle f|(\hat{\pi}_x - i\hat{\pi}_y)|i\rangle\right|^2 \end{aligned} \tag{5.33}$$

There is the opposite sign on all the $\hat{\pi}_y$ for the left polarization result. Remembering to divide by 2 because this is a double counting, we get now, for **polarization averaging**,

$$S_R = \frac{-\omega}{2m_e\hbar}\sum_{fi}\frac{(w_i - w_f)}{\omega_{if}}\frac{\left|\langle f|\hat{\pi}_x - i\hat{\pi}_y|i\rangle\right|^2}{\omega + i\gamma + \omega_{if}} \tag{5.34}$$

$$S_L = \frac{-\omega}{2m_e\hbar}\sum_{fi}\frac{(w_i - w_f)}{\omega_{if}}\frac{\left|\langle f|\hat{\pi}_x + i\hat{\pi}_y|i\rangle\right|^2}{\omega + i\gamma + \omega_{if}}. \tag{5.35}$$

When right polarization is identified by helicity $\nu = -1$ and left by helicity $\nu = +1$, these can be combined into one formula,

$$S_\nu = \frac{-\omega}{2m_e\hbar}\sum_{fi}\frac{(w_i - w_f)}{\omega_{if}}\frac{\left|\langle f|\hat{\pi}_x + i\nu\hat{\pi}_y|i\rangle\right|^2}{\omega + i\gamma + \omega_{if}} \quad \begin{cases}\nu = +1 = L \\ \nu = -1 = R\end{cases} \tag{5.36}$$

We can also do the symmetrization into occupied (i) and unoccupied (f) bands, which makes more sense at low temperature. This is really just splitting the sum into two, and swapping the indices. The i index is about half of the states, and the f index is the other half of the states, so this is not double counting. We've done this before. It gives initially

$$\sum_{fi} \to \sum_i^o\sum_f^u \frac{(w_i - w_f)}{\omega_{if}}\frac{\langle i|\hat{v}_a|f\rangle\langle f|\hat{v}_b|i\rangle}{\omega + i\gamma + \omega_{if}} + \sum_i^u\sum_f^o \frac{(w_i - w_f)}{\omega_{if}}\frac{\langle i|\hat{v}_a|f\rangle\langle f|\hat{v}_b|i\rangle}{\omega + i\gamma + \omega_{if}} \tag{5.37}$$

Switching the names $i \leftrightarrow f$ in the second sum, and then reversing $\omega_{fi} = -\omega_{if}$, etc., gives two terms that add with the same sign, so the susceptibility from **polarization averaging** is

$$\chi_{ab} = \frac{ne^2}{m_e^2\hbar(\omega + i\gamma)}\sum_i^o\sum_f^u \frac{(w_i - w_f)}{\omega_{if}}\left\{\frac{\langle i|\hat{\pi}_a|f\rangle\langle f|\hat{\pi}_b|i\rangle}{\omega + i\gamma + \omega_{if}} + \frac{\langle i|\hat{\pi}_b|f\rangle\langle f|\hat{\pi}_a|i\rangle}{\omega + i\gamma - \omega_{if}}\right\}. \tag{5.38}$$

or

$$\chi_{ab} = \frac{ne^2}{\hbar(\omega + i\gamma)}\sum_i^o\sum_f^u \frac{(w_i - w_f)}{\omega_{if}}\left\{\frac{\langle i|\hat{v}_a|f\rangle\langle f|\hat{v}_b|i\rangle}{\omega + i\gamma + \omega_{if}} + \frac{\langle i|\hat{v}_b|f\rangle\langle f|\hat{v}_a|i\rangle}{\omega + i\gamma - \omega_{if}}\right\}. \tag{5.39}$$

In a form with dimensionless factors times a dimensionless sum, this is

$$\chi_{ab} = \frac{-ne^2}{m_e\omega(\omega+i\gamma)} \times S_{ab}, \tag{5.40}$$

$$S_{ab} = \frac{-\omega}{m_e\hbar}\sum_i^o\sum_f^u \frac{(w_i-w_f)}{\omega_{if}}\left\{\frac{\langle i|\hat{\pi}_a|f\rangle\langle f|\hat{\pi}_b|i\rangle}{\omega+i\gamma+\omega_{if}} + \frac{\langle i|\hat{\pi}_b|f\rangle\langle f|\hat{\pi}_a|i\rangle}{\omega+i\gamma-\omega_{if}}\right\}, \tag{5.41}$$

$$S_{ab} = \frac{-m_e\omega}{\hbar}\sum_i^o\sum_f^u \frac{(w_i-w_f)}{\omega_{if}}\left\{\frac{\langle i|\hat{v}_a|f\rangle\langle f|\hat{v}_b|i\rangle}{\omega+i\gamma+\omega_{if}} + \frac{\langle i|\hat{v}_b|f\rangle\langle f|\hat{v}_a|i\rangle}{\omega+i\gamma-\omega_{if}}\right\}. \tag{5.42}$$

Also going to the formulas for right ($\nu=-1$) and left ($\nu=+1$) circular polarizations, we have

$$S_\nu = \frac{-\omega}{2m_e\hbar}\sum_i^o\sum_f^u \frac{(w_i-w_f)}{\omega_{if}}\left\{\frac{|\langle f|\hat{\pi}_x+i\nu\hat{\pi}_y|i\rangle|^2}{\omega+i\gamma+\omega_{if}} + \frac{|\langle f|\hat{\pi}_x-i\nu\hat{\pi}_y|i\rangle|^2}{\omega+i\gamma-\omega_{if}}\right\}, \begin{cases}\nu=+1=L\\ \nu=-1=R\end{cases}. \tag{5.43}$$

5.2 Current averaging: The plasma current term due to $\hat{\rho}_0$

For the first term in the current density, it seems to be the same as the plasma term found earlier.

$$\langle\mathbf{v}\rangle_0 = \frac{1}{m_e}\left[\mathrm{Tr}\{\hat{\rho}_0\mathbf{p}\} - \frac{e}{c}\mathrm{Tr}\{\hat{\rho}_0(\mathbf{A}+\tilde{\mathbf{A}})\}\right] \tag{5.44}$$

The averaged momentum in the unperturbed state is zero. Further, the average of the DC vector potential (symmetric gauge) gives something that does not oscillate. That leaves only the average of the oscillating field, performed over some volume smaller than the wavelength, so that the dipole approximation is valid. Let me look carefully at the averaging of the vector potential terms. If we did this by first finding the local space-dependent current density, one would need to use the local operator, as shown in other notes,

$$\hat{j}_A(r,t) = \frac{-e^2}{m_e c}|r\rangle\langle r|\hat{\mathbf{A}}_{\rm tot}(\hat{r},t) \tag{5.45}$$

It's expectation value gives the current density at some point (not averaged over volume yet)

$$\begin{aligned}\mathbf{j}_A(r,t) &= \mathrm{Tr}\left\{\hat{\rho}_0\hat{j}_A\right\} = \sum_k\langle k|\sum_i w_i|i\rangle\langle i|\frac{-e^2}{m_e c}|r\rangle\langle r|\hat{\mathbf{A}}_{\rm tot}(\hat{r},t)|k\rangle \\ &= \frac{-e^2}{m_e c}\mathbf{A}_{\rm tot}(\mathbf{r},t)\sum_k w_k|\langle r|k\rangle|^2 = \frac{-e^2}{m_e c}\left[\mathbf{A}+\mathbf{A}_q e^{i(\mathbf{q}\cdot\mathbf{r}-(\omega+i\gamma)t)}\right]\sum_k w_k\left|\psi_k(\mathbf{r})\right|^2\end{aligned} \tag{5.46}$$

Then the averaging over the system volume of interest is made at this point, using the dipole approximation. Adding up the response of N electrons, the result for the part that oscillates at frequency ω is

$$\mathbf{J}_A = \frac{N}{V}\int d^3r\ \mathbf{j}_A(r,t) = \frac{-ne^2}{m_e c}\mathbf{A}_q e^{i\mathbf{q}\cdot\mathbf{r}_c}e^{-i(\omega+i\gamma)t} \tag{5.47}$$

where $\mathbf{r}_c$ is the center of the system. That gives

$$\langle\mathbf{v}\rangle_0 = -\frac{e}{m_e c}\mathbf{A}_q e^{i\mathbf{q}\cdot\mathbf{r}_c}e^{-i(\omega+i\gamma)t} \tag{5.48}$$

The averaged current density is only due to this term,

$$\mathbf{J}_0 = \mathbf{J}_A = -\frac{ne^2}{m_e c}\mathbf{A}_q e^{i\mathbf{q}\cdot\mathbf{r}_c}e^{-i(\omega+i\gamma)t} = -\frac{ne^2}{m_e c}\cdot\frac{c}{i(\omega+i\gamma)}\mathbf{E} = -i\omega\tilde{\chi}_0(\omega)\cdot\mathbf{E} \tag{5.49}$$

This uses the electric field at the center of the system. This leads to one contribution to the susceptibility,

$$\tilde{\chi}_0(\omega) = -\frac{ne^2}{m_e\omega(\omega+i\gamma)}\mathbf{1} \tag{5.50}$$

The $\mathbf{1}$ means the matrix is diagonal. That is the same plasmon term as found earlier, including the effect of electron damping. There is no effect due to the DC magnetic field here.

5.3 The current terms due to $\hat{\rho}_1$ and the perturbation

Next, consider the other contributions. $\hat{\rho}_1$ already oscillates at frequency ω. It involves a sum over "initial" and "final" states. Also, the only averaged velocity terms that can oscillate at frequency ω are the terms from averaging of $\mathbf{p}$ and $\mathbf{A}$, the DC field. One ignores the terms that would involve averaging of $\tilde{\mathbf{A}}$ using $\hat{\rho}_1$, because both of these oscillate at ω, giving a term oscillating at 2ω, which we don't care about here (a nonlinear term). So the desired average is

$$\langle \mathbf{v} \rangle_1 = \frac{1}{m_e} \left[\mathrm{Tr}\{\hat{\rho}_1 \mathbf{p}\} - \frac{e}{c} \mathrm{Tr}\{\hat{\rho}_1 (\mathbf{A} + \tilde{\mathbf{A}})\} \right] \rightarrow \frac{1}{m_e} \left[\mathrm{Tr}\{\hat{\rho}_1 \mathbf{p}\} - \frac{e}{c} \mathrm{Tr}\{\hat{\rho}_1 \mathbf{A}\} \right] \tag{5.51}$$

Do the second term using local space-dependent current density operator, involving only the DC vector potential this time,

$$\hat{j}_A(r) = \frac{-e^2}{m_e c} |r\rangle\langle r| \hat{\mathbf{A}}(\hat{r}) \tag{5.52}$$

The expectation value is the current density at point $\mathbf{r}$. Need to use the change in the density operator:

$$\begin{aligned}
\mathbf{j}_A(r,t) &= \mathrm{Tr}\left\{ \hat{\rho}_1 \hat{j}_A \right\} = \sum_k \langle k| \sum_{fi} \frac{(w_i - w_f)|f\rangle\langle f|H_1|i\rangle\langle i|}{\hbar(\omega + i\gamma) + (E_i - E_f)} \frac{-e^2}{m_e c} |r\rangle\langle r| \hat{\mathbf{A}}(\hat{r}) |k\rangle \\
&= \frac{-e^2}{m_e c} \mathbf{A}(\mathbf{r}) \sum_{fi} \frac{(w_i - w_f)\langle f|H_1|i\rangle\langle i|r\rangle\langle r|f\rangle}{\hbar(\omega + i\gamma) + (E_i - E_f)} \\
&= \frac{-e^2}{m_e c} \mathbf{A}(\mathbf{r}) \sum_{fi} \frac{(w_i - w_f)\langle r|f\rangle\langle f|H_1|i\rangle\langle i|r\rangle}{\hbar(\omega + i\gamma) + (E_i - E_f)} \\
&= \frac{-e^2}{m_e c} \mathbf{A}(\mathbf{r}) \sum_{fi} \frac{(w_i - w_f)\psi_f(r)\langle f|H_1|i\rangle\psi_i^*(r)}{\hbar(\omega + i\gamma) + (E_i - E_f)}
\end{aligned} \tag{5.53}$$

The state k had to match state f to get the second line. We want the volume average of this. The vector potential is proportional to $\mathbf{B}$. The difference of probabilities, for pairs of states that might contribute, is either large (for band to band transitions) or of the order of B (for an intraband transition where $\Delta m = \pm 1$). So this term is hard to evaluate in the most general case. My expectation is that it comes out small. If it could be shown to be an odd function of position, the average would be zero. Or, if some symmetry between the indices might show that swapping i, f gives the opposite sign??

But, it can be looked at another way. The trace can be performed using the matrix elements of the operators. These are

$$\hat{\rho}_{1,fi} = \frac{(w_i - w_f)\langle f|H_1|i\rangle}{\hbar(\omega + i\gamma) + (E_i - E_f)}, \qquad \hat{j}_{A,if} = \frac{-e^2}{m_e c} \langle i|r\rangle\langle r|\hat{\mathbf{A}}(\hat{r})|f\rangle. \tag{5.54}$$

Then the trace is matrix multiplication and summing on the diagonal,

$$\mathbf{j}_A(\mathbf{r},t) = \sum_{fi} \hat{\rho}_{1,fi}\, \hat{j}_{A,if} \tag{5.55}$$

Do the averaging over the volume V in this expression, scaled for N electrons, assuming the dipole approximation for the perturbation term H_1,

$$\mathbf{J}_{A,1} = \frac{N}{V} \int d^3r \sum_{fi} \hat{\rho}_{1,fi}\, \hat{j}_{A,if} = \frac{N}{V} \sum_{fi} \hat{\rho}_{1,fi} \int d^3r\, \hat{j}_{A,if} \tag{5.56}$$

This averaging of the current operator contains an identity operation,

$$\int d^3r\, \hat{j}_{A,if} = \int d^3r\, \frac{-e^2}{m_e c} \langle i|r\rangle\langle r|\hat{\mathbf{A}}(\hat{r})|f\rangle = \frac{-e^2}{m_e c} \langle i|\hat{\mathbf{A}}(\hat{r})|f\rangle. \tag{5.57}$$

Then the desired current expression is rather simple!

$$\begin{aligned}\mathbf{J}_{A,1} &= n\sum_{fi}\hat{\rho}_{1,fi}\frac{-e^2}{m_e c}\langle i|\hat{\mathbf{A}}(\hat{r})|f\rangle \\ &= \frac{-ne^2}{m_e c}\sum_{fi}\frac{(w_i-w_f)\langle f|H_1|i\rangle\langle i|\hat{\mathbf{A}}(\hat{r})|f\rangle}{\hbar(\omega+i\gamma)+(E_i-E_f)}\end{aligned} \tag{5.58}$$

One can also insert the perturbation matrix element, and get

$$\mathbf{J}_{A,1} = \frac{-ne^2}{m_e c}\cdot\frac{-e}{i(\omega+i\gamma)m_e}\sum_{fi}\frac{(w_i-w_f)\langle f|(E_x\hat{\pi}_x+E_y\hat{\pi}_y)|i\rangle\langle i|\hat{\mathbf{A}}(\hat{r})|f\rangle}{\hbar(\omega+i\gamma)+(E_i-E_f)} \tag{5.59}$$

There is also the term due to the momentum current. Follow the same approach. The operator to be averaged is the symmetrized one,

$$\hat{j}_m(r) = \frac{e}{2m_e}\Big[|r\rangle\langle r|\hat{\mathbf{p}}+\hat{\mathbf{p}}|r\rangle\langle r|\Big] \tag{5.60}$$

Its matrix elements are surprisingly simple,

$$\hat{j}_{m,if} = \frac{e}{2m_e}\langle i|\Big[|r\rangle\langle r|\hat{\mathbf{p}}+\hat{\mathbf{p}}|r\rangle\langle r|\Big]|f\rangle \tag{5.61}$$

such that the averaged matrix element is

$$\frac{N}{V}\int d^3r\ \hat{j}_{m,if} = \frac{ne}{m_e}\langle i|\hat{\mathbf{p}}|f\rangle \tag{5.62}$$

The averaging works as follows:

$$\begin{aligned}\mathbf{J}_{m,1} &= n\int d^3r\ \mathrm{Tr}\Big\{\hat{\rho}_1\hat{j}_m\Big\} = n\sum_{fi}\hat{\rho}_{1,fi}\ \int d^3r\ \hat{j}_{m,if} = \\ &= \frac{ne}{m_e}\sum_{fi}\frac{(w_i-w_f)\langle f|H_1|i\rangle\langle i|\hat{\mathbf{p}}|f\rangle}{\hbar(\omega+i\gamma)+(E_i-E_f)}\end{aligned} \tag{5.63}$$

At this point one can see this isn't much different from the previous result. Both can be combined into one expression that involves the operator $\mathbf{p}-\frac{e}{c}\mathbf{A}$, that is

$$\mathbf{J}_1 = \frac{ne}{m_e}\sum_{fi}\frac{(w_i-w_f)\langle f|H_1|i\rangle\langle i|\hat{\mathbf{p}}-\frac{e}{c}\hat{\mathbf{A}}(\hat{r})|f\rangle}{\hbar(\omega+i\gamma)+(E_i-E_f)} \tag{5.64}$$

$$= \frac{-ne^2}{i(\omega+i\gamma)m_e^2}\sum_{fi}\frac{(w_i-w_f)\langle f|(E_x\hat{\pi}_x+E_y\hat{\pi}_y)|i\rangle\langle i|\left[\hat{\mathbf{p}}-\frac{e}{c}\hat{\mathbf{A}}(\hat{r})\right]|f\rangle}{\hbar(\omega+i\gamma)+(E_i-E_f)} \tag{5.65}$$

Need to keep in mind, this involves only the DC vector potential. Also, note that the $\vec{\pi}$ operator is the same as $\hat{\mathbf{p}}-\frac{e}{c}\hat{\mathbf{A}}(\hat{r})$!

5.4 Finding the susceptibility and permittivity – Current averaging

It was found above that $\mathbf{J}_0$ is a diagonal response, while $\mathbf{J}_1$ has off-diagonal response. In other words, write out the currents in x and y directions, as caused by E_x and E_y in the optical field. Consider the total volume-averaged current density, $\mathbf{J}=\mathbf{J}_0+\mathbf{J}_1$. One has for the x-component of current density due to E_x,

$$J_{x,x} = \frac{-ne^2}{i(\omega+i\gamma)m_e}\left\{1+\frac{1}{m_e}\sum_{fi}\frac{(w_i-w_f)\langle i|\hat{\pi}_x(\hat{r})|f\rangle\langle f|\hat{\pi}_x(\hat{r})|i\rangle}{\hbar(\omega+i\gamma)+(E_i-E_f)}\right\}\ E_x \tag{5.66}$$

In the same fashion, the current density along x due to E_y is

$$J_{x,y} = \frac{-ne^2}{i(\omega+i\gamma)m_e}\left\{0 + \frac{1}{m_e}\sum_{fi}\frac{(w_i - w_f)\langle i|\hat{\pi}_x(\hat{r})|f\rangle\langle f|\hat{\pi}_y(\hat{r})|i\rangle}{\hbar(\omega+i\gamma)+(E_i-E_f)}\right\}E_y \tag{5.67}$$

(I swapped the order of matrix elements to give them the same ordering as the indices on $\mathbf{J}$.) That's a clean expression. Let me switch to the notation $i \to k$ and $f \to k'$, and use i, j for coordinate indices to write it generally as

$$J_{ij} = \frac{-ne^2}{i(\omega+i\gamma)m_e}\left\{\delta_{ij} + \frac{1}{m_e}\sum_{kk'}\frac{(w_k - w_{k'})\langle k|\hat{\pi}_i|k'\rangle\langle k'|\hat{\pi}_j|k\rangle}{\hbar(\omega+i\gamma)+(E_k-E_{k'})}\right\}E_j \tag{5.68}$$

Then with a division by $-i\omega$ and removing the electric field, gives the susceptibility,

$$\chi_{ij}(\omega) = \frac{-ne^2}{m_e\omega(\omega+i\gamma)}\left\{\delta_{ij} + \frac{1}{m_e}\sum_{kk'}\frac{(w_k - w_{k'})\langle k|\hat{\pi}_i|k'\rangle\langle k'|\hat{\pi}_j|k\rangle}{\hbar(\omega+i\gamma)+(E_k-E_{k'})}\right\} \tag{5.69}$$

Then one can read off the dimensionless sum as defined earlier,

$$\chi_{ij} = \frac{-ne^2}{m_e\omega(\omega+i\gamma)}\left(\delta_{ij} + S_{ij}\right), \tag{5.70}$$

$$S_{ij} = \frac{1}{m_e\hbar}\sum_{kk'}\frac{(w_k - w_{k'})\langle k|\hat{\pi}_i|k'\rangle\langle k'|\hat{\pi}_j|k\rangle}{\omega+i\gamma+\omega_{kk'}} \tag{5.71}$$

This then leads to the dielectric function by $\epsilon(\omega) = 1 + 4\pi\chi(\omega)$,

$$\epsilon_{ij}(\omega) = \delta_{ij} - \frac{4\pi ne^2}{m_e\omega(\omega+i\gamma)}\left\{\delta_{ij} + \frac{1}{m_e}\sum_{kk'}\frac{(w_k - w_{k'})\langle k|\hat{\pi}_i|k'\rangle\langle k'|\hat{\pi}_j|k\rangle}{\hbar(\omega+i\gamma)+(E_k-E_{k'})}\right\} \tag{5.72}$$

One can check that the terms in the sum are dimensionless.

For circular polarization problems, however, we want to get $\epsilon_R = \epsilon_{xx} - i\epsilon_{xy}$ and $\epsilon_L = \epsilon_{xx} + i\epsilon_{xy}$, as was shown in a previous section. For reference, these are seen to be

$$\epsilon_R(\omega) = 1 - \frac{4\pi ne^2}{m_e\omega(\omega+i\gamma)}\left\{1 + \frac{1}{m_e}\sum_{fi}\frac{(w_i - w_f)\langle i|\hat{\pi}_x|f\rangle\langle f|\hat{\pi}_x - i\hat{\pi}_y|i\rangle}{\hbar(\omega+i\gamma)+(E_i-E_f)}\right\} \tag{5.73}$$

$$\epsilon_L(\omega) = 1 - \frac{4\pi ne^2}{m_e\omega(\omega+i\gamma)}\left\{1 + \frac{1}{m_e}\sum_{fi}\frac{(w_i - w_f)\langle i|\hat{\pi}_x|f\rangle\langle f|\hat{\pi}_x + i\hat{\pi}_y|i\rangle}{\hbar(\omega+i\gamma)+(E_i-E_f)}\right\} \tag{5.74}$$

There isn't really any lack of symmetry between x and y, with the transformations done earlier we know that this is equivalent to using the dimensionless sums as

$$S_R = \frac{1}{m_e\hbar}\sum_{fi}\frac{(w_i - w_f)\langle i|\hat{\pi}_x|f\rangle\langle f|\hat{\pi}_x - i\hat{\pi}_y|i\rangle}{\omega+i\gamma+\omega_{if}} = \frac{1}{2m_e\hbar}\sum_{fi}\frac{(w_i - w_f)\left|\langle f|\hat{\pi}_x - i\hat{\pi}_y|i\rangle\right|^2}{\omega+i\gamma+\omega_{if}} \tag{5.75}$$

$$S_L = \frac{1}{m_e\hbar}\sum_{fi}\frac{(w_i - w_f)\langle i|\hat{\pi}_x|f\rangle\langle f|\hat{\pi}_x + i\hat{\pi}_y|i\rangle}{\omega+i\gamma+\omega_{if}} = \frac{1}{2m_e\hbar}\sum_{fi}\frac{(w_i - w_f)\left|\langle f|\hat{\pi}_x + i\hat{\pi}_y|i\rangle\right|^2}{\omega+i\gamma+\omega_{if}} \tag{5.76}$$

Combined into a single equation,

$$S_\nu = \frac{1}{2m_e\hbar}\sum_{fi}\frac{(w_i - w_f)\left|\langle f|\hat{\pi}_x + i\nu\hat{\pi}_y|i\rangle\right|^2}{\omega+i\gamma+\omega_{if}}, \quad \begin{cases}\nu = +1 = L \\ \nu = -1 = R\end{cases}. \tag{5.77}$$

5.4.1 Symmetrizing for occupied and unoccupied bands

In all the above expressions there are unrestricted sums over the states. But in a common situation, some states can be considered "occupied", with values of w_k near one in equilibrium, and some other states are considered "unoccupied", with values of w_k very near zero. Even without this distinction, the sums can be re-arranged, by defining k and k' as belonging to two different categories (i.e., lower energy occupied states and higher energy unoccupied states). Then explicitly writing the term where k is occupied and k' unoccupied, and, another term where k is unoccupied and k' is occupied, we have for the sum appearing in the susceptibility χ_{ij} or the permittivity ϵ_{ij},

$$\sum_{kk'} \to \sum_{k}^{o}\sum_{k'}^{u}(w_k - w_{k'})\frac{\langle k|\hat{\pi}_i|k'\rangle\langle k'|\hat{\pi}_j|k\rangle}{\hbar(\omega+i\gamma)+\hbar\omega_{kk'}} + \sum_{k}^{u}\sum_{k'}^{o}(w_k - w_{k'})\frac{\langle k|\hat{\pi}_i|k'\rangle\langle k'|\hat{\pi}_j|k\rangle}{\hbar(\omega+i\gamma)+\hbar\omega_{kk'}} \tag{5.78}$$

Here I inserted also the definition of the transition frequency,

$$\omega_{kk'} \equiv \frac{E_k - E_{k'}}{\hbar}. \tag{5.79}$$

The labels k and k' can be swapped on the second term, which reverses the overall sign and the sign of the transition frequency. The two terms then can be combined, and this gives

$$\sum_{kk'} \to \frac{1}{\hbar}\sum_{k}^{o}\sum_{k'}^{u}(w_k - w_{k'})\left\{\frac{\langle k|\hat{\pi}_i|k'\rangle\langle k'|\hat{\pi}_j|k\rangle}{\omega+i\gamma+\omega_{kk'}} - \frac{\langle k|\hat{\pi}_j|k'\rangle\langle k'|\hat{\pi}_i|k\rangle}{\omega+i\gamma-\omega_{kk'}}\right\} \tag{5.80}$$

Generally one would apply this with the occupieds being those states below the Fermi level and the unoccupieds being the states above the Fermi level. This separation only really makes good sense at low temperature (compared to the Fermi temperature, which is usually very high). Finally it means the sums for the two polarizations are

$$S_\nu = \frac{1}{2m_e\hbar}\sum_{i}^{o}\sum_{f}^{u}(w_i - w_f)\left\{\frac{|\langle f|\hat{\pi}_x + i\nu\hat{\pi}_y|i\rangle|^2}{\omega+i\gamma+\omega_{if}} - \frac{|\langle f|\hat{\pi}_x - i\nu\hat{\pi}_y|i\rangle|^2}{\omega+i\gamma-\omega_{if}}\right\}, \quad \begin{cases}\nu=+1=L\\ \nu=-1=R\end{cases}. \tag{5.81}$$

5.5 Application to free or quasi-free electrons?

The simplest test is to apply the last formula to a free electron gas, possibly in a confined system, where one is not using the usual Landau levels. Instead, the electrons have kinetic energy and the coupling of angular momentum to the magnetic field. There is no potential $U(\mathbf{r})$ (although in some sense I want the electrons confined within some radius). It is as if there is a single band, split by the magnetic field according to the energy term $-m\mu_B B$. The electrons could be in something like the confined states of a spherical system as discussed earlier. Or they may be in a single band with some effective mass, hence the idea of quasi-free electrons. But to have truely free electrons, they could be in plane wave states in an unbounded system.

The states k and k' can be any two states of the band, distinguished by whatever quantum numbers are necessary and azimuthal quantum index m. We restrict the sum to terms when m changes only by ±1, in accordance with a selection rule for absorption/emission of photons (due to matrix elements of the momentum operator). So considering just the parts due to momentum currents, the states must change m by ±1. For the moment, ignore the m.e.s of the $\hat{\mathbf{A}}$ operator.

So the states needed should be simultaneous eigenstates of $\mathbf{p}^2$ and $\mathbf{L}^2$ and L_z, for a Hamiltonian,

$$H_0 = \frac{\mathbf{p}^2}{2m_e} - \frac{eB}{2m_e c}L_z. \tag{5.82}$$

But we know the eigenstates here. They are products of spherical Bessel functions and spherical

harmonics. The allowed states, in an unbounded system[3], can be written,

$$\psi_{klm} = Cj_l(kr)Y_{lm}(\theta,\phi), \qquad E_{klm} = \frac{\hbar^2 k^2}{2m_e} - m\mu_B B. \tag{5.83}$$

The energy does not depend on the magnitude of $\mathbf{L}$, only on its z-component. There is a radial momentum energy and a magnetic energy. The radial momentum is a continuum of states in an unbounded system, unlike what was found for the confined system. For any chosen $l \geq 0$, the magnetic quantum number is $m = 0, \pm 1, \pm 2, ... \pm l$.

It will be useful to know the currents in the state, in the sense of what is the action of the momentum operator $\mathbf{p} = (p_x, p_y, p_z)$ on them. This can probably be done most efficiently instead using the spherical components, $\mathbf{p} = (p_r, p_\theta, p_\phi)$, and transforming the results to Cartesian components.

But really, need the matrix elements of $\mathbf{p}$ between these states. From the trick used earlier, we know the following matrix elements between two states:

$$\langle f|\hat{\pi}_x|i\rangle = \langle f|\frac{im_e}{\hbar}[H_0, x]|i\rangle = \frac{im_e}{\hbar}(E_f - E_i)\langle f|x|i\rangle \tag{5.84}$$

The same can be done for y, and for z it works too although there is no A_z. So the momentum m.e.s become dipole m.e.s. Then when *these* are evaluated within the spherical harmonics, the selection rules come out: $\Delta l = \pm 1$, and $\Delta m = 0, \pm 1$. Further, if there was a transition at fixed k, the energy would not change unless m changes, too. So $\Delta m = 0$ can be allowed only if k also changes. The matrix elements needed can be expressed as

$$\langle f|\hat{\pi}|i\rangle = im_e\omega_{fi}\ \langle f|\,\mathbf{r}\,|i\rangle, \qquad \omega_{fi} \equiv \frac{E_f - E_i}{\hbar}. \tag{5.85}$$

The energy splittings due to the magnetic field come in due to changes in m, and those energy changes are linearly proportional to B. However, that is only true when considering transitions at fixed wave vector k. So without getting the matrix elements and their total dependence on k, k', and l, m, it is not easy to see the main change in dielectric function with magnetic field.

5.5.1 Transition matrix elements–States of defined l and m

True "free electrons" in a magnetic field are in Landau levels. However, electrons in bands in a nanoparticle are believed to be in states with a well-defined angular momentum. This section applies to that kind of situation. See a later section for the calculation for electrons in Landau levels, that can be solved exactly.

One can try to get the general dipole matrix element, which is a "standard" QM calculation. The matrix elements have an angular part and a radial part. Let the final state have wave vector k', angular momentum $l' = 1$, some $m' = -l' ... + l'$, and similarly for the initial state. In some notes on Legendre functions and spherical harmonics I figured out the angular part of these matrix elements. Let the states' wave functions be described in some general way (not necessarily just truely free particles) as products of radial and angular parts,

$$\psi_{klm} = R_{kl}(r)Y_{lm}(\Omega) \tag{5.86}$$

For the free particles the radial functions are the spherical Bessel functions. The typical general matrix element needed is

$$\langle k'l'm'|\mathbf{r}|klm\rangle = \int dr\ r^2\, R_{k'l'}(r)\, r\, R_{kl}(r) \int d\Omega\ Y_{l'm'}(\Omega)\, \hat{r}(\Omega)\, Y_{lm}(\Omega) = I_{k'l'kl}\, I_\Omega. \tag{5.87}$$

[3] An important caution. This model really does not work! In a truly unbounded system the correct states are the Landau levels! So this needs to be done with more care. One can see that the Hamiltonian (5.83) is unstable in the sense that there is no well-defined ground state. It has states of very high l and large m with arbitrary negative energy. But that is inconsistent with the original KE Hamiltonian from which it was derived, whose energies are all positive. This present Hamiltonian really only can be applied for a system confined in some volume, so that there are only discrete wavevectors k allowed. The k should really be those produced from the zeros of the Bessel function.

The angular kernel is the unit vector with components (r_x, r_y, r_z), given by

$$\hat{r}(\Omega) = \hat{x}\sin\theta\cos\phi + \hat{y}\sin\theta\sin\phi + \hat{z}\cos\theta = \hat{x}r_x + \hat{y}r_y + \hat{z}r_z. \tag{5.88}$$

The angular matrix elements (I_Ω) were found as follows, depending on which component is considered. The definitions are like this, and similar for r_y and r_z,

$$I_{\Omega x} = \langle l'm'|r_x|lm\rangle = \int d\Omega\; Y^*_{l'm'}(\Omega)\,(\sin\theta\cos\phi)\,Y_{lm}(\Omega) \tag{5.89}$$

These are

$$\langle l+1, m+1|r_x|lm\rangle = +\frac{1}{2}\sqrt{\frac{(l+m+1)(l+m+2)}{(2l+1)(2l+3)}} \qquad \Delta l = +1,\ \Delta m = +1. \tag{5.90}$$

$$\langle l-1, m+1|r_x|lm\rangle = -\frac{1}{2}\sqrt{\frac{(l-m-1)(l-m)}{(2l-1)(2l+1)}} \qquad \Delta l = -1,\ \Delta m = +1. \tag{5.91}$$

$$\langle l+1, m-1|r_x|lm\rangle = -\frac{1}{2}\sqrt{\frac{(l-m+1)(l-m+2)}{(2l+1)(2l+3)}} \qquad \Delta l = +1,\ \Delta m = -1. \tag{5.92}$$

$$\langle l-1, m-1|r_x|lm\rangle = +\frac{1}{2}\sqrt{\frac{(l+m-1)(l+m)}{(2l-1)(2l+1)}} \qquad \Delta l = -1,\ \Delta m = -1. \tag{5.93}$$

Obviously these determine the selection rules. For r_y the results are very similar, but due to the relation between sine and cosine, i.e., $\cos\phi = \frac{1}{2}(e^{i\phi} + e^{-\phi})$, and $\sin\phi = \frac{1}{2i}(e^{i\phi} - e^{-\phi})$, there is a simple symmetry. The matrix elements of r_y are those of r_x, but multiplied by $\mp i$ for $\Delta m = \pm 1$, respectively:

$$\langle l+1, m+1|r_y|lm\rangle = -\frac{i}{2}\sqrt{\frac{(l+m+1)(l+m+2)}{(2l+1)(2l+3)}} \qquad \Delta l = +1,\ \Delta m = +1. \tag{5.94}$$

$$\langle l-1, m+1|r_y|lm\rangle = +\frac{i}{2}\sqrt{\frac{(l-m-1)(l-m)}{(2l-1)(2l+1)}} \qquad \Delta l = -1,\ \Delta m = +1. \tag{5.95}$$

$$\langle l+1, m-1|r_y|lm\rangle = -\frac{i}{2}\sqrt{\frac{(l-m+1)(l-m+2)}{(2l+1)(2l+3)}} \qquad \Delta l = +1,\ \Delta m = -1. \tag{5.96}$$

$$\langle l-1, m-1|r_y|lm\rangle = +\frac{i}{2}\sqrt{\frac{(l+m-1)(l+m)}{(2l-1)(2l+1)}} \qquad \Delta l = -1,\ \Delta m = -1. \tag{5.97}$$

Finally for $r_z = \cos\theta$, the basic integral is

$$I_{\Omega z} = \langle l'm'|r_z|lm\rangle = \int d\Omega\; Y^*_{l'm'}(\Omega)\,(\cos\theta)\,Y_{lm}(\Omega) \tag{5.98}$$

And this gives two results,

$$\langle l+1, m|r_z|lm\rangle = \sqrt{\frac{(l-m+1)(l+m+1)}{(2l+1)(2l+3)}} \qquad \Delta l = +1,\ \Delta m = 0. \tag{5.99}$$

$$\langle l-1, m|r_z|lm\rangle = \sqrt{\frac{(l-m)(l+m)}{(2l-1)(2l+1)}} \qquad \Delta l = -1,\ \Delta m = 0. \tag{5.100}$$

5.6 Permittivity for circular polarizations–States with defined l and m

This section applies to electrons in states of specified angular momentum, but not in Landau levels. It could apply to electrons in band states.

I imagine the situation of high symmetry where the light is propagating along the z-axis. In that case we don't have any need for these z components. Further, it gives an obvious symmetry between the matrix elements for r_x and r_y. Especially, we want some simple combinations to produce $\epsilon_R = \epsilon_{xx} - i\epsilon_{xy}$ and $\epsilon_L = \epsilon_{xx} + i\epsilon_{xy}$, where there are the following needed symmetry relations

$$\langle f|r_y|i\rangle = -i\Delta m\langle f|r_x|i\rangle, \qquad \Delta m = \pm 1. \tag{5.101}$$

The same kind of relation applies to matrix elements of the velocity,

$$\langle f|\hat{v}_y|i\rangle = -i\Delta m\langle f|\hat{v}_x|i\rangle, \qquad \Delta m = \pm 1. \tag{5.102}$$

The product that appears in the sum for defining ϵ_{xx} is

$$\epsilon_{xx} \sim \sum_{fi} g_{fi} \left|\langle f|\hat{v}_x|i\rangle\right|^2 \tag{5.103}$$

On the other hand, one sees the similar factors needed for ϵ_{xy},

$$\epsilon_{xy} \sim \sum_{fi} g_{fi}\langle i|\hat{v}_x|f\rangle\langle f|\hat{v}_y|i\rangle = \sum_{fi} g_{fi}\langle i|\hat{v}_x|f\rangle(-i\Delta m)\langle f|\hat{v}_x|i\rangle = \sum_{fi} g_{fi}(-i\Delta m)\left|\langle f|\hat{v}_x|i\rangle\right|^2. \tag{5.104}$$

These are the same terms but just modified by $(-i\Delta m)$. When these two parts are combined to get the dielectric function for right circular polarization, one has

$$\epsilon_R = \epsilon_{xx} - i\epsilon_{xy} \sim \sum_{fi} g_{fi}\left[1 - i(-i\Delta m)\right]\left|\langle f|\hat{v}_x|i\rangle\right|^2 = \sum_{fi} g_{fi}(1-\Delta m)\left|\langle f|\hat{v}_x|i\rangle\right|^2. \tag{5.105}$$

As the only choices are $\Delta m = \pm 1$, it is seen that only the terms with $\Delta m = -1$ contribute here. This is due to the fact that right circular photons have negative helicity. For left circular photons the situation is opposite, they have positive helicity, and only the terms with $\Delta m = +1$ contribute:

$$\epsilon_L = \epsilon_{xx} + i\epsilon_{xy} \sim \sum_{fi} g_{fi}\left[1 + i(-i\Delta m)\right]\left|\langle f|\hat{v}_x|i\rangle\right|^2 = \sum_{fi} g_{fi}(1+\Delta m)\left|\langle f|\hat{v}_x|i\rangle\right|^2. \tag{5.106}$$

5.6.1 From averaging the current density

So now, based on these results, combine them to get something useful to summarize how to calculate these permittivities. The previous expressions for ϵ_R and ϵ_L, based on **averaging the current density**, become as follows:

$$\epsilon_R = 1 - \frac{4\pi n e^2}{m_e\omega(\omega+i\gamma)}\left\{1 + \frac{m_e}{\hbar}\sum_{fi}\frac{(w_i - w_f)(1-\Delta m)|\langle f|\hat{v}_x|i\rangle|^2}{\omega + i\gamma + \omega_{if}}\right\} \tag{5.107}$$

$$\epsilon_L = 1 - \frac{4\pi n e^2}{m_e\omega(\omega+i\gamma)}\left\{1 + \frac{m_e}{\hbar}\sum_{fi}\frac{(w_i - w_f)(1+\Delta m)|\langle f|\hat{v}_x|i\rangle|^2}{\omega + i\gamma + \omega_{if}}\right\} \tag{5.108}$$

One can see that the factor $1 - \Delta m$ is twice a Kronecker delta function. When $\Delta m = +1$ it gives zero, but when $\Delta m = -1$, it gives a value of 2. The factor $1 + \Delta m$ is equal to 2 only in the opposite case. These are both represented by

$$1 + \nu\Delta m = 2\delta_{\Delta m = \nu} \tag{5.109}$$

So these two formulas are equivalent to the one formula for the sum,

$$S_\nu = \frac{2m_e}{\hbar}\sum_{fi}\frac{(w_i - w_f)\delta_{\Delta m,\nu}|\langle f|\hat{v}_x|i\rangle|^2}{\omega + i\gamma + \omega_{if}} \tag{5.110}$$

Now I want to write this for the case of occupied and unoccupied states. Let me consider first the permittivity ϵ_R for right circular polarization which is controlled by the constraint $\Delta m = m_f - m_i = -1$. Of course, which is "final" and which is "initial" is somewhat arbitrary. So doing the change to $i \to k = o$ for occupied and $f \to k' = u$ for unoccupied, and vice-versa, as presented earlier, we have an expression for the dimensionless summation S_R that is needed,

$$S_R = \frac{1}{m_e}\sum_{fi} \to \frac{m_e}{\hbar}\sum_{k}^{o}\sum_{k'}^{u}(w_k - w_{k'})|\langle k'|\hat{v}_x|k\rangle|^2\left\{\frac{1-(m_{k'}-m_k)}{\omega + i\gamma + \omega_{kk'}} - \frac{1-(m_k - m_{k'})}{\omega + i\gamma - \omega_{kk'}}\right\} \tag{5.111}$$

Really the funny factors involving Δm are meant to be delta functions enforcing the selection rules. But by this symmetrization, one sees that he first term has $\Delta m = m_{k'} - m_k = -1$, while the second has $\Delta m = m_{k'} - m_k = +1$. When either one is satisfied, these have the value $1 \mp \Delta m = 2$. So instead I'll take the 2 out front and write them as Kronecker delta functions:

$$S_R = \frac{1}{m_e}\sum_{fi} \to \frac{2m_e}{\hbar}\sum_{k}^{o}\sum_{k'}^{u}(w_k - w_{k'})|\langle k'|\hat{v}_x|k\rangle|^2\left\{\frac{\delta_{m_{k'}=m_k-1}}{\omega + i\gamma + \omega_{kk'}} - \frac{\delta_{m_{k'}=m_k+1}}{\omega + i\gamma - \omega_{kk'}}\right\} \tag{5.112}$$

These deltas don't do anything special within the braces, however, they select out different possible transitions from the sum. So the two terms can't be any further combined until the actual transitions are specified. For example, this requires one to say if the transitions are from a p-band to an s-band or a d-band. Then the particluar Δm that are present can be analyzed for their contributions in these terms. Then the dielectric function is calculated from the expression,

$$\epsilon_R = 1 - \frac{4\pi n e^2}{m_e\omega(\omega + i\gamma)}(1 + S_R). \tag{5.113}$$

For the permittivity associated with left circular polarization, in the original formula only the terms with $\Delta m = +1$ contributed. Now the organization into occupied and unoccupied states leads to a similar expression for sum S_L but only with the sign of Δm reversed,

$$S_L = \frac{1}{m_e}\sum_{fi} \to \frac{2m_e}{\hbar}\sum_{k}^{o}\sum_{k'}^{u}(w_k - w_{k'})|\langle k'|\hat{v}_x|k\rangle|^2\left\{\frac{\delta_{m_{k'}=m_k+1}}{\omega + i\gamma + \omega_{kk'}} - \frac{\delta_{m_{k'}=m_k-1}}{\omega + i\gamma - \omega_{kk'}}\right\} \tag{5.114}$$

Then obviously this produces the related permittivity according to

$$\epsilon_L = 1 - \frac{4\pi n e^2}{m_e\omega(\omega + i\gamma)}(1 + S_L). \tag{5.115}$$

Apparently the two polarizations can be combined into one formula depending on ν, the symmetrized sums needed are

$$S_\nu = \frac{2m_e}{\hbar}\sum_{k}^{o}\sum_{k'}^{u}(w_k - w_{k'})|\langle k'|\hat{v}_x|k\rangle|^2\left\{\frac{\delta_{m_{k'}=m_k+\nu}}{\omega + i\gamma + \omega_{kk'}} - \frac{\delta_{m_{k'}=m_k-\nu}}{\omega + i\gamma - \omega_{kk'}}\right\} \tag{5.116}$$

Keep in mind: the only terms that contribute must have angular momentum l change by ± 1. There are slightly different matrix elements for those two cases, as shown above. One can say that therefore, only terms related to interband transitions are present. If there is only a single band (i.e., only one value for l), then there is nothing in the sums. To proceed further, it is best to do a more concrete example.

5.6.2 From averaging the electric polarization

By using averaging of the **electric polarization**, if we start from the sums needed, in terms of the velocity operators as,

$$S_\nu = \frac{-m_e\omega}{\hbar}\sum_i^o\sum_f^u \frac{(w_i-w_f)}{\omega_{if}}\left\{\frac{\langle i|\hat{v}_x|f\rangle\langle f|\hat{v}_x+i\nu\hat{v}_y|i\rangle}{\omega+i\gamma+\omega_{if}}+\frac{\langle i|\hat{v}_x|f\rangle\langle f|\hat{v}_x-i\nu\hat{v}_y|i\rangle}{\omega+i\gamma-\omega_{if}}\right\}, \tag{5.117}$$

and do the same kinds of operations, we get that the first term applies for $\Delta m=+1$ and the second for $\Delta m=-1$. That is, we have very simply, mostly repeating some previous algebra,

$$\langle f|\hat{v}_x+i\nu\hat{v}_y|i\rangle = \langle f|\hat{v}_x|i\rangle + (i\nu)(-i\Delta m)\langle f|\hat{v}_x|i\rangle = (1+\nu\Delta m)\langle f|\hat{v}_x|i\rangle. \tag{5.118}$$

That again has the same Kronecker delta as encountered earlier. The second term is similar,

$$\langle f|\hat{v}_x-i\nu\hat{v}_y|i\rangle = \langle f|\hat{v}_x|i\rangle - (i\nu)(-i\Delta m)\langle f|\hat{v}_x|i\rangle = (1-\nu\Delta m)\langle f|\hat{v}_x|i\rangle. \tag{5.119}$$

So again applying

$$1+\nu\Delta m=\delta_{\Delta m=\nu},\quad 1-\nu\Delta m=\delta_{\Delta m=-\nu}, \tag{5.120}$$

the sums needed for electric polarization averaging are

$$S_\nu = \frac{-2m_e\omega}{\hbar}\sum_i^o\sum_f^u \frac{(w_i-w_f)}{\omega_{if}}\left|\langle f|\hat{v}_x|i\rangle\right|^2\left\{\frac{\delta_{m_f=m_i+\nu}}{\omega+i\gamma+\omega_{if}}+\frac{\delta_{m_f=m_i-\nu}}{\omega+i\gamma-\omega_{if}}\right\}, \tag{5.121}$$

Note the differences compared to the current density approach: 1) opposite overall sign; 2) factor ω/ω_{if}; 3) same signs on the two contributions.

5.7 Permittivity of Landau level free electrons–from current density

In the last couple of sub-sections I studied the matrix elements for quasi-free electrons, where an approximate Hamiltonian was used. However, as mentioned there, really one has a different Hamiltonian for the electrons, that must be positive definite. The Hamiltonian (5.83) has negative energies, which is a serious problem with it. The only way to use that type of Hamiltonian is if the system has some geometrical confinement, so that instead of arbitrary continuum of k, there are band values like $k_{ln}=x_{ln}/R$, determined by the zeros of the spherical Bessel functions for electrons confined in a system of radius R. This would insure positive energies. At some point that calculation could be useful, so I have not cut it out of this document.

Now I consider an unbounded system, where the electrons really should be described by Landau levels. These states actually are very well defined, and have all positive energies. In addition, the needed matrix elements for the Faraday rotation problem are easy to find. I should have done this calculation first! The energies of the states, including their motion along the z-axis (parallel to $\mathbf{B}$) are

$$E_{nlk} = \left(n+\frac{1}{2}\right)\hbar\omega_B + \frac{\hbar^2k^2}{2m_e} \tag{5.122}$$

where n is the principle quantum number, $l=n_b-n$ where n_b is the number of b-quanta, giving the angular momentum component $l\hbar$ along z, and $p=p_z=\hbar k$ is a continuous conserved quantity, being the component of momentum parallel to the $\mathbf{B}$-field. The corresponding wave functions in real space vary as

$$\psi_{nlk} = R_{nl}(\rho)e^{il\phi}e^{ikz} \qquad \text{for state} \qquad |nlk\rangle. \tag{5.123}$$

The main thing one needs to be able to calculate are the matrix elements of $\hat{\pi}_x$ and $\hat{\pi}_y$ between two of these states. But these states are eigenstates of the number operator $N=a^\dagger a$ (with eigenvalue n) and $M\equiv b^\dagger b$ (eigenvalue n_b), as well as the angular momentum operator $L=\hbar(b^\dagger b-a^\dagger a)$ (with

eigenvalue $l\hbar$, where $l = n_b - n$). The states are essentially harmonic oscillator-like, and can be constructed from the $n = 0$, $n_b = 0$ ground state as shown earlier,

$$|n, n_b\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} \frac{(b^\dagger)^{n_b}}{\sqrt{n_b!}} |0, 0\rangle \tag{5.124}$$

Either n_b or l must be specified. In terms of angular momentum, there is a simple change,

$$|n, l\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} \frac{(b^\dagger)^{n+l}}{\sqrt{(n+l)!}} |0, 0\rangle \tag{5.125}$$

but then one must remember the constraint that $n + l \geq 0$.

The π operators, though, are expressed in terms of the energy creation and annihilation operators:

$$\hat{\pi}_x = \sqrt{\frac{m\hbar\omega_B}{2}}\ (a + a^\dagger), \quad \hat{\pi}_y = \frac{1}{i}\sqrt{\frac{m\hbar\omega_B}{2}}\ (a - a^\dagger), \tag{5.126}$$

These don't have any dependence on l (or n_b) and not on the longitudinal motion, k. So those quantum numbers are conserved in the transitions. This makes finding the required matrix elements fairly trivial. For harmonic oscillator operators we have the usual relations,

$$a|n\rangle = \sqrt{n}\ |n-1\rangle, \qquad a^\dagger|n\rangle = \sqrt{n+1}\ |n+1\rangle. \tag{5.127}$$

Then here the results for matrix elements are (treating k as discrete although really it is continuous)

$$\langle n'l'k'|\hat{\pi}_x|nlk\rangle = \sqrt{\frac{m_e\hbar\omega_B}{2}}\ \left[\sqrt{n}\ \delta_{n',n-1} + \sqrt{n+1}\ \delta_{n',n+1}\right] \delta_{ll'}\delta_{kk'} \tag{5.128}$$

$$\langle n'l'k'|\hat{\pi}_y|nlk\rangle = -i\sqrt{\frac{m_e\hbar\omega_B}{2}}\ \left[\sqrt{n}\ \delta_{n',n-1} - \sqrt{n+1}\ \delta_{n',n+1}\right] \delta_{ll'}\delta_{kk'} \tag{5.129}$$

We also know that for ϵ_R it is good to know the matrix elements of $(\hat{\pi}_x - i\hat{\pi}_y)$, whereas, for ϵ_L is it good to know the matrix elements of $(\hat{\pi}_x + i\hat{\pi}_y)$. But these are also very easy, because recall that these operator combinations are proportional to the creation/annihilation operators:

$$a = \sqrt{\frac{1}{2m_e\hbar\omega_B}}\ (\hat{\pi}_x + i\hat{\pi}_y), \quad a^\dagger = \sqrt{\frac{1}{2m_e\hbar\omega_B}}\ (\hat{\pi}_x - i\hat{\pi}_y). \tag{5.130}$$

Then these matrix elements good for ϵ_R are found to be

$$\langle n'l'k'|(\hat{\pi}_x - i\hat{\pi}_y)|nlk\rangle = \sqrt{2m_e\hbar\omega_B}\ \langle n'l'k'|a^\dagger|nlk\rangle = \sqrt{2m_e\hbar\omega_B}\sqrt{n+1}\ \delta_{n',n+1}\delta_{ll'}\delta_{kk'}. \tag{5.131}$$

That shows the final state must have *one more* energy quantum than the initial state. Since n_b did not change, the final state has one quantum *less* of angular momentum. The matrix elements good for ϵ_L are found to be similar,

$$\langle n'l'k'|(\hat{\pi}_x + i\hat{\pi}_y)|nlk\rangle = \sqrt{2m_e\hbar\omega_B}\ \langle n'l'k'|a|nlk\rangle = \sqrt{2m_e\hbar\omega_B}\sqrt{n}\ \delta_{n',n-1}\delta_{ll'}\delta_{kk'}. \tag{5.132}$$

and of course now the final state has one quantum *less* of energy, but one quantum *more* of angular momentum. These are really unusual requirements. Again, though, the distinction of "initial" and "final" isn't a physical one, once the sums are evaluated that give the susceptibility, etc.

For ϵ_R, the combination that appears in its sum can be written, taking state $|i\rangle$ as $|nlk\rangle$ and state $|f\rangle$ as $|n'l'k'\rangle$,

$$\begin{aligned}\langle nlk|\hat{\pi}_x|n'l'k'\rangle\langle n'l'k'|(\hat{\pi}_x - i\hat{\pi}_y)|nlk\rangle \quad &= \quad \sqrt{\frac{m_e\hbar\omega_B}{2}}\ \left[\sqrt{n'}\ \delta_{n,n'-1} + \sqrt{n'+1}\ \delta_{n,n'+1}\right] \delta_{ll'}\delta_{kk'} \\ &\times \quad \sqrt{2m_e\hbar\omega_B}\sqrt{n+1}\ \delta_{n',n+1}\delta_{ll'}\delta_{kk'}. \end{aligned} \tag{5.133}$$

In the first part I had to swap the n and n' indices. But now one sees that the only part that can survive is where $n' = n + 1$, so this reduces to

$$\langle nlk|\hat{\pi}_x|n'l'k'\rangle\langle n'l'k'|(\hat{\pi}_x - i\hat{\pi}_y)|nlk\rangle = m_e\hbar\omega_B\ (n+1)\ \delta_{n',n+1}\,\delta_{ll'}\delta_{kk'}. \tag{5.134}$$

Doing the same thing for the product that will appear in ϵ_L, one has only a contribution from $n' = n - 1$ and the result is easily found,

$$\langle nlk|\hat{\pi}_x|n'l'k'\rangle\langle n'l'k'|(\hat{\pi}_x + i\hat{\pi}_y)|nlk\rangle = m_e\hbar\omega_B\ (n)\ \delta_{n',n-1}\,\delta_{ll'}\delta_{kk'}. \tag{5.135}$$

Then next, figure out the sums S_R and S_L. Here I will not yet try to do any expression using occupied and unoccupied states. Go to the original expression for ϵ_R, we need the following sum,

$$\begin{aligned} S_R &= \frac{1}{m_e\hbar}\sum_{n'k'l'}\sum_{nkl}\frac{w_n - w_{n'}}{\omega + i\gamma + \omega_{nn'}}\,(m_e\hbar\omega_B\ (n+1)\ \delta_{n',n+1}\,\delta_{ll'}\delta_{kk'}) \\ S_R &= \omega_B\sum_{nkl}\frac{(n+1)(w_n - w_{n+1})}{\omega + i\gamma - \omega_B}, \qquad \text{where} \quad \omega_{nn'} = \omega_{n,n+1} = -\omega_B. \end{aligned} \tag{5.136}$$

Then the associated permittivity is

$$\epsilon_R = 1 - \frac{4\pi ne^2}{m_e\omega(\omega + i\gamma)}(1 + S_R). \tag{5.137}$$

There is not much difference for the other polarization, except that the transition is downward instead:

$$\begin{aligned} S_L &= \frac{1}{m_e\hbar}\sum_{n'k'l'}\sum_{nkl}\frac{w_n - w_{n'}}{\omega + i\gamma + \omega_{nn'}}\,(m_e\hbar\omega_B\ (n)\ \delta_{n',n-1}\,\delta_{ll'}\delta_{kk'}) \\ S_L &= \omega_B\sum_{nkl}\frac{(n)(w_n - w_{n-1})}{\omega + i\gamma + \omega_B}, \qquad \text{where} \quad \omega_{nn'} = \omega_{n,n-1} = +\omega_B. \end{aligned} \tag{5.138}$$

Then this associated permittivity is

$$\epsilon_L = 1 - \frac{4\pi ne^2}{m_e\omega(\omega + i\gamma)}(1 + S_L). \tag{5.139}$$

5.7.1 The summands for ϵ_{xx} and ϵ_{xy}

For completeness also write out what is needed for the Cartesian elements of the permittivity matrix. Here instead we need the following products of matrix elements. For ϵ_{xx}, there is

$$\begin{aligned} \langle nlk|\hat{\pi}_x|n'l'k'\rangle\langle n'l'k'|\hat{\pi}_x|nlk\rangle &= |\langle n'l'k'|\hat{\pi}_x|nlk\rangle|^2 = \\ &= \left|\sqrt{\frac{m_e\hbar\omega_B}{2}}\ \left[\sqrt{n}\ \delta_{n',n-1} + \sqrt{n+1}\ \delta_{n',n+1}\right]\delta_{ll'}\delta_{kk'}\right|^2 \\ &= \frac{1}{2}m_e\hbar\omega_B\left[(n+1)\ \delta_{n',n+1} + n\,\delta_{n',n-1}\right]\delta_{ll'}\delta_{kk'} \end{aligned} \tag{5.140}$$

The two terms are mutually exclusive, which is why there is no cross term in the square. For ϵ_{xy}, there is

$$\begin{aligned} \langle nlk|\hat{\pi}_x|n'l'k'\rangle\langle n'l'k'|\hat{\pi}_y|nlk\rangle &= \sqrt{\frac{m_e\hbar\omega_B}{2}}\ \left[\sqrt{n'}\ \delta_{n,n'-1} + \sqrt{n'+1}\ \delta_{n,n'+1}\right]\delta_{ll'}\delta_{kk'} \\ &\times\ (-i)\sqrt{\frac{m_e\hbar\omega_B}{2}}\ \left[\sqrt{n}\ \delta_{n',n-1} - \sqrt{n+1}\ \delta_{n',n+1}\right]\delta_{ll'}\delta_{kk'} \\ &= \frac{i}{2}m_e\hbar\omega_B\left[(n+1)\ \delta_{n',n+1} - n\,\delta_{n',n-1}\right]\delta_{ll'}\delta_{kk'} \end{aligned} \tag{5.141}$$

Then the sums that are needed to get these ϵ components are clearly related to those for the circular polarizations,

$$\begin{aligned} S_{xx} &= \frac{1}{m_e\hbar}\sum_{n'k'l'}\sum_{nkl}\frac{w_n - w_{n'}}{\omega + i\gamma + \omega_{nn'}}\left(\frac{1}{2}m_e\hbar\omega_B\ \left[(n+1)\ \delta_{n',n+1} + n\ \delta_{n',n-1}\right]\delta_{ll'}\delta_{kk'}\right) \\ S_{xx} &= \frac{\omega_B}{2}\sum_{nkl}\left\{\frac{(n+1)(w_n - w_{n+1})}{\omega + i\gamma - \omega_B} + \frac{n(w_n - w_{n-1})}{\omega + i\gamma + \omega_B}\right\} \end{aligned} \tag{5.142}$$

The values of $\omega_{nn'}$ are opposite on the two terms, because the first is an upward transition and the second is a downward transition. Find a similar result for the sum for ϵ_{xy},

$$\begin{aligned} S_{xy} &= \frac{1}{m_e\hbar}\sum_{n'k'l'}\sum_{nkl}\frac{w_n - w_{n'}}{\omega + i\gamma + \omega_{nn'}}\left(\frac{i}{2}m_e\hbar\omega_B\ \left[(n+1)\ \delta_{n',n+1} - n\ \delta_{n',n-1}\right]\delta_{ll'}\delta_{kk'}\right) \\ S_{xy} &= \frac{i\omega_B}{2}\sum_{nkl}\left\{\frac{(n+1)(w_n - w_{n+1})}{\omega + i\gamma - \omega_B} - \frac{n(w_n - w_{n-1})}{\omega + i\gamma + \omega_B}\right\} \end{aligned} \tag{5.143}$$

That these are correct is clear, because they are related to the circular polarization sums by the simple relations,

$$S_R = S_{xx} - iS_{xy}, \qquad S_L = S_{xx} + iS_{xy}. \tag{5.144}$$

5.7.2 Finding the sums

In all of these sums, the denominators are constants that can come out front. Recall also that the w_n are the state probabilities, with $\sum_{n=0}^{\infty} w_n = 1$ and $w_n = e^{-\beta E_n}/Z$ where β is the inverse temperature and Z is the partition function. The state energies depend only on n. So these sums are related to expectation values of the number operator, $N = a^\dagger a$.

Consider first the sum S_L for left polarization, expression (5.138). One part of it is the following sum:

$$\sum_{n=0}^{\infty} n\, w_n = \langle n\rangle. \tag{5.145}$$

The other part is a sum that can be transformed into this also, because its $n = 0$ term gives nothing. So the other term has its sum really start at $n = 1$. Doing a shift of its index, there is

$$\sum_{n=1}^{\infty} n\, w_{n-1} = \sum_{n=0}^{\infty}(n+1)w_n = \langle n\rangle + 1. \tag{5.146}$$

But S_L involves the difference of these two sums. So there is a cancellation, and the result is too simple!

$$S_L = \frac{\omega_B}{\omega + i\gamma + \omega_B}\sum_{lk}\left[\langle n\rangle - (\langle n\rangle + 1)\right] = \frac{-\omega_B}{\omega + i\gamma + \omega_B}\sum_{lk} 1 \tag{5.147}$$

The last sum over l and k I am going to take as some constant g, which is probably unity (although technically it should be the degeneracy of any Landau level, which is enormous and depends on the system volume). The reason is the way the normalization has been set up, that this sum is normalized for an individual electron. This may seem mathematically absurd, but we have already accounted for N electrons in a factor contained in the density of electrons per unit volume. This seems a little suspicous, only because I have some lack of total understanding about the normalization that was given to the density matrix. This should be clarified better at some point. So ignoring those slight "technicalities", the left polarization sum should be

$$S_L = \frac{-g\omega_B}{\omega + i\gamma + \omega_B}. \tag{5.148}$$

Consider next the sum S_R in (5.136) needed for ϵ_R and right circular polarization. One has very directly

$$\sum_{n=0}^{\infty}(n+1)\,w_n = \langle n\rangle + 1. \tag{5.149}$$

The other sum needs the index shifted, which makes it effectively start at $n = 1$:

$$\sum_{n=0}^{\infty}(n+1)\,w_{n+1} = \sum_{n=1}^{\infty} n\,w_n = \sum_{n=0}^{\infty} n\,w_n = \langle n\rangle \tag{5.150}$$

This is true because the $n = 0$ term makes no contribution to the sum. So now we have

$$S_R = \frac{\omega_B}{\omega + i\gamma - \omega_B}\sum_{lk}\left[\langle n\rangle + 1 - \langle n\rangle\right] = \frac{+\omega_B}{\omega + i\gamma - \omega_B}\sum_{lk} 1 \tag{5.151}$$

Again with the final sum set to some value g, the result is very simple,

$$S_R = \frac{+g\omega_B}{\omega + i\gamma - \omega_B}. \tag{5.152}$$

The two results for S_R and S_L are related one to the other by switching the sign of ω_B.

For the Cartesian components, we have

$$S_{xx} = \frac{S_R + S_L}{2} = \frac{1}{2}\left\{\frac{+g\omega_B}{\omega + i\gamma - \omega_B} + \frac{-g\omega_B}{\omega + i\gamma + \omega_B}\right\} = \frac{g\omega_B^2}{(\omega + i\gamma)^2 - \omega_B^2} \tag{5.153}$$

$$S_{xy} = i\frac{S_R - S_L}{2} = \frac{i}{2}\left\{\frac{+g\omega_B}{\omega + i\gamma - \omega_B} - \frac{-g\omega_B}{\omega + i\gamma + \omega_B}\right\} = \frac{ig\omega_B(\omega + i\gamma)}{(\omega + i\gamma)^2 - \omega_B^2} \tag{5.154}$$

5.7.3 Results for Landau-level free electrons

Now the right-circular polarization result for permittivity is seen to be

$$\epsilon_R = 1 - \frac{4\pi ne^2}{m_e\omega(\omega + i\gamma)}\left[1 + \frac{g\omega_B}{\omega + i\gamma - \omega_B}\right] \longrightarrow 1 - \frac{4\pi ne^2}{m_e\omega}\cdot\frac{1}{\omega + i\gamma - \omega_B} \tag{5.155}$$

The last expression is the limit when $g = 1$, which is the value I think it should have. Then for left polarization there is similarly,

$$\epsilon_L = 1 - \frac{4\pi ne^2}{m_e\omega(\omega + i\gamma)}\left[1 - \frac{g\omega_B}{\omega + i\gamma + \omega_B}\right] \longrightarrow 1 - \frac{4\pi ne^2}{m_e\omega}\cdot\frac{1}{\omega + i\gamma + \omega_B} \tag{5.156}$$

The Cartesian components are also found quickly,

$$\epsilon_{xx} = 1 - \frac{4\pi ne^2}{m_e\omega(\omega + i\gamma)}\left[1 + \frac{g\omega_B^2}{(\omega + i\gamma)^2 - \omega_B^2}\right] \longrightarrow 1 - \frac{4\pi ne^2}{m_e\omega}\cdot\frac{\omega + i\gamma}{(\omega + i\gamma)^2 - \omega_B^2} \tag{5.157}$$

$$\epsilon_{xy} = 0 - \frac{4\pi ne^2}{m_e\omega(\omega + i\gamma)}\left[0 + \frac{ig\omega_B(\omega + i\gamma)}{(\omega + i\gamma)^2 - \omega_B^2}\right] \longrightarrow -i\frac{4\pi ne^2}{m_e\omega}\cdot\frac{\omega_B}{(\omega + i\gamma)^2 - \omega_B^2} \tag{5.158}$$

Now one can see that curiously, after all this work to do the quantum mechanics correctly, these last two results agree exactly with the expression (3.38) found with the classical theory for damped electrons! But it was necessary to include the damping factor $i\gamma$ with ω in the relation connecting $\mathbf{J}$ and $\mathbf{P}$, as well as using the limiting value of the lk sum, $g = 1$. Still, this was a good test problem for getting all the details correct.

Also, a caution is needed. In the theory to this point, I did not worry about the sign of e, the charge of the carriers. It is contained in the definition of ω_B, which is linearly proportional to e. If the carriers are really negative electrons, then keep in mind that this would make ω_B a negative number, when comparing with experimental results and especially comparing the results at right and left polarizations!

6 Band to band transitions in a semiconductor/metal

So far the general theory for ϵ_R and ϵ_L was 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.

That is presented in *Dielectrics: Part C*. Go there for the story of how the magnetic field enters and gives a simple contribution, or in fact, a simple modification of the expression for the dielectric functions for the two circular polarizations.